



Malika Zghal

Development of Liquid-Sprays Numerical Modelling Approaches for Low-
Emission Gas Turbine Combustion Systems

SATM
PhD in Aerospace

PhD
Academic Year: 2020 - 2024

Supervisor: Dr. Xiaoxiao Sun
Associate Supervisor: Prof. Vishal Sethi, Prof. Pierre Gauthier

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Abstract

Computational Fluid Dynamics (CFD) is used to guide the design of novel low-emission gas turbine combustion technologies. For combustion systems using liquid fuels, injecting the spray in crossflow, coupled with enhanced turbulence can achieve superior mixing characteristics and reduce emissions. The development of advanced mixing technologies requires accurate predictions of the spray characteristics. However, atomization is often modelled using the Lagrangian approach with deterministic breakup models instead of the higher-fidelity interface-capturing methods, such as Volume-of-Fluid (VOF), due to their high computational cost. The breakup models used in state-of-the-art CFD and developed specifically for liquid jets in crossflow (LJIC) rely on empirical constants and/or correlations that need to be calibrated with experimental data, which is not practical. The practicability of modelling LJIC could be improved by using a stochastic secondary droplet (SSD) breakup model that does not require exhaustive calibration. A better compromise between computational cost and accuracy could also be achieved by coupling the Lagrangian and VOF approaches. However, very few studies have assessed or validated their predictive capabilities for LJIC, especially for fuels and under more representative gas turbine conditions.

This research aimed to improve the practicability of modelling turbulent liquid fuel jets in crossflow (LFJIC) and to contribute to the knowledge of the Lagrangian and hybrid approach through new assessment and validation work. Lower and higher-fidelity modelling approaches for turbulent LFJIC were assessed and validated using experimental data over a wide range of pressures, momentum flux ratios and Weber numbers. This comprised an investigation of the effects of different sub-models and boundary conditions on the flow properties, predictive capabilities, and computational cost. This collaborative research between Cranfield University and Siemens Energy has led to the development and validation of novel stochastic numerical methodologies as well as a better understanding of LFJIC modelling. The hybrid resolved method proposed offers superior predictive capabilities for the overall droplet velocities and droplet diameters in the leeward region but is on average 17 times more computationally expensive than the URANS Lagrangian methodology. The optimized stripping method proposed reduces the cost of the hybrid approach by 78% and the average relative difference between their predictions is less than 15%. Thus, their trade-offs between accuracy and computational cost were deemed reasonable and guidelines were formulated to help determine the most suitable methodology for future research work on turbulent LFJIC. The research outcomes are already being used to hasten the design, development, and delivery of novel low-emission gas turbine combustion systems.

Keywords: CFD, VOF, Lagrangian, Liquid Jets in Crossflow, Atomization, Breakup

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*In loving memory of my grandfather,
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List of Abbreviations

3D	Three Dimensions
AMG	Algebraic Multigrid
AMR	Adaptive Mesh Refinements
BDF	Backward Difference Multi-Step
BDF1	1st Order Backward Difference Multi-Step
BDF2	2nd Order Backward Difference Multi-Step
BLS	Boundary-Layer-Stripping
CBP	Column Breakup Point
CFD	Computational Fluid Dynamics
CLSVOF	Coupled Level Set/Volume-Of-Fluid
CPU	Central Processing Unit
CSF	Continuum Surface Force
CVP	Counter-Rotating Vortex Pair
DNS	Direct Numerical Simulations
FAR	Fuel-Air Ratio
FEA	Finite Element Analysis
FGVT	Fine Grid Volume Tracking
HPC	High-Performance Computing
HRIC	High-Resolution Interface Capturing
HTP	High Temperature and Pressure
HTSP	High Temperature and Standard Pressure
JIC	Jet In Crossflow
KH	Kelvin-Helmholtz
KHRT	Kelvin-Helmholtz Rayleigh-Taylor
LES	Large Eddy Simulation
LFJIC	Liquid Fuel Jet In Crossflow
LIF	Laser-Induced Fluorescence
LISA	Linearized Instability Sheet Atomization
LJIC	Liquid Jet In Crossflow
LS	Level-Set
MIM	Multiple Injector Model
NVD	Normalized Variable Diagram

ODE	Ordinary Differential Equation
OPR	Overall Pressure Ratio
PDPA	Phase Doppler Particle Analyzer
PIV	Particle Image Velocimetry
PS	Parcel Stream
RANS	Reynolds-Averaged Navier-Stokes
RD	Reitz-Diwakar
RLSG	Refined Level-Set Grid
RT	Rayleigh-Taylor
SEM	Synthetic Eddy Method
SGS	Subgrid-Scale
SMD	Sauter Mean Diameter
SOA	State-Of-the-Art
SSD	Stochastic Secondary Droplet
STHP	Standard Temperature and High Pressure
STP	Standard Temperature and Pressure
TAB	Taylor's Analogy Breakup
TKE	Turbulent Kinetic Energy
URANS	Unsteady Reynolds-Averaged Navier-Stokes
URF	Under-Relaxation Factor
VOF	Volume-Of-Fluid
WALE	Wall-Adapting Local Eddy-Viscosity

List of Symbols

A_{blob}	Actual surface area of the blob
A_{cd}	Interaction Area density
A_p	Projected Area of the particle
α_G	Volume fraction of the gas phase
α_L	Volume fraction of the liquid phase
α_{blob}	Volume fraction of the blob
α_i	Volume fraction of phase i
α_p	Volume fraction of the Lagrangian particle
B_1	SSD Breakup parameter
$C_{D_{sphere}}$	Drag coefficient of an undistorted droplet
C_D	Drag force coefficient
Co_{max}	Maximum Lagrangian phase courant numbers
Co_{min}	Minimum Lagrangian phase courant numbers
$(D_{p,s})_{Target}$	Target stripped droplet diameter
D_H	Hydraulic diameter
D_{blob}	Diameter of the blob
D_{crit}	Critical droplet diameter
$D_{p,s}$	Diameter of the stripped droplet
D_p	Diameter of the particle
D_s	Diameter of a stable droplet
Δx_{cell}	Characteristic length of the cell
Δt_{CPU}	Solver CPU time per time step normalized by the total number of cpus
$\Delta t_{Lag.}$	Time difference after activating the VOF-Lagrangian transition model
Δt	Physical time-step
Δ	Grid filtered width
t_p	Local parcel time-step
d	Diameter of the plain orifice injector
ε_{SGS}	Subgrid-scale dissipation rate
η	Void fraction
ε	Dissipation rate
F_b	Body force
F_d	Drag force

F_p	Pressure gradient force
F_s	Surface force
$F_{\sigma,T}$	Tangential component of the surface tension force
$F_{\sigma,n}$	Normal component of the surface tension force
F_σ	Surface tension force between VOF phases
H	Rectangular cross-section Height
J	Momentum flux ratio
K_3	SSD Normal velocity coefficient
k_{SGS}	Subgrid scale turbulent kinetic energy
k	Turbulent kinetic energy
κ	Mean curvature of the interface
L_{AMR}	Adapted cell size
L_{cell}	Cell size
l_{cd}	Characteristic interaction length scale
l_e	Eddy length scale
l_t	Turbulent length scale
Λ	Wavelength of the KHRT instabilities (KHRT model)
L	Length of the plain orifice injector
$(\dot{m}_{L,s}'')_{Target}$	Mass Flux targeted for the stripped droplets
$(m_{L,s})_{Target}$	Mass targeted for the stripped droplets
$\dot{m}_p$	Mass transfer rate
$m_{L,s}$	Mass of the continuous liquid phase that can be stripped
m_L	Mass of the continuous liquid phase available in the interface cell
$m_{p,s}$	Mass of the stripped particles
m_p	Mass of the particle
μ_G	Dynamic viscosity of the continuous gas phase
μ_{H2O}	Dynamic viscosity of water
μ_L	Dynamic viscosity of the continuous liquid phase
μ_{jet}	Dynamic viscosity of the jet
μ_t	Turbulent eddy viscosity
μ	Dynamic viscosity of the continuous phase (mixture)
Ma	Mach number
$\dot{n}_\pi$	Particle flow rate
$n_{\pi,s}$	Number of particles stripped
n_π	Number of particles per parcel

Ω	Growth rate of the KHRT instabilities (KHRT breakup model)
Oh	Ohnesorge number
P_g	Gas pressure
Q_t	Convective heat transfer
Q	Q-criterion
R_G	Ideal gas constant
$Re_{g,d}$	Reynolds number of the droplet based on the gas phase properties
Re_g	Reynolds number of the crossflow gas (before the injector)
Re_{jet}	Reynolds number of the jet (before injection)
Re_p	Reynolds number of the particle
R_p	Position vector of the particle
r_{crit}	Critical droplet radius
$r_{p,c}$	Radius of the child particle
r_p	Radius of the parent particle
ρ	Density of the continuous phase (mixture)
ρ_G	Density of the continuous gas phase
ρ_L	Density of the continuous liquid phase
ρ_g	Density of the crossflow gas (before the injector)
ρ_i	Density of the phase i
ρ_{jet}	Density of the liquid jet (before injection)
ρ_p	Density of the particle
R	Curvature of the plain orifice injector
S_{v_x}	Cumulative net transfer rate of axial momentum
S_{v_y}	Cumulative net transfer rate of vertical momentum
S_E	Transfer rate of energy between the phases
S_M	Transfer rate of mass between the phases
S_{SGS}	Subgrid-scale strain rate
S_v	Transfer rate of momentum between the phases
S_α	Momentum source term of the phase volume fraction
S	Modulus of the mean strain rate tensor
σ	Surface tension
τ_Λ	Instabilities lifetime (KHRT model)
$\tau_{R,p}$	Residence time of the particle
τ_{bu}	Breakup time
τ_c	Eddy transit time

τ_e	Eddy time scale
τ_l	Eddy interaction time
τ_t	Turbulent time scale
τ_v	Momentum-relaxation time scale
$\mathbf{T}$	Viscous stress tensor
$\emptyset$	Sphericity of the blob
u_{p_x}	Axial component of the droplet velocity
u_{p_y}	Vertical component of the droplet velocity
URF_{tw}	Under-relaxation factor of the two-way coupling solver
$\bar{u}$	Local Reynolds-averaged velocity
u_e	Eddy velocity scale
u_g	Velocity of the crossflow gas (before the injector)
u_{jet}	Velocity of the jet (before injection)
$u_{p,c}$	Velocity of the child droplet
u_p	Velocity of the particle
u_s	Slip velocity
u_y	Vertical component of the continuous phase velocity
u	Velocity of the continuous phase
u'	Fluctuating eddy velocity
V_{α_i}	Volume of the cell occupied by phase i
V_{cell}	Volume of the cell
V_p	Volume of the particle
$ W_{bu} $	SSD scaling factor for the parent droplet velocity
$We_{L\Delta}$	Characteristic liquid Weber number
We_{crit}	Critical weber number
We_g	Gas weber number
We_{jet}	Jet Weber number
We	Weber number
W	Rectangular cross-section width
$\langle \xi^2 \rangle$	Second logarithmic moment of the breakup spectrum function of the SSD breakup model
$\langle \xi \rangle$	First logarithmic moment of the breakup spectrum function of the SSD breakup model
x_{CBP}	Column breakup length
y_{CBP}	Column breakup height
y_{TAB}	Normalized droplet distortion (TAB distortion model)

y_{max}	Maximum height reached by the droplets at a given distance
∇P_{static}	Static pressure gradient of the continuous phase

List of Publications

Peer-Reviewed Journal Publications:

M. Zghal, P. Gauthier, X. Sun, C. Wijesinghe, and V. Sethi, “Validation and Assessment of a Hybrid VOF-Lagrangian Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow,” *Journal of Engineering for Gas Turbines and Power*, vol. 146, no. 8, Feb. 2024, <https://doi.org/10.1115/1.4064218>.

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Industrial Research and Development Report:

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1 Introduction

To alleviate global environmental concerns, various legislative bodies have set highly ambitious targets to reduce emissions within the next 10 years [e.g. 1, 2, 3]. Many countries are joining efforts to achieve “net-zero by 2050”, such as the United Kingdom, Canada and Germany [1, 4]. Thus, it is critical for the industrial and academic communities to work together to reduce emissions of harmful pollutants from both stationary and aero gas turbines, such as CO, unburned hydrocarbons, soot, CO₂ and NO_x. This work stems from a collaborative research effort between Cranfield University and Siemens Energy.

For combustion systems using liquid fuel injectors, superior fuel-air mixing characteristics can be achieved to reduce emissions by introducing the spray transversely into crossflowing air, which enhances the atomization and evaporation process [5, 6, 7, 8]. These processes can be further enhanced by the turbulent flow properties, jet penetration (high momentum flux ratio) and aerodynamic effects on the breakup properties (high Weber numbers) [7, 9, 10]. The development of such advanced mixing technologies and the design work of low-emission gas turbine combustion systems is often guided by Computational Fluid Dynamics (CFD) simulations to predict changes in the combustion performance and emissions. Considering the significant influence of the spray characteristics on the combustion process [5], robust numerical tools that can accurately predict the atomization process are urgently needed to accelerate the development of more sustainable technologies.

Atomization modelling is often facilitated by using the Lagrangian approach coupled with breakup models rather than the high-fidelity interface-capturing methods, such as Volume-of-Fluid (VOF) [11] or Level-Set (LS) [12, 13], due to their high computational cost. The breakup models used in state-of-the-art (SOA) CFD mostly rely on empirical constants and correlations that need to be calibrated with experimental data to produce accurate predictions [5, 14]. However, their predictive capabilities for liquid jets in crossflow (LJIC) have been mostly assessed for water sprays under low pressure [15, 16, 17, 18, 19, 20, 21, 22, 23]. Although further work could be done to validate their suitability for liquid fuel jets in crossflow (LFJIC) under more representative gas turbine conditions, they are unlikely suitable for such applications without conducting further

improvement or calibration work. This is due to their heavy dependence on model constants originally derived from experiments of sprays in quiescent or coflowing air at atmospheric conditions or using water [24, 25]. This implies the need to have access to experimental data for the specific injector and operating conditions studied, which is not a realistic expectation when atomization modelling is used in the context of an iterative research and development process. In addition, calibrating the model constants can be extremely time-consuming without any guarantee that the expected accuracy can be achieved [e.g. 26, 27]. Moreover, the calibration process would likely need to be repeated when studying different operating conditions or injector configurations considering their significant influence on the atomization characteristics [7, 9, 14, 28].

These concerns surrounding the practicability of lower-fidelity atomization models in SOA CFD also extend to the few breakup models specifically developed to account for the particularities of jets in crossflows (JIC). Indeed, they are also based on these deterministic breakup models and/or rely on empirical correlations to predict the column breakup and shedding process [29, 30, 31, 32]. Moreover, their application is mostly limited to breakup regimes that are not representative of the turbulence and atomization levels of gas turbine combustors [29, 31, 32].

Thus, to facilitate the development of low-emission gas turbine technologies, further work needs to be done to improve the practicability of the Lagrangian approach for LJIC, especially for more representative gas turbine conditions. This could be achieved by using a novel Stochastic Secondary Droplet (SSD) breakup model that relies significantly less on experimental data by considering the breakup process to be random in nature [33, 34]. However, its accuracy for LJIC has only been assessed for water sprays under low pressures and Weber numbers [35, 36, 37] or low momentum flux ratios [38]. In fact, very few studies have validated the predictive capabilities of the Lagrangian approach for LJIC with fuel datasets regardless of the breakup model used [27, 30, 31, 32, 38].

A better compromise between computational cost and accuracy could also potentially be achieved by directly coupling the Lagrangian approach with an interface-capturing method. This hybrid approach would allow to predict the primary breakup process and account for the effect of the injector geometry on the spray characteristics without relying on deterministic models or empirical correlations. However, its validation for LJIC has

been mostly confined to the near-field region [35, 36, 39, 40] and often only for the trajectory [35, 39]. In addition, the few studies conducted to validate its predictions in the far-field region used deterministic breakup models [40, 41]. Moreover, their conditions were limited to low Weber numbers [35, 36, 39, 40, 41] and often to low momentum flux ratios [35, 40, 41] using either water at ambient pressure [35, 36, 41] or non-turbulent jets [39, 40, 41].

Therefore, there is a significant need for more research on the numerical modelling of turbulent LFJIC under more representative gas turbine conditions. In particular, further work needs to be done to help fill the gaps in knowledge on the predictive capabilities of the SSD breakup model, Lagrangian approach and hybrid approach for such applications. Furthermore, to facilitate and hasten the delivery of low-emission technologies, the academic and industrial gas turbine communities need more robust and practical numerical tools for modelling turbulent LFJIC with both the lower and higher-fidelity approaches.

1.1 Aims And Objectives

The overall scientific aim of the research was to improve the practicability of modelling turbulent liquid-fuel jets in crossflows, especially for more representative gas turbine conditions. As described earlier in Chapter 1, this was done by proposing novel numerical methodologies for modelling turbulent LFJIC that:

- use a stochastic breakup model to rely significantly less on having prior knowledge of the spray characteristics and to reduce the need for calibrating model constants to obtain accurate predictions, thus shortening the time cost of modelling LJIC.
- reduce the computational cost of using the higher-fidelity atomization modelling approaches to account for the effect of the injector geometry and liquid jet column on the spray characteristics, thus enabling the use of CFD to guide the design of novel low-emission injectors.

To achieve the aim of the research, the following research objectives were formulated:

1. Evaluate if the SSD breakup model can achieve predictive capabilities for LFJIC that are similar to the deterministic breakup models used in SOA CFD or specifically developed for this application by:
 - Evaluating their current accuracy as reported in the literature.
 - Assessing their baseline (non-calibrated) predictive capabilities.
2. Assess, validate, and develop high and low-fidelity atomization modelling methodologies for turbulent LFJIC that require minimal or no calibration over a wide range of conditions as outlined above.
3. Assess, validate, and develop stochastic numerical methodologies that improve the practicability of using the higher-fidelity interface capturing methods (VOF) for modelling turbulent LFJIC.
4. Ensure the trade-off between the practicability and accuracy of the proposed numerical methodologies is reasonable by comparing their predictive capabilities to the calibrated deterministic breakup models as reported in the literature.
5. Help fill the gaps in knowledge on the different atomization modelling approaches (Lagrangian and hybrid) and the SSD breakup model through new assessment and validation work (see definitions below) leading to new findings and a better understanding of LFJIC modelling.
6. Disseminate the research outcomes to the academic and industrial gas turbine communities and provide recommendations to improve the capabilities in atomization modelling for turbulent LFJIC of the CFD software Simcenter STAR-CCM+ (Siemens Digital Industries Software).

Details of the assessment, validation and development of the numerical methodologies referenced above are elaborated below:

- **Assessment:** Investigate the effect of different sub-models (Lagrangian, VOF, VOF-Lagrangian, Turbulence or Flow solvers) and boundary conditions (test section, injector diameter, operating conditions, and crossflow velocity profile) on:
 - Spray properties (Droplet velocity, trajectory, width and Sauter Mean Diameter) and related predictive capabilities (see **validation***).

- Turbulent Flow characteristics (velocities, wake regions, recirculation zones, Lagrangian turbulent interactions, turbulent viscosity, turbulent length and time scales, vortices).
- Two-way coupled interactions (Eulerian-Lagrangian, VOF-Lagrangian and VOF phases).
- Computational cost.
- **Development:** Use the results and conclusions from the assessment work to form an optimal numerical methodology for predicting the spray characteristics (see **validation***) of LFJIC for the lower (Lagrangian) and higher-fidelity (VOF-Lagrangian) approaches by:
 - Down-selecting and combining the different sub-models assessed.
 - Proposing new modifications to existing models (i.e. VOF-Lagrangian stripping transition criterion).
 - Proposing new implementation strategies to impose specific parameters (Lagrangian courant numbers, stripping mass flux, Adaptive Mesh Refinement settings, VOF-Lagrangian transition criterion).
- ***Validation:** Compare the spray characteristics predicted by the different sub-models, approaches and numerical methodologies developed to experimental data available in the literature. The operating conditions, test section and injector used in the experiments are replicated numerically to impose the boundary conditions, numerical domain, and injector settings. Experimental correlations derived from similar experiments are used to complete the dataset.
- **Numerical methodology:** Recommended combination of models, sub-models, schemes, and specific parameters that have been validated (see **validation***). This includes guidelines to aid its implementation for trade-offs between cost and accuracy depending on the intended application.

1.2 Thesis Structure

The thesis comprises 7 chapters, namely the introduction (Chapter 1), literature review (Chapter 2), core research work (Chapter 3 to Chapter 6), overall discussion and

conclusion (Chapter 7). The “core” research chapters are presented in the format of standalone publications, thus directly contributing to the 6th research objective:

- Chapter 3, Chapter 4 and Chapter 5 each correspond to one of the 3 peer-reviewed publications published as part of the research outcome.
- Chapter 6 is a manuscript ready for submission.

The core research chapters each include the following sections: Abstract, Introduction, Numerical Set-up, Methodology, Results, Discussion, Conclusion and Acknowledgements. It should be noted that Chapter 3 and Chapter 4 incorporate the discussion section into the result section and that Chapter 5 and Chapter 6 have an additional section dedicated to discussing the computational cost. Furthermore, each core research chapter includes a review of the relevant literature and provides specific recommendations for future work.

To produce a coherent narrative for the thesis, Chapter 2 provides contextual and technical details that supplement the information presented in the core research chapters. Moreover, Chapter 7 provides an overall discussion that establishes connections between the main research outcomes from each core research chapter. The thesis structure is further detailed below:

- **Chapter 2:** Provides important background information to ensure the completeness of the thesis. This includes a literature review on the physical processes of LJIC, the fundamental CFD equations, an overview of the different atomization modelling approaches and details of the selection process for the validation datasets (experimental literature review). This chapter also contributes to addressing the 1st research objective by reviewing the current predictive capabilities of the different atomization modelling approaches as reported in the literature.
- **Chapter 3:** Presents the research work done to improve the practicability of the Lagrangian approach for turbulent LFJIC by assessing the effect of different Lagrangian sub-models and flow solvers. The non-calibrated predictive capabilities of the SSD and SOA deterministic breakup models were also compared, which further contributes to achieving the 1st research objective. This

peer-reviewed paper was presented at an international conference and published in the conference proceedings of *The American Society of Mechanical Engineers (ASME) 2022 Turbomachinery Technical Conference and Exposition* :

- [42] M. Zghal, X. Sun, P. Q. Gauthier, and V. Sethi, “Validation and Assessment of a Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow,” in *Proceedings of the ASME Turbo Expo 2022: Turbomachinery Technical Conference and Exposition. Volume 2: Coal, Biomass, Hydrogen, and Alternative Fuels; Controls, Diagnostics, and Instrumentation; Steam Turbine*, Rotterdam, Netherlands, June 2022. <https://doi.org/10.1115/GT2022-83166>.
- **Chapter 4:** Presents the research work done to further improve the predictive capabilities of the Lagrangian approach with the SSD breakup model for turbulent LFJIC by assessing the effect of turbulence modelling and the sensitivity to different boundary conditions. This peer-reviewed journal publication has been published in *Atomization and Sprays*:
 - [43] M. Zghal, X. Sun, P. Gauthier, and V. Sethi, “Validation of a Stochastic Breakup Model for Turbulent Jets In High-Speed Crossflow: Assessment of Turbulent Interactions and Sensitivity to Boundary Conditions,” *Atomization and Sprays*, vol. 33, no. 4, pp. 25–54, Jan. 2023, <https://doi.org/10.1615/AtomizSpr.2023041220>.
- **Chapter 5:** Presents the research work done to improve the practicability of using the higher-fidelity methods to model LFJIC by coupling the VOF approach with the lower-cost Lagrangian approach based on the stochastic methodology previously developed. It also focuses on improving the predictive capabilities of LES for modelling turbulent LFJIC. This peer-reviewed paper was published in the *Journal of Engineering for Gas Turbine and Power* and was presented at the international conference *ASME 2023 Turbomachinery Technical Conference and Exposition*:
 - [44] M. Zghal, P. Gauthier, X. Sun, C. Wijesinghe, and V. Sethi, “Validation and Assessment of a Hybrid VOF-Lagrangian Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow,” *Journal of Engineering*

for Gas Turbines and Power, vol. 146, no. 8, Feb. 2024,
<https://doi.org/10.1115/1.4064218>.

- **Chapter 6:** Presents the research work done to improve the practicability of the VOF-Lagrangian approach for turbulent LFJIC by optimizing the hybrid numerical methodology previously developed and proposing a stochastic VOF-Lagrangian stripping transition model. This manuscript is ready for submission:
 - M. Zghal, P. Gauthier, X. Sun, and V. Sethi, "An Optimized VOF-Lagrangian Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow", 2024. [To be submitted].
- **Chapter 7:** Provides an overview of the main research outputs by summarizing the numerical methodologies developed and comparing their predictive capabilities to those reported in the literature for LJIC, which addresses the 4th research objective. The achievement of the 5th research objective is further supported by articulating the novelty, contribution, and impact of the work, which includes a reference to the experimental rig facility developed using the proposed numerical methodologies as presented in Appendix A. The research limitations are also addressed and recommendations are made for future work, thus contributing to fulfilling the last research objective.

Figure 1-1 illustrates in more technical detail the structure of the work done in each core research chapter to fulfill the aim and objectives described in *section 1.1*. In particular, it shows how the 2nd and 3rd objectives were addressed by providing an overview of the assessment, validation, and development of the lower and higher-fidelity numerical methodologies. Furthermore, the arrows indicate how the research findings from each core research chapter were used to inform the work done in the following chapter. Indeed, the numerical methodology developed in Chapter 3 provided the baseline numerical set-up (drag coefficient, flow solver, breakup model and SSD model parameters) used in Chapter 4 (blue arrow at the top left). The research findings from Chapter 4 oriented the work towards higher-fidelity interface capturing methods, which is the subject of Chapter 5 (grey arrow at the bottom left). The conclusions from the latter motivated the development of a lower-cost hybrid approach as presented in Chapter 6 (grey arrow at the bottom right).

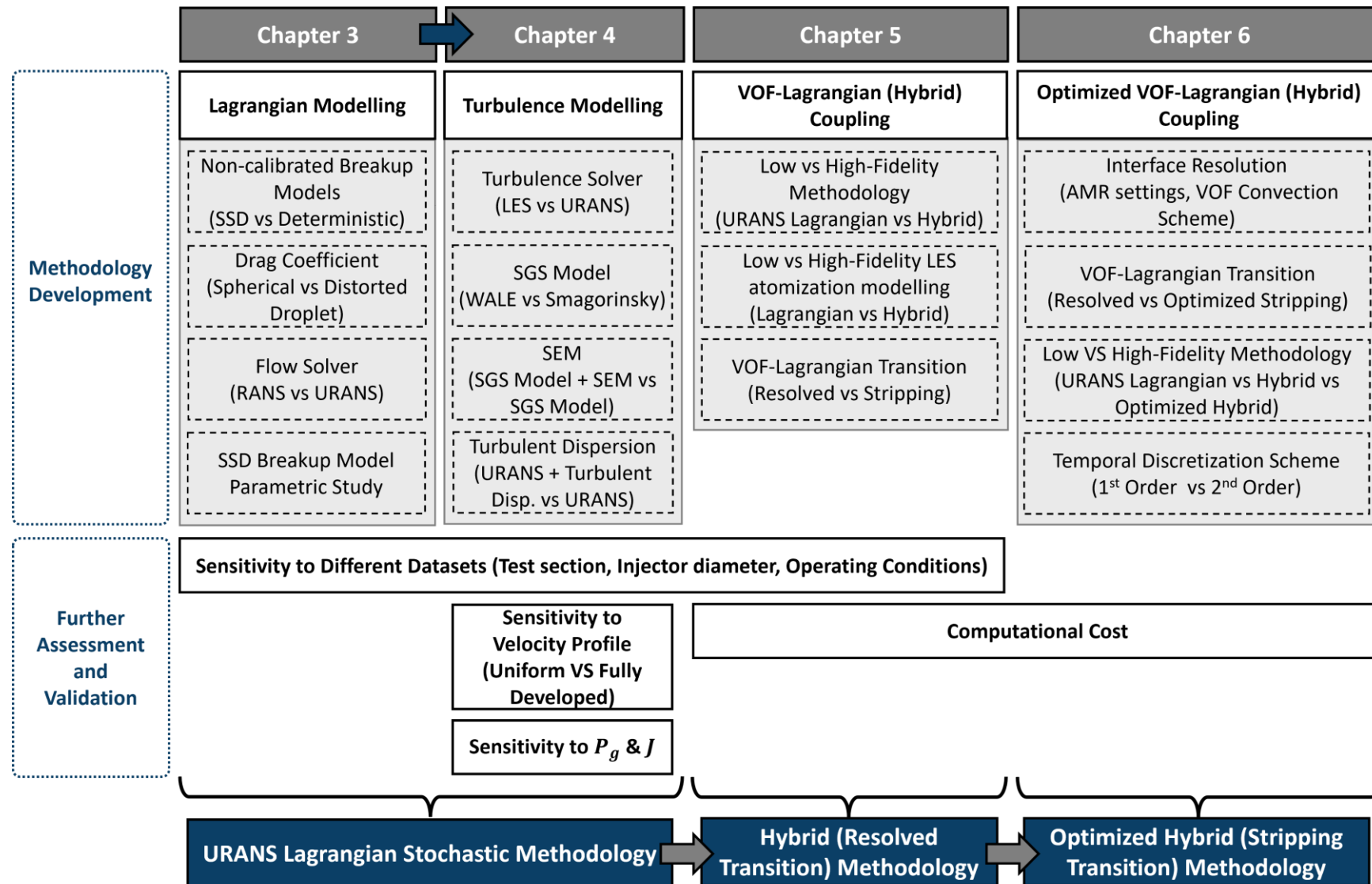


Figure 1-1: Overview of the core chapters' structure and research work conducted.

It is important to note that some of the most important numerical models are described more than once in the thesis due to the core chapters representing standalone papers. This is also true for the description of the general research context, which is often provided in the first or second paragraph of the introduction sections. Although the discussion surrounding the numerical models and research context varies from one core chapter to another, the intended message is essentially the same. **Table 1-1** indicates where in the thesis the descriptions of the various numerical models are provided. In instances where a numerical model is described in multiple locations, a recommendation is provided by the author for the section in which the most comprehensive details of the model are available, which is indicated by the highlighted grey cells.

Table 1-1: Sections and equations describing the numerical models.

Model	Section (equations)			
	Chapter 3	Chapter 4	Chapter 5	Chapter 6
Lagrangian Two-way coupling (steady)	3.3.1 (3-1 to 3-3)			
Lagrangian Two-way coupling (unsteady)		4.3.1 (4-1 to 4-2)	5.3.2 (5-9 to 5-10)	
Two-way coupling steady URF	3.4 (3-29)			
Local parcel time step	3.3.1 (3-4)	4.3.1 (4-8)		
Lagrangian conservation of linear momentum	3.3.1 (3-7)	4.3.1 (4-7)	5.3.3 (5-13)	
Pressure Gradient Force	3.3.1 (3-5)	4.3.1 (4-4)	5.3.3 (5-11)	
Drag Force	3.3.1 (3-6)	4.3.1 (4-5)	5.3.3 (5-12)	
Drag Coefficient (Spherical Droplet)	3.3.2 (3-11)			
Drag Coefficient (TAB Distortion)	3.3.2 (3-8, 3-10)	4.3.2 (4-9 to 4-12)		
RD Breakup Model	3.3.3 (3-12 to 3-17)			
KHRT Breakup Model	3.3.4 (3-18 to 3-22)			
SSD Breakup Model	3.3.5 (3-23 to 3-28)	4.3.3 (4-13 to 4-18)	5.3.3 (5-14 to 5-19)	
Surface Force		4.3.1 (4-3)		
Slip velocity		4.3.1 (4-6)		
Turbulent Dispersion		4.3.4 (4-19 to 4-24)		
Turbulence RANS		4.3.5 (4-25 to 4-26)		
Turbulence LES		4.3.6 (4-27 to 4-28)		

Fully Developed Velocity Profile		4.4.2 (4-30 to 4-31)		
VOF			5.3.1 (5-1 to 5-4)	6.3.1 (6-1 to 6-2)
Continuum Surface Force			5.3.1 (5-5 to 5-6)	
VOF-Lagrangian resolved Transition			5.3.2 (5-7 to 5-8)	6.3.2 (6-3 to 6-5)
VOF-Lagrangian stripping Transition				6.3.2 (6-6 to 6-11)
Temporal Discretization Scheme				6.3.3 (6-12 to 6-13)

2 Literature Review

2.1 Fundamentals of Liquid Jets in Crossflow

Liquid fuel injectors are essential parts of combustion chambers because they provide the energy source needed to produce the power required by a wide range of applications, such as gas turbines in the aerospace and power generation field. Once injected into the combustion chamber, the liquid jet is divided into small droplets by going through a primary and secondary breakup process. The resulting droplet cloud then evaporates and mixes with the air, which leads to the combustion process. This research focuses on liquid jets in crossflow (LJIC) considering this injector configuration is expected to be the optimal design of advanced-mixing technologies for low-emission gas turbines due to their enhanced mixing characteristics [6, 9, 10]. Thus, the objective of this section is to provide a summary of the important physical processes involved in the formation of transverse sprays. The atomization process of LJIC is illustrated in **Figure 2-1**.

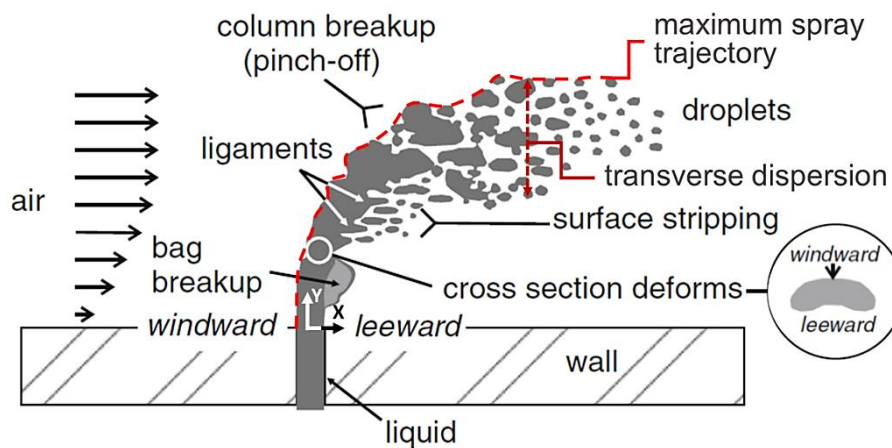


Figure 2-1: Atomization process of a liquid jet in crossflow (Adapted from Sedarsky et al. [45]; Reproduced with permission from Springer Nature).

The primary breakup process refers to the atomization of the liquid jet column that forms large droplets and ligaments near the injector [7, 9]. The secondary breakup process occurs further downstream of the injector and is defined as the atomization of the primary droplets and ligaments that form even smaller droplets due to aerodynamic and capillary effects [7, 9]. The windward spray region refers to the liquid column surface and droplets that first interact with the crossflowing air, the leeward spray region refers to the droplets located in the wake of the jet column close to the wall and the core spray region refers to the droplets located in between. The transverse dispersion of the droplet is defined as the

difference between the maximum and minimum droplet position on the Y axis at a given axial distance. The latter refers to the horizontal distance (X axis) from the liquid injector. The spray width or radial dispersion refers to the absolute difference between the maximum and minimum droplet position on the Z axis (not shown in **Figure 2-1**) at a given axial distance. The spray trajectory corresponds to the transverse position of the droplets located at the windward interface (i.e. maximum position on Y axis).

The physical processes involved in the formation of gaseous jets in crossflow (JIC) can help provide further insight into the flow field characteristics of LJIC [9, 25, 39]. Similar to gaseous JIC, the jet column bends under the effect of aerodynamic forces when the liquid penetrates the crossflowing air stream [e.g. 7, 29]. For gaseous JIC, the resulting flow field can be divided into a near-field and far-field region, which differ by the local deflection of the jet column [e.g. 9, 10]. In the former, the jet deflection is not significant while in the latter it is almost parallel to the gaseous crossflow [e.g. 9, 46, 47]. Although these flow field characteristics can also be extended to LJIC, the near-field region is also characterized by the primary breakup process. Thus, the terms primary breakup region and near-field region are often used interchangeably in the literature to refer to the zone downstream of the injector that includes the liquid jet column, ligaments, and larger droplets [e.g. 9, 25, 48]. However, the distance away from the injector where the flow field transitions to the secondary breakup region has not been clearly defined to the best knowledge of the author. This is likely due to the experimental challenges involved in measuring the large droplets and ligaments formed during the primary breakup process [25, 39, 49, 50, 51]. Despite these limitations, the minimum length of the primary breakup region could be considered equal to the column breakup length, which is further discussed in *section 2.1.4*.

Another similarity that can be drawn between liquid and gaseous JIC is the different vortex structures within the near-field and far-field regions generated from the interactions between the penetrating fluid and crossflowing gas stream [9, 25, 39]. As shown in **Figure 2-2**, the transverse penetration of the jet column creates an adverse pressure gradient that generates horseshoe vortices and induces instabilities near the jet surface that generate shear layer vortices [10, 52]. These vortex structures are located in the near-field region upstream of the jet column [10, 52]. The crossflowing air stream

entrains the shear-layer vortices downstream of the jet column to form a counter-rotating vortex pair (CVP) that propagates in the far-field region. Wake vortices are also generated downstream of the jet column [10, 52]. The flow field characteristics of LJIC are further analyzed numerically in Chapter 6.

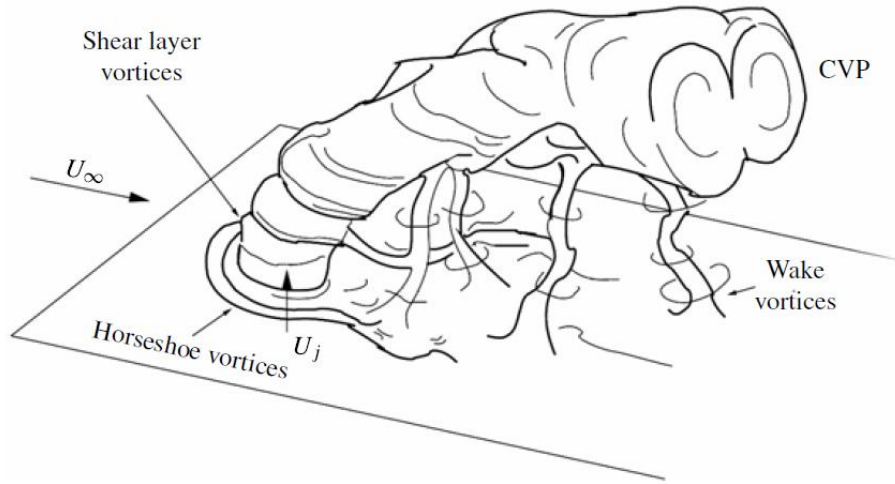


Figure 2-2: Important vortex structures of jets in crossflow (Reproduced from [10] with permission from Cambridge University Press).

The atomization process and spray characteristics of LJIC in both breakup regions depend on the properties of the liquid and air as well as the injector design [7, 9, 28]. Regardless of the injector type or configuration used, their influences on the spray formation and characteristics are commonly expressed through non-dimensional parameters [5, 7, 9, 14, 28]. To better understand the different mechanisms involved in the formation of LJIC, these non-dimensional parameters must be first defined in the context of the atomizer type studied. Although this research focuses on the plain orifice injectors as further explained in *section 2.4.1*, a brief overview of the different types of atomizers that could be positioned in a crossflow is first provided. The effect of the non-dimensional parameters and injector design on the spray characteristics of plain orifice injectors are then presented.

2.1.1 Injector Types

This section introduces the principle behind the plain orifice injector and highlights that the research gaps in knowledge on LJIC extend to any other type of atomizer. As shown in **Figure 2-3**, the different types of injector designs can be classified into 3 main categories: pressure, rotary and twin-fluid atomizers [28].

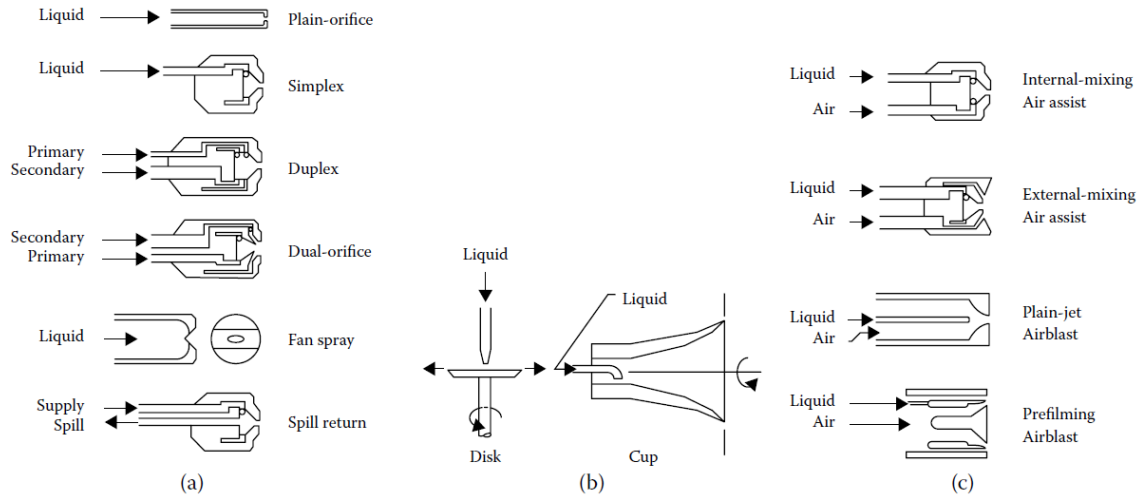


Figure 2-3: Different types of liquid injectors: a) Pressure atomizers b) Rotary atomizers c) twin-fluid atomizers (Reproduced with permission of CRC Press, Taylor & Francis Group, from [28]; permission conveyed through Copyright Clearance Center, Inc.).

Pressure atomizers work by flowing the liquid through small orifices to generate a high-pressure drop [5, 28]. In other words, the atomization process relies on converting the energy from the pressure into kinetic energy [5, 28]. Plain orifice injectors are pressure atomizers that use a single small orifice to generate a solid liquid jet column, which is often circular [7, 28]. Further details on the specific design features of plain orifice injectors and their influence on the spray characteristics are provided in *section 2.1.5*. Rotary injectors rely on centrifugal forces to atomize the liquid via a rotating plate [7, 28] while twin-fluid atomizers rely on the interaction of the liquid with high-velocity air [5, 7, 28].

The experimental gaps in knowledge on LJIC using plain orifice injectors are presented in *Appendix A.1*. Furthermore, *section 2.4.4* presents the experimental data available on turbulent liquid fuel jets in crossflow (LFJIC) at standard temperatures. In comparison, very few studies have been conducted on LJIC using other types of atomizers or injectors [53, 54, 55]. Most experimental studies on more complex injectors in crossflow have been carried out using air-blast atomizers [54, 56, 57, 58, 59, 60, 61, 62, 63] and effervescent sprays (aerated injectors) [64, 65, 66]. Although these types of twin-fluid atomizers are commonly used in gas turbines [5, 28], their installation in a crossflow configuration is expected to be challenging depending on the combustor type due to the need to flow high-pressure air through them. A few studies have also been done using

rotary atomizers [55, 67, 68, 69], but their application is mostly relevant to the agricultural industry [28]. The experimental studies that have assessed the spray characteristics achieved by positioning other types of pressure atomizers in crossflow have mostly used hollow cone sprays [70] or simplex injectors [53, 71, 72, 73], which are often referred to as pressure-swirl injectors [28].

Pressure-swirl injectors are commonly used in gas turbines [5, 28] and similarly to plain orifice injectors, their installation in a crossflow configuration is deemed likely to be less challenging than twin-fluid atomizers (i.e. does not require adapting the air delivery system to ensure sufficient air is fed to the injector for the atomization process). However, further experimental work needs to be done to fill the gaps in knowledge on their spray characteristics when positioned in crossflow. This could be achieved by adapting the experimental rig facility designed and commissioned based on the research findings, which is presented in Appendix A. This aspect is further discussed in Chapter 7 by addressing the research limitations and formulating recommendations for future work.

2.1.2 Non-Dimensional Parameters

As previously mentioned, the atomization process of LJIC is often characterized by non-dimensional parameters that are a function of the following air and liquid properties: dynamic viscosity, density, velocity and surface tension (σ). It is important to note that these non-dimensional parameters also evolve with the local flow properties, hence why the breakup models defined in the core research chapters often use the corresponding values for the continuous phase and liquid droplets. However, the breakup regime maps and empirical correlations available in the literature to predict the spray characteristics are defined based on the initial fluid properties. Thus, the non-dimensional parameters presented in this section rely on the liquid properties at the exit of the injector (μ_{jet} , ρ_{jet} and u_{jet}) and the air crossflow properties upstream of the injector (μ_g , ρ_g and u_g). As for the characteristic length scale, the initial jet diameter is considered equal to the exit diameter of the plain orifice injector (d instead of D_p) [7].

One of the most important parameters that characterize jets in crossflow is the momentum flux ratio J defined in equation (2-1), which indicates the ability of the transverse fluid to penetrate the crossflowing air stream [e.g. 7, 9]. Higher values of J are often associated

with a higher penetration of the liquid jet column as discussed in *section 2.1.4* [9, 74]. If the crossflow fluid is considered to be an ideal gas, then increasing the pressure P_g will have the opposite effect. It is important to note that the impact of increasing the temperature T_g on the spray penetration is not as straightforward due to the effect of evaporation on the windward droplets, especially in the far-field region [9, 74].

$$J = \frac{\rho_{jet} u_{jet}^2}{\rho_g u_g^2} = \left(\frac{\rho_{jet} u_{jet}^2}{u_g^2} \right) \left(\frac{T_g R_G}{P_g} \right) \quad (2-1)$$

Where R_G is the ideal gas constant. The Reynolds number for the liquid jet column relative to the jet properties Re_{jet} is defined below [7, 9, 14]. Some studies prefer using the gas properties to represent the influence of the turbulent crossflow on the liquid jet column and droplets [e.g. 48, 75, 76, 77, 78]. It should be noted that the related droplet gas Reynolds number $Re_{g,d}$ defined in equation (2-3) differs from the Reynolds number of the air crossflow upstream of the injector Re_g presented in equation (2-4), which is proportional to the hydraulic diameter D_H of the test section [79].

$$Re_{jet} = \frac{\rho_{jet} u_{jet} d}{\mu_{jet}} \quad (2-2)$$

$$Re_{g,d} = \frac{\rho_g u_g d}{\mu_g} \quad (2-3)$$

$$Re_g = \frac{\rho_g u_g D_H}{\mu_g} \quad (2-4)$$

Another important set of non-dimensional parameters is the Weber numbers, which have been heavily correlated to the breakup regimes of LJIC [e.g. 80, 81, 82, 83]. The liquid jet Weber number We_{jet} and gas Weber number We_g defined below indicates the importance of the corresponding fluid (i.e. liquid or gas) inertial force relative to the liquid surface tension force [7, 9].

$$We_{jet} = \frac{\rho_{jet} u_{jet}^2 d}{\sigma} \quad (2-5)$$

$$We_g = \frac{\rho_g u_g^2 d}{\sigma} \quad (2-6)$$

$$We = \frac{\rho_g u_s^2 d}{\sigma} = \frac{\rho_g (u_g - u_{jet})^2 d}{\sigma} \quad (2-7)$$

As seen in equation (2-7), a few studies also use an alternative definition of We_g based on the slip velocity u_s [e.g. 84, 85, 86]. It should be noted that We_g has also been called

the aerodynamic Weber number [e.g. 48, 81, 87], Weber number [e.g. 84, 85, 86] and crossflow Weber number [e.g. 82, 88]. Although there is not a clear consensus in the literature on the terminology that should be used to distinguish We_g from We , the latter is simply referred to in this work as the Weber number and the former as the gas Weber number.

In addition to the different Weber numbers and Reynolds numbers, the breakup regimes of LJIC have also been described using the Ohnesorge number Oh defined below [51, 89, 90].

$$Oh = \frac{\sqrt{We_{jet}}}{Re_{jet}} = \frac{\mu_{jet}}{\sqrt{\sigma \rho_{jet} d}} \quad (2-8)$$

This last non-dimensional parameter combines Re_{jet} and We_{jet} as an alternative way of representing the ratio of viscous to surface tension forces [7, 9, 14].

2.1.3 Breakup Regimes

Several experimental studies on LJIC have classified the characteristics of the primary breakup process into two principal modes: the column breakup and surface breakup [7, 9, 51, 80, 89, 91, 92, 93, 94, 95], which are represented in **Figure 2-1**. The latter is described as the stripping of large droplets and ligaments from the unbroken liquid column [7, 9, 51, 80, 89, 93, 96]. The column breakup process is described as the breakup of the liquid column into large droplets and ligaments due to the growth of axial instabilities and waves on its surface, which are induced by aerodynamic, inertial and surface tension forces [9, 14, 51, 80, 89, 92, 93, 94]. These instabilities cause the jet column to oscillate and deform, which ultimately leads to its breakup downstream of the injector [7, 9, 97]. At the location of the column breakup point (CBP), the liquid jet is replaced by large droplets and ligaments that will go through a secondary breakup process [7, 9].

In addition to the column and surface breakup, different experimental studies have also identified mixed modes or transition regimes, such as the bag, multi-mode and shear breakup [9, 48, 51, 80, 81, 87, 89, 91, 98, 99]. These breakup regimes are characteristics of non-turbulent jets ($Re_{jet} \leq 3000$ [9, 82]) and often defined by the We_g , J or Oh as

shown in **Figure 2-4**. A visual representation of the non-turbulent breakup modes is provided in **Figure 2-5**.

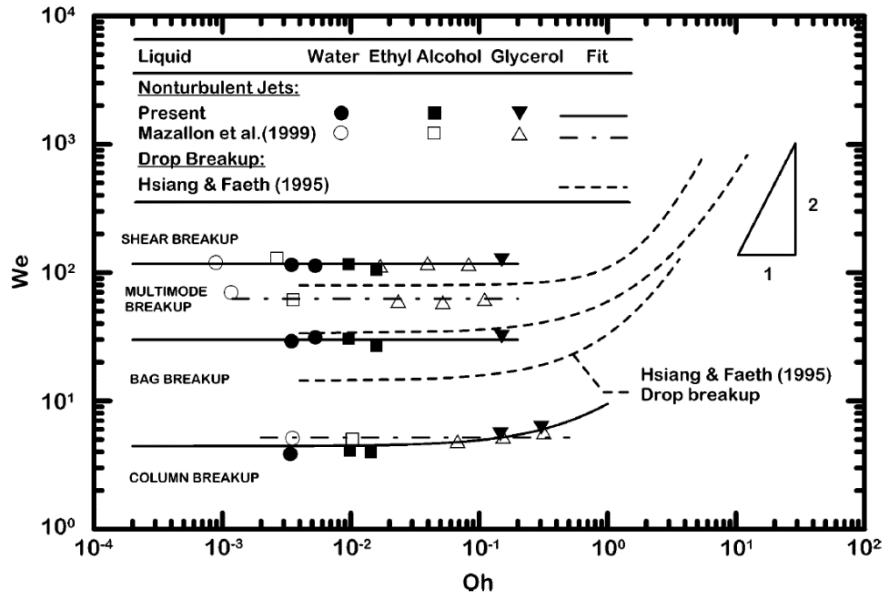


Figure 2-4: Breakup regime map for non-turbulent LJIC proposed by Sallam et al. [89]
(Reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.).

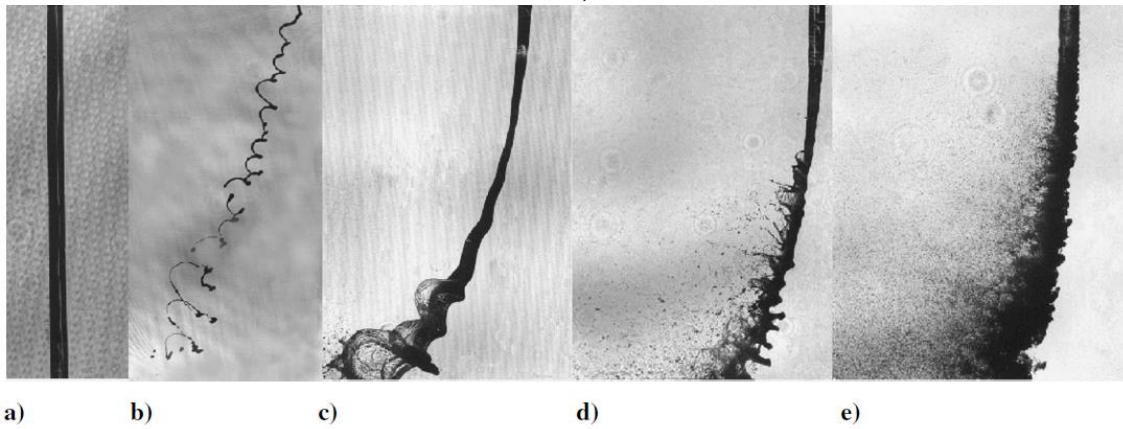


Figure 2-5: Shadowgraph images of a non-turbulent LJIC (water at ambient conditions) for different breakup regimes: a) No crossflow/breakup ($We_g = 0$), b) Column ($We_g = 3$), c) Bag ($We_g = 8$), d) Multi-mode ($We_g = 30$), and d) Shear ($We_g = 220$) breakup regimes
(From [89]; reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.).

While multiple breakup regime maps have been proposed in the literature for non-turbulent LJIC over a wide range of operating conditions [48, 51, 80, 81, 87, 89, 90, 91, 95, 98, 99, 100, 101, 102, 103] as reviewed in detail by Broumand and Birouk [9], fewer

studies have been done to characterize the primary breakup process of turbulent LJIC. Furthermore, there is not yet a clear consensus on the different breakup modes involved. Although a few studies have reported that the turbulent breakup regimes are similar to non-turbulent LJIC [82, 97, 104, 105] especially at lower Re_{jet} or proposed non-turbulent breakup regime maps using both high and low Re_{jet} datasets [81, 87, 89, 91, 98], others have observed two new breakup modes that can occur over a wide range of jet Reynolds numbers [82, 83, 106]: an aerodynamic and non-aerodynamic/turbulent breakup process. The latter is characterized by the stripping of ligaments and droplets from the windward interface, which are caused by turbulence-induced instabilities resulting from the liquid flow properties [9, 82, 106]. The former is characterized by the different non-turbulent LJIC breakup modes previously described [82, 106]. These new turbulent breakup modes are primarily a function of the jet Weber Number We_{jet} and momentum flux J as shown in Figure 2-6.

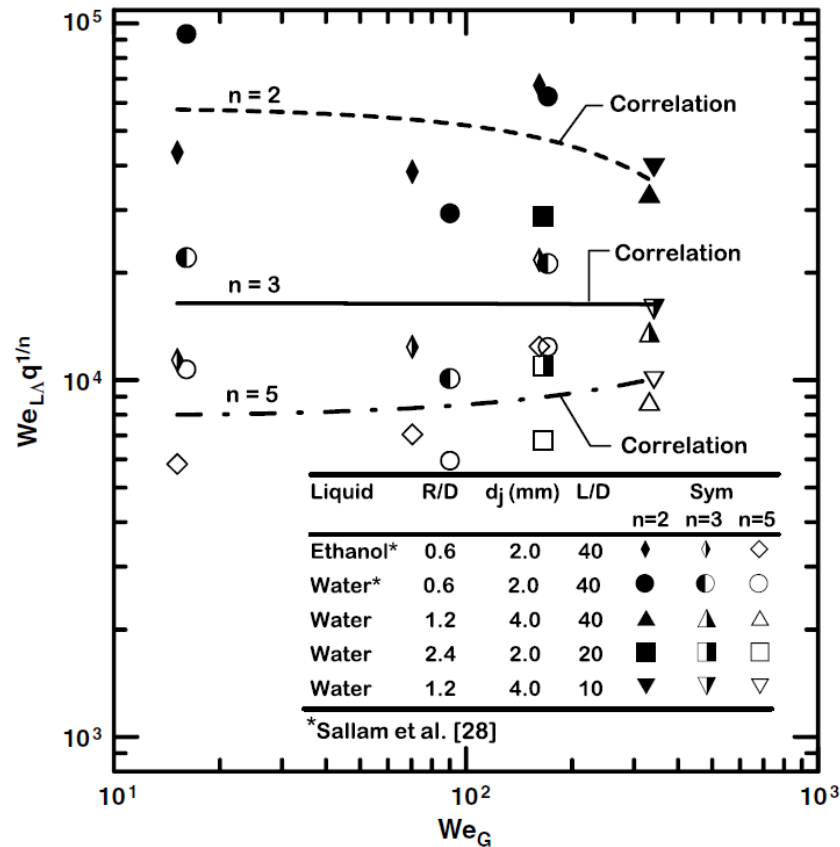


Figure 2-6: Breakup regime map proposed by Osta and Sallam [106] for turbulent LJIC (“q” represents the momentum flux ratio, reference indicated at the bottom corresponds to [82]) (Reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.).

The transition between both modes depends on the characteristic liquid Weber number We_{LA} proposed by Wu and Faeth [107], which consists of replacing d in equation (2-5) by a characteristic length scale. Considering the latter equals 1/8 of the nozzle diameter [107], the left axis of the breakup regime map shown in **Figure 2-6** equals 1/8 of We_{jet} multiplied by J . Sallam et al. [82] initially proposed to add an exponent of 1/3 to the momentum flux ratio, but their research group later tried different exponential values ranging from 1/5 to 1/2 [106]. Both studies concluded that turbulent LJIC transitions from the aerodynamic to non-aerodynamic/turbulent breakup mode above the horizontal line defined by $J^{1/3}We_{jet}/8 \approx 17000$ regardless of We_g or Re_{jet} [82, 106]. **Figure 2-7** illustrates the turbulent breakup regimes of LJIC.

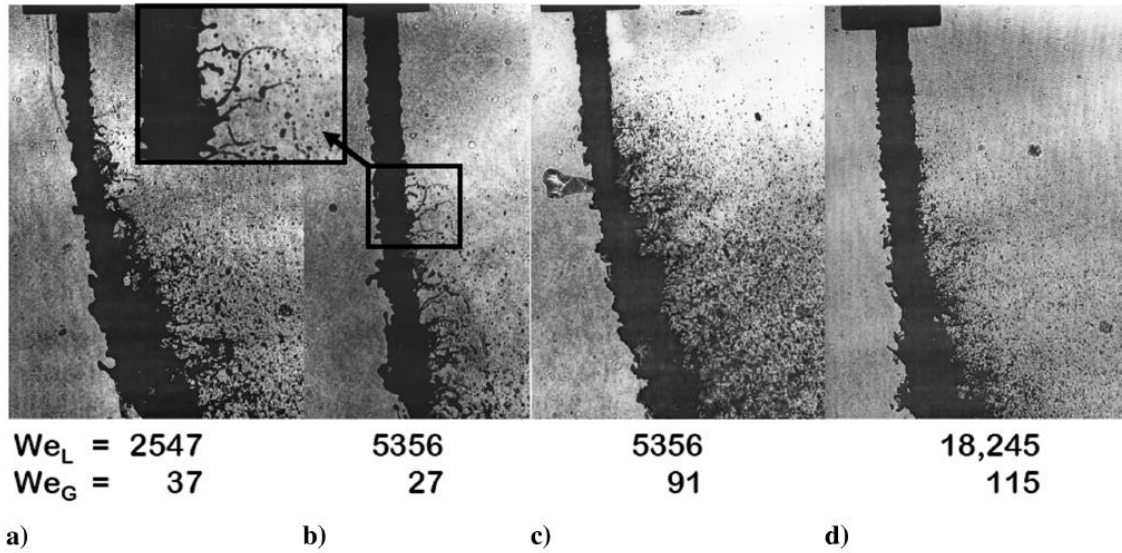


Figure 2-7: Shadowgraph images of a turbulent LJIC for different $J^{1/3}We_{jet}/8$ values (images a) to c) are water jets while d) is alcohol): a) 1304, b) 3904 c) 2603 d) 12345 (From [88]; reprinted by permission of the American Institute of Aeronautics and Astronautics, Inc.).

2.1.4 Spray Characteristics

This section summarizes the influence of the non-dimensional parameters on the most relevant spray characteristics of LJIC for gas turbine applications. Sprays are generally characterized by the properties of the droplets located at a given distance downstream of the injector, which includes the distribution of their diameter and velocity [5, 7, 14, 28]. For reacting flow applications, the Sauter Mean Diameter (SMD) given in equation (2-9) is commonly used to evaluate the droplet sizes as it can easily be incorporated in simple

analysis to determine if sufficient evaporation can be achieved to ensure the ignition and combustion process [7, 14, 28].

$$SMD = \left(\sum n_{\pi} D_p^3 \right) / \left(\sum n_{\pi} D_p^2 \right) \quad (2-9)$$

Where n_{π} is the number of droplets. Very few studies available in the literature on LJIC have proposed empirical correlations to predict the SMD, especially for turbulent LJIC as shown in **Table 2-1**. However, they mostly all agree that increasing We_g yields a smaller SMD due to the enhanced atomization process [48, 84], which has been corroborated by other studies on LJIC [81, 108]. This effect has been attributed more directly to the related increase in crossflow gas velocity u_g [81, 91]. The SMD has also been observed to decrease at higher Reynolds numbers for both phases and/or upstream of the injector [77, 78, 84]. Increasing the momentum flux ratio J also tends to reduce the SMD [48, 81, 91], but it has been found to have less impact at higher pressures [84, 91, 109]. Although decreasing We_{jet} has been reported to decrease the SMD [84], very few studies have established a direct connection between both parameters. Instead, it has been observed to have no significant impact at low pressure [110] and other studies suggested that the influence of the viscosity and density ratios on the SMD are more important [48, 111].

Table 2-1: Empirical correlations proposed in the literature for the SMD of a turbulent liquid jet in crossflow.

Reference	SMD
Song et al. [48]	$d \left[0.267 We_g^{0.44} J^{0.08} \left(\frac{\rho_{jet}}{\rho_g} \right)^{0.3} \left(\frac{\mu_{jet}}{\mu_g} \right)^{-0.16} \right]^{-1}$
Amighi [84]	$(d) e^{10.34} We_g^{-0.04} We_{jet}^{-0.07} \left(\frac{\sqrt{We_g}}{Re_{g,d}} \right)^{0.04} Oh^{2.1}$ $= (d) e^{10.34} We_g^{-0.02} We_{jet}^{0.98} Re_{g,d}^{-0.04} Re_{jet}^{-2.1}$
Becker and Hassa [91]	$429 (\rho_g u_g^2)^{-0.24}$

The impact of the non-dimensional parameters on the droplet velocity u_p has been associated with their respective effect on the SMD. Indeed, a few studies have reported that increasing J , We_g or We increases the droplet velocity as it produces smaller droplets

[81, 108, 110]. Thus, smaller droplets are transported at a much faster speed in the far-field region [9].

For LJIC in particular, the spray trajectory is another important factor used to assess the performance of the injector [7, 9, 28]. As shown in **Table 2-2**, the experimental studies on LJIC available in the literature agree that increasing the momentum flux ratio J increases the spray trajectory regardless of the test conditions. The relationship between J and P_g defined in equation (2-1) also implies they all consider that higher-pressure conditions reduce the penetration. The important influence of the momentum flux ratio is further supported by the exhaustive literature reviews conducted recently by Broumand and Birouk [9] as well as Yoon [74] on the empirical correlations for the spray trajectory. Apart from this common feature, **Table 2-2** shows there are great discrepancies between the spray trajectory correlations available in the literature, which can be related to differences in the test conditions. In fact, Yoon [74] found they have been proposed in 6 different formats that all depend on the momentum flux ratio but vary based on their functional form (i.e. power-law, logarithmic or exponential) and the non-dimensional parameters included.

Table 2-2: Empirical correlations proposed in the literature for the maximum spray trajectory of a liquid jet in crossflow.

Conditions	Reference	Maximum Spray Trajectory (y/d)
STP	Wu et al. [80]	$1.37J^{0.5} \left(\frac{x}{d}\right)^{0.5}$
	Tambe et al. [81]	$1.55J^{0.53} \ln \left(1.66 \left(\frac{x}{d}\right) + 1\right)$
	Elshamy et al. [99]	$5.38J^{0.467} \left(\frac{x}{d}\right)^{0.281} We_g^{-0.119}$
	Farvardin et al. [111]	$3.688J^{0.430} \left(\frac{x}{d}\right)^{0.384} We_g^{-0.085} \left(\frac{\mu_{jet}}{\mu_{H2O}}\right)^{-0.222}$
	Wu et al. [112]	$4.3J^{0.33} \left(\frac{x}{d}\right)^{0.33}$
	Lin et al. [113]	$2.42J^{0.48} \left(\frac{x}{d}\right)^{0.24}$
	Iyogun et al. [114]	$1.997J^{0.444} \left(\frac{x}{d}\right)^{0.444}$

	Birouk et al. [115]	$\begin{cases} 1.997J^{0.444} \left(\frac{x}{d}\right)^{0.444} & \text{for } \frac{x}{d} < 12 \\ 1.627J^{0.47} \left(\frac{x}{d}\right)^{0.46} \left(\frac{\mu_{jet}}{\mu_{H2O}}\right)^{0.079} & \text{for } \frac{x}{d} \geq 12 \end{cases}$
	Brown et al. [116]	$1.1J^{0.55} \left(\frac{x}{d}\right)^{0.34}$
	Song. Y et al. [117]	$2.398J^{0.442} \left(\frac{x}{d}\right)^{0.264}$
	Olyaei & al. [118]	$1.21J^{0.624} \left(\frac{x}{d}\right)^{0.501} We^{-0.152}$
	Stenzler et al. [119]	$2.898J^{0.430} \left(\frac{x}{d}\right)^{0.384} We_g^{-0.11} \left(\frac{\mu_{jet}}{\mu_{H2O}}\right)^{-0.108}$
HTSP	Lakhamraju [87]	$1.971J^{0.438} \ln\left(1.279\left(\frac{x}{d}\right) + 1\right) \left(\frac{T_g}{294K}\right)^{-0.236}$
	Stenzler et al. [119]	$2.630J^{0.442} \left(\frac{x}{d}\right)^{0.390} We_g^{-0.088} \left(\frac{\mu_{jet}}{\mu_{H2O}}\right)^{-0.027}$
	Yoon et al. [120]	$2.241J^{0.402} \left(\frac{x}{d}\right)^{0.41}$
STHP	Song et al. [48]	$\begin{cases} 1.163J^{0.557} \left(\frac{x}{d}\right)^{0.463} We_g^{0.111} \left(\frac{\rho_{jet}}{\rho_g}\right)^{-0.052} \left(\frac{\mu_{jet}}{\mu_g}\right)^{-0.086} & \text{for } \frac{x}{d} < 8 \\ 4.391J^{0.556} \left(\frac{x}{d}\right)^{0.214} We_g^{-0.011} \left(\frac{\rho_{jet}}{\rho_g}\right)^{-0.082} \left(\frac{\mu_{jet}}{\mu_g}\right)^{-0.053} & \text{for } \frac{x}{d} \geq 8 \end{cases}$
	Becker and Hassa [91]	$1.48J^{0.42} \ln\left(3.56\left(\frac{x}{d}\right) + 1\right)$
	Elshamy et al. [99]	$4.95J^{0.424} \left(\frac{x}{d}\right)^{0.279} We_g^{-0.076} \left(\frac{P_g}{P_{atm}}\right)^{-0.051}$
	Freitag and Hassa [109]	$1.6J^{0.4} \ln\left(3.81\left(\frac{x}{d}\right) + 1\right)$
	Ragucci et al. [121]	$2.698J^{0.441} \left(\frac{x}{d}\right)^{0.367} \left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{-0.069}$
HTP	Bellofiore et al. [75]	$0.909J^{0.476} \left(\frac{x}{d}\right)^{0.35} \left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{-0.128} Re_{g,d}^{0.135}$
	Amighi [84]	$\begin{aligned} & 13.31 \left(\frac{x}{d} + 0.5\right)^{0.27} We_g^{-0.25} We_{jet}^{0.40} \left(\frac{\sqrt{We_g}}{Re_{g,d}}\right)^{-0.20} Oh^{0.65} \\ & = 13.31J^{0.4} \left(\frac{x}{d} + 0.5\right)^{0.27} We_g^{0.04} Re_{g,d}^{0.20} Oh^{0.65} \\ & = 13.31 \left(\frac{x}{d} + 0.5\right)^{0.27} We_g^{-0.35} We_{jet}^{0.725} Re_{g,d}^{0.20} Re_{jet}^{-0.65} \end{aligned}$

	Ragucci et al. [122]	$2.28J^{0.442} \left(\frac{x}{d}\right)^{0.367} \left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{-0.015} \left(\frac{\mu_{jet}}{\mu_{g,300K}}\right)^{0.186}$
	Li et al. [123]	$1.44J^{0.4356} \ln\left(1.06\left(\frac{x}{d}\right) + 1\right) We_g^{0.01147} \left(\frac{T_g}{280K}\right)^{0.295}$
	Lubarsky et al. [124]	$1.9866J^{0.5} \left[\left(1 + 0.7403\left(\frac{x}{d}\right)\right)^{-1} + \ln\left(1 + 0.7403\left(\frac{x}{d}\right)\right) \right]$

Regardless of the test conditions (e.g. standard temperature and pressure (STP), standard temperature and high-pressures (STHP), etc.), turbulent properties, or liquid used, most experimental studies have reported that the spray trajectory only depends on J [80, 81, 91, 109, 112, 113, 114, 116, 117, 120, 124]. Many other studies also consider the effect of the gas Weber number either through We_g or We [48, 84, 99, 111, 118, 119, 123] or by including the ratio of gas density to surface tension (ρ_g/σ) [75, 121, 122]. Although some correlations derived from experiments with LFJIC account directly or indirectly for the effect of the liquid viscosity μ_{jet} [48, 84, 111, 115, 119, 122], very few include the jet density ρ_{jet} [48, 84] or the jet velocity to surface tension ratio (u_{jet}^2/σ) [75, 121, 122]. This suggests that most studies on LJIC consider that We_{jet} does not have a significant impact on the spray trajectory. This is also true for the turbulent properties of both fluids considering very few correlations include the effect of any Reynolds numbers [75, 84]. Among the studies conducted at higher pressure and/or temperature, very few have proposed correlations that directly include the effect of P_g [99] or T_g [87, 123]. This is most likely because they are already accounted for through the gas properties, which are either directly included in the correlation [48, 75, 121, 122] or indirectly through non-dimensional parameters that depend on μ_g [48, 75, 84] or ρ_g [48, 75, 84, 91, 109, 119, 120, 121, 122, 123, 124].

It is also possible to observe in **Table 2-2** that the studies available in the literature on the spray trajectory of LJIC sometimes disagree on the effect of a given parameter. While most correlations including the effect of We_g or We consider that higher values reduce the spray penetration [48, 75, 84, 99, 111, 118, 119, 121, 122], Li et al. [123] have reported otherwise. Song et al. [48] have also observed that the effect of We_g differs between the near-field and far-field regions. There is also no clear consensus on the effect of the liquid viscosity considering some correlations predict that the spray will penetrate less with

more viscous liquids [48, 111, 119] while others consider the opposite [84, 115, 122]. There are also some disagreements between the studies that directly include the effect of T_g . Although Li et al. [123] have reported higher spray trajectories for higher temperature and pressure (HTP) conditions, Lakhamraju [87] reported otherwise for high temperature and standard pressure (HTSP) conditions. These discrepancies could be explained by the different measurement techniques, experimental conditions and liquid properties used [9, 74]. As explained in the following section, differences in the design of the plain orifice injector used to conduct the experiments could also be responsible for these discrepancies [9, 74].

In addition to the spray trajectory, a few studies have provided information on the location of the CBP as shown in **Table 2-3** for turbulent LJIC. Although fewer correlations have been established between the non-dimensional parameters and the length of the CBP x_{CBP} , a few studies have reported the latter to increase with higher pressures or jet velocities u_{jet} [75, 121, 122] and with lower momentum flux ratios [121, 122] or surface tension [75, 84, 121, 122]. Furthermore, according to Broumand and Birouk [9], the liquid column breakup lengths reported by different experimental studies on LJIC vary between $8 \leq x_{CBP}/d \leq 12$ regardless of the turbulent properties of the liquid jet. On the other hand, the height of the CBP y_{CBP} has been strongly correlated to the non-dimensional parameters, especially the momentum flux ratio as higher values increase the penetration of the liquid jet column [75, 106, 118, 121, 122]. Similarly to the length of the CBP, higher jet velocities have also been associated with higher y_{CBP} values [121, 122]. Moreover, decreasing We has also been reported to increase the jet column penetration [84, 118].

Table 2-3: Empirical correlations proposed in the literature for the length and height of the column breakup point of a turbulent liquid jet in crossflow.

Reference	Column Breakup Point (CBP) Location	
	CBP Length (x_{CBP}/d)	CBP Height (y_{CBP}/d)
Bellofiore et al. [75]	$3.794 \left(\frac{\rho_g u_{jet}^2 d}{\sigma} \right)^{0.366}$	$1.499 J^{0.476} Re_{g,d}^{0.135}$
Amighi [84]	$3709 We^{0.09} We_{jet}^{0.01} \left(\frac{\sqrt{We}}{Re_{g,d}} \right)^{0.1} Oh^{0.88}$	$27.33 We_g^{-0.29} We_{jet}^{0.45} \left(\frac{\sqrt{We_g}}{Re_{g,d}} \right)^{-0.19} Oh^{0.69}$
	$=$ $3709 We^{0.14} We_{jet}^{0.45} Re_{g,d}^{-0.1} Re_{jet}^{-0.88}$	$=$ $27.33 We_g^{-0.385} We_{jet}^{0.795} Re_{g,d}^{0.19} Re_{jet}^{-0.69}$

Lee et al. [88]	5.2	N/A
Osta and Sallam [106]	5.2-8.0	$\begin{cases} 3.3J^{0.5} & \text{for } L/d = 10 \\ 3.1J^{0.5} & \text{for } L/d = 20 \\ 2.7J^{0.5} & \text{for } L/d = 40 \end{cases}$
Olyaei and Kebriaee [118]	12.5	$7.35J^{0.433}We^{-0.173}$
Ragucci et al. [121]	$3.687J^{-0.068}\left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{0.420}$	$4.355J^{0.416}\left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{0.085}$
Ragucci et al. [122]	$4.17J^{-0.095}\left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{0.382}\left(\frac{\mu_g}{\mu_{g,300K}}\right)^{0.044}$	$3.85J^{0.387}\left(\frac{\rho_g u_{jet}^2 d}{\sigma}\right)^{0.126}\left(\frac{\mu_g}{\mu_{g,300K}}\right)^{0.202}$
Lubarsky et al. [124]	1-4	N/A
Prakash et al. [125]	6-4	18-26

While there are plenty of correlations available for the transverse dispersion of the spray, little is known about the radial dispersion of LJIC. However, the few studies that have provided empirical correlations for the spray width have only correlated it to the momentum flux ratio as shown in **Table 2-4**. Thus, higher momentum flux ratios have been associated with wider LJIC sprays.

Table 2-4: Empirical correlations proposed in the literature for the radial dispersion of liquid jet in crossflow.

Reference	Spray Width (z/d)
Becker and Hassa [91]*	$2.32J^{0.09}\left(\frac{x}{d}\right)^{0.32}$
Song et al. [126]*	$0.560J^{0.4}\left(\frac{x}{d}\right)^{0.6}$
Wu et al. [127]	$7.86J^{0.17}\left(\frac{x}{d}\right)^{0.33}$
* Half spray width	

The correlations presented in **Table 2-1**, **Table 2-2** and **Table 2-4** were used to design a test section to conduct experiments of non-turbulent and turbulent LFJIC over a wide range of pressures, temperatures, Weber numbers and momentum flux ratios. The design and development work are presented in *Appendix A.6*.

2.1.5 Plain Orifice Injector Design

To complement the information provided in *section 2.1.4* regarding the effect of the non-dimensional parameters on the spray characteristics of LJIC, this section summarizes the effect of the injector design. As previously mentioned, this research focuses on the plain orifice injector, which is a type of pressure atomizer that uses a single orifice to atomize the liquid [7, 28]. Its main design features are shown in **Figure 2-8**.

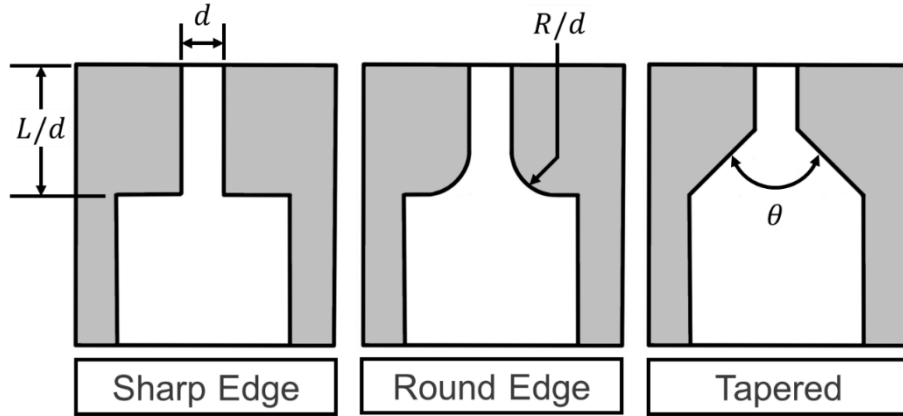


Figure 2-8: Plain orifice injector design.

Despite its simple design, the geometric features of the plain orifice injector strongly influence the spray characteristics of LJIC. To the best knowledge of the author, a vast majority of the empirical correlations proposed in the literature depend on the size of the injector diameter d . As presented in *section 2.1.4*, experimental studies on LJIC have reported that the SMD and the column breakup length are proportional to d apart from a few exceptions (i.e. [91]). The correlations shown in **Table 2-1** and **Table 2-3** indicate that larger orifices tend to produce larger droplets and enhance the axial penetration of the liquid jet column. Although the influence of the injector diameter on the spray trajectory and width is not as straightforward, the correlations proposed in the literature all strongly depend on non-dimensional parameters that vary with d as shown in **Table 2-2** and **Table 2-4**. This is also true for those that only depend on the momentum flux ratio considering the jet velocity u_{jet} is inversely proportional to d^2 when expressed as a function of the liquid mass flow rate through the injector. Replacing u_{jet} by the latter in the jet Weber and Reynolds numbers equations defined in *section 2.1.2* also reveals that injectors with larger diameters are less likely to generate turbulent jets and more likely to

exhibit a behaviour associated with the aerodynamic breakup regime described in *section 2.1.3*.

Other design features of the plain orifice injector have been reported to have an impact on the spray characteristics, such as the orifice length to diameter ratio (L/d). The latter has been shown to have an impact on both the primary breakup process (i.e. formation of ligaments and droplets, ligament size, column breakup point) [83, 106, 125] and secondary breakup process (i.e. spray penetration, SMD) [116, 125]. A few studies have found that increasing L/d increases the frequency and size of the ligaments shed from the liquid jet column [83, 106], reduces the axial and vertical penetration of the latter [83, 106, 125], lowers the maximum spray trajectory [116, 125] and enhances the secondary atomization process thus resulting in smaller SMD values in the far-field region [125]. These results have been attributed to larger L/d ratios reducing the discharged coefficient [116] and likely enhancing the turbulence level of the liquid at the orifice exit [83, 106]. A few studies have also assessed the effect of the injector's edge curvature (R/d) [106, 124] and found that it also has an impact on the primary [106, 124] and secondary [124] breakup process. Lubarsky et al. [124] have reported that using a sharp edge instead of a round edge increases the spray trajectory, reduces the liquid jet column penetration, and increases the SMD within the windward spray region. These observations have also been attributed to the sharp edge's effect on the discharge coefficient [124, 126] and on the turbulent characteristics at the injector's orifice [106, 124], which are similar to the effect of larger L/d ratios. Brown et al. [116] have also shown that using a tapered injector inlet yields a higher spray trajectory compared to using a sharp edge design because it increases the discharge coefficient.

The effect on the spray characteristics of the different plain orifice design features described in this section was considered to design the injector that will be used to produce exhaustive datasets of LFJIC. The design of the plain orifice injector for the experimental rig facility developed is presented in *Appendix A.3.2*.

2.2 General Governing Equations for Computational Fluid Dynamics

This section presents an overview of the fundamental equations used in Computational Fluid Dynamics (CFD) to study and predict complex flow phenomena [128]. The motion

of Newtonian fluid flow is governed by the Navier-Stokes equations, which prescribe the conservation of mass, momentum and energy as indicated below [129, 130].

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho u) = 0 \quad (2-10)$$

$$\frac{\partial (\rho v)}{\partial t} + \nabla \cdot (\rho u \otimes u) = -\nabla \cdot (PI) + \nabla \cdot (T) + F_b \quad (2-11)$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot (\rho E u) = -\nabla \cdot (Pu) + \nabla \cdot (T)u - \nabla \cdot (q) + F_b u \quad (2-12)$$

Where F_b represents the body forces such as gravity and I is the identity tensor.

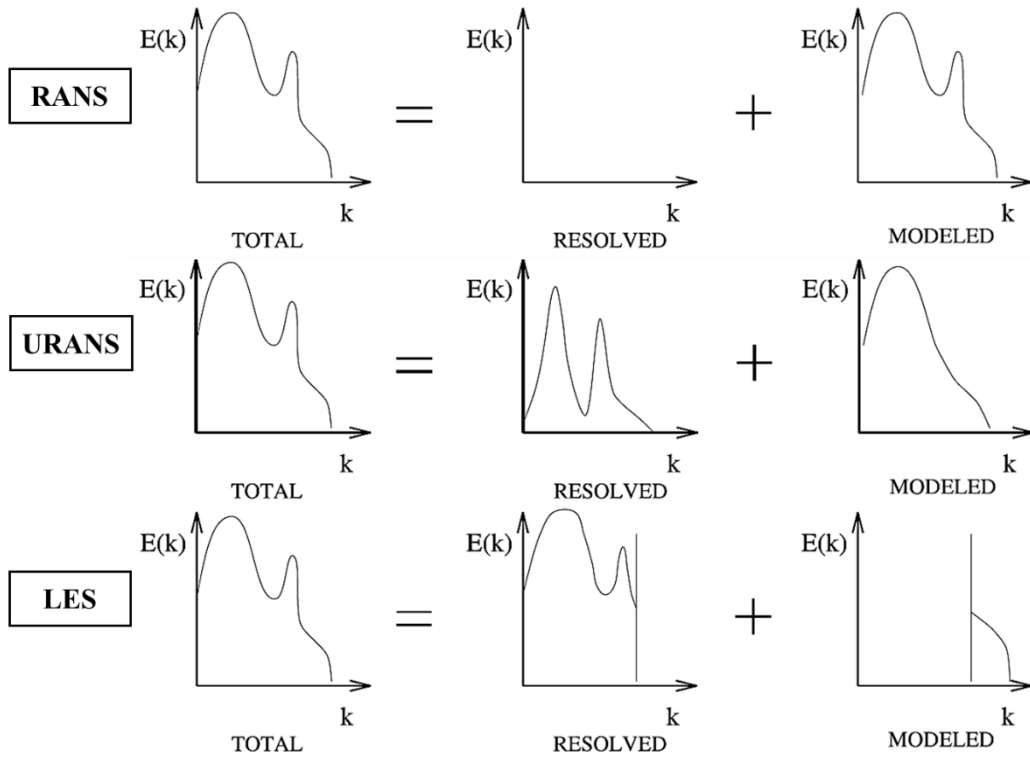


Figure 2-9: Symbolic difference in the energy spectrum decomposition between RANS, URANS and LES (Adapted from [128]. Reproduced by permission from Springer Nature; permission conveyed through Copyright Clearance Center, Inc.).

The methods used to solve these equations for turbulent flows depend on the type of numerical simulation performed, which should be selected by taking into consideration the level of accuracy, applicability, and practicability required for the specific engineering application involved [131]. In addition to the differences in the time-dependence nature of their solution (steady or unsteady), the main types of simulations used in state-of-the-art (SOA) CFD also differ by their decomposition of the energy spectrum as shown in **Figure 2-9** [128]. The Reynolds-Averaged Navier-Stokes (RANS) simulation is a lower-

fidelity and lower-cost tool that can be used to obtain a mean representation of a fluctuating flow field. While RANS relies on turbulence models to compute the statistical average of the solution, Direct Numerical Simulations (DNS) can fully resolve all turbulent scales but at the expense of the computational cost [129, 131, 132]. Alternative methods have been developed to simulate turbulent unsteady flows at a lesser cost than DNS, such as Large Eddy Simulations (LES) and unsteady RANS (URANS) [129]. Although LES uses subgrid-scale (SGS) models to represent the smaller dissipative scales filtered (also known as the Kolmogorov scales [131]), it is considered a higher-fidelity approach because it resolves at least 80% [131] of the energy spectrum [128, 131]. Despite modern advancements in High-Performance Computing (HPC), further improvements are still needed before LES can be fully incorporated into the CFD workflow for iterative design processes. URANS is a lower-fidelity tool that can be used to obtain an unsteady solution of the flow field by resolving a small portion of the lower-frequency modes [128].

With RANS, the pressure P , velocity u , total energy E and heat flux q values that govern the fluid motion are separated into a fluctuating φ' and mean $\bar{\varphi}$ component as seen in equation (2-13). The mean transport equations for the mass, momentum and energy are then obtained by replacing the solution variables inside the corresponding Navier-Stokes equations with their respective mean component. [128, 130]

$$\varphi = \begin{cases} \bar{\varphi} + \varphi' & \text{RANS} \\ \tilde{\varphi} + \varphi' & \text{LES} \end{cases} \quad (2-13)$$

With LES, the mean component is replaced by a filtered variable $\tilde{\varphi}$ and substituting the solution variables with the latter yields the filtered Navier-Stokes transport equations. The viscous stress tensor T is also decomposed into a mean or filtered component depending on the turbulence approach used as shown in equation (2-14). It can also be observed that an additional term is added to close the governing equations, which depends on the mean strain rate $\mathbb{S}$ and turbulent viscosity μ_t . [128, 130]

$$T = \begin{cases} \bar{T} + T_{RANS} & \text{RANS} \\ \tilde{T} + T_{SGS} & \text{LES} \end{cases} \quad (2-14)$$

$$T_{RANS} = 2\mu_t\mathbb{S} - \frac{2}{3}(\mu_t\nabla \cdot \bar{u})I \quad (2-15)$$

$$\mathbf{T}_{SGS} = 2\mu_t \mathbb{S} - \frac{2}{3}(\mu_t \nabla \cdot \tilde{\mathbf{u}})\mathbf{I} \quad (2-16)$$

To compute the RANS stress tensor $\mathbf{T}_{RANS}$ defined in equation (2-15), the turbulent terms are derived from the eddy viscosity model selected (e.g. Realizable k-epsilon [133]). The LES turbulent stress tensor $\mathbf{T}_{SGS}$ depends on the chosen SGS model (e.g. Wall-Adapting Local Eddy-Viscosity (WALE) [134]) [128, 130]. As for URANS, the Navier-Stokes solution variables are decomposed into all three components (i.e. mean, filtered and fluctuating) and the RANS viscous stress tensor is applied [128]. The different RANS turbulence models and SGS models utilized in this research are described in further detail in Chapter 4.

2.3 Overview of Atomization Models

This section presents an overview of the different atomization approaches used to model LJIC. The introduction sections of the core research chapters present a more in-depth description of the approaches and breakup models assessed in this research. **Table 1-1** previously presented at the end of *section 1.2* indicates where their governing equations can be found within the core research chapters. As shown in **Figure 2-10**, there are mainly three different approaches that are widely used for modelling atomization: the higher-fidelity interface capturing (and/or tracking) methods, the lower-fidelity Lagrangian approach (also referred to as Lagrangian-Eulerian) and the hybrid approach. The latter consists of coupling the Lagrangian approach with the interface capturing method.

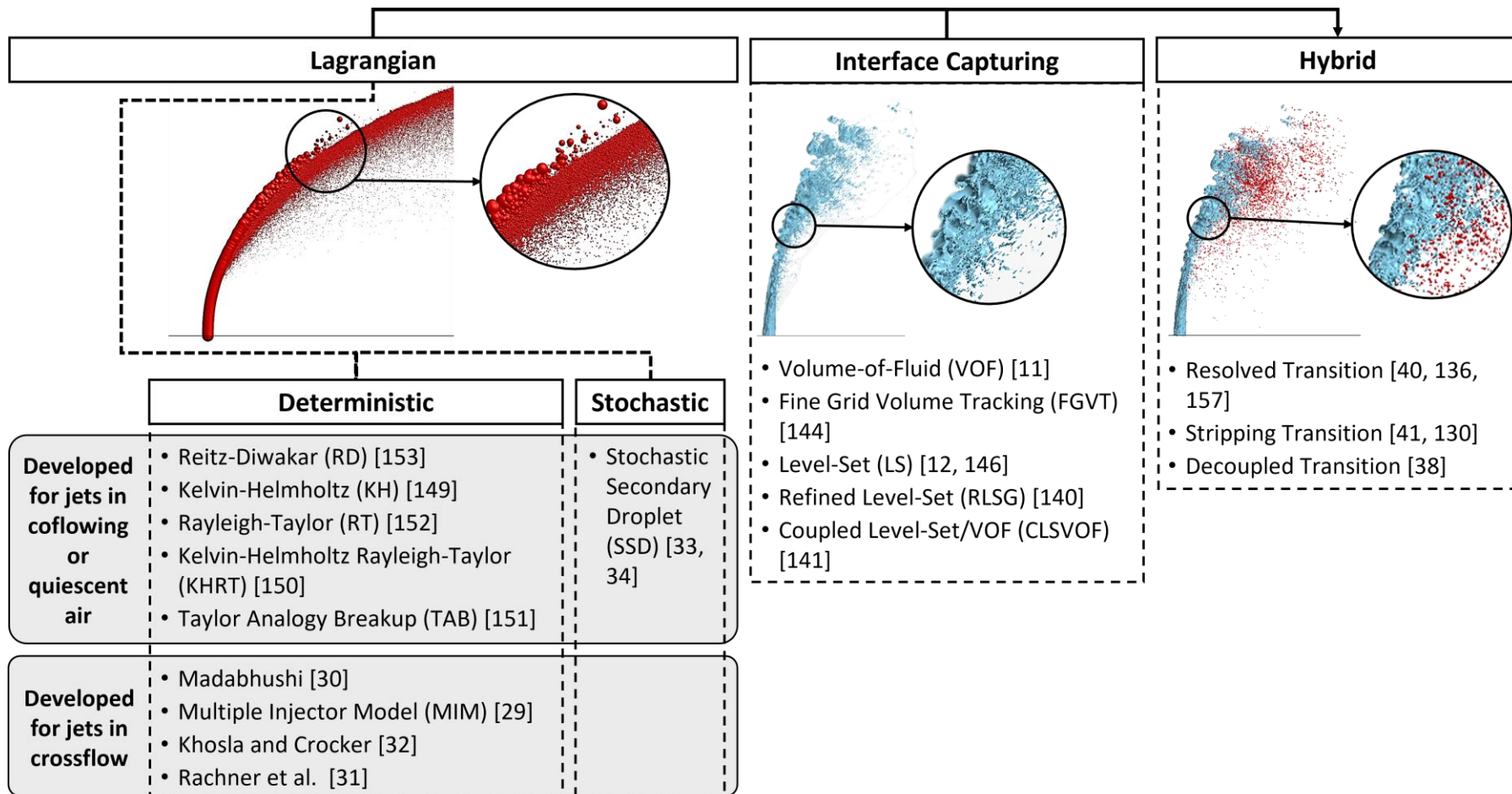


Figure 2-10: Atomization modelling approaches and secondary breakup models.

The interface-capturing methods use the Eulerian framework to resolve the interface between the liquid and gas phases [7, 132]. These methods can be classified as higher-fidelity atomization modelling approaches due to their ability to model the dense spray region and fine droplet cloud without relying on empirical correlations [24, 41, 135, 136]. Thus, they are more suitable for Large Eddy Simulations (LES) and Direct Numerical Simulations (DNS) [e.g. 132, 137, 138, 139]. They are able to capture the important processes involved in the atomization of LJIC, such as the shedding of ligaments from the surface of the jet column [e.g. 25, 35, 135]. Furthermore, these higher-fidelity methods model the continuous phase flowing inside the injector, which enables accounting for the effect of the injector design on the spray characteristics. However, they require a fine mesh resolution to accurately capture the interface position [13, 135 and reference therein, 140] and impose restrictions on the time-step size [13, 135, 141], which can be in the order of micro to nanoseconds [41]. As for the mesh size, it is often in the order of hundreds of million elements even for small numerical domains [38, 137, 138, 142] and well over 30 million elements [39, 143] even when using Adaptive Mesh Refinements (AMR) techniques to constrain the finer mesh resolution to the interface region [140]. Moreover, higher-order schemes and more robust sub-models are often needed to accurately capture the surface curvature [140, 141] and to account for the surface tension force effects, especially for flows with large density gradients [13, 140, 144]. Thus, the main drawback of the interface-capturing methods is their high computational cost, which makes them non-practical for engineering applications [132, 135, 145], especially for processes that involve high Weber and Reynolds numbers [135, 138].

There are multiple types of interfaces capturing and tracking methods, such as the Level-Set (LS) methods [12, 146], Fine Grid Volume Tracking (FGVT) [144] method and Volume-of-Fluid (VOF) [11] approach. One of the fundamental differences between the LS method and the VOF approach lies in the representation of the interface, which affects the computation of the curvature. The latter uses the volume fraction to capture the interface [11] while the LS method uses a set of points corresponding to the “zero level-set of a smooth function” [12]. Although not relying on the volume fraction simplifies the computation of the curvature, it tends to introduce important numerical errors, especially when the free surface gets severely distorted and/or disintegrates [141]. As a result, the

interface capturing approaches based on the LS method are prone to mass conservation issues [13, 140, 141]. Different alternative approaches have been developed to address this problem, such as the Coupled Level Set/VOF (CLSVOF) [141] method or the Refined Level-Set Grid (RLSG) method [140]. A more in-depth comparison between the VOF approach and the different interface capturing methods can be found in Sussman et al. [141] for the LS methods and in Duarte et al. [135] for the FGVT approach. Duarte et al. [135] have also compared the predictive capabilities of the VOF and FGVT approach for LJIC to the results reported by Herrmann [35] using the RLSG method [140].

Most numerical studies available in the literature on LJIC that use the higher-fidelity interface capturing methods either rely on the VOF approach [26, 27, 36, 38, 40, 41, 135, 137, 142] or the CSLVOF method [25, 39, 137, 143], which is likely to avoid the mass imbalance problems of the LS method. Moreover, the latter is likely more prone to numerical errors when modelling LJIC considering it involves strong aerodynamic effects that cause the free surface to bend and separate. It should also be noted that most numerical studies using the hybrid method to model LJIC have used the VOF approach [26, 27, 36, 38, 40, 41]. Indeed, very few studies have used the CLSVOF-Lagrangian [25, 39] or the RLSG-Lagrangian approach [35]. This could be due to the CSLVOF method requiring additional correction schemes to damp the important fluctuations that are likely to occur and affect the curvature derivative [140, 147]. The RLSG method was developed to address this issue by reducing the need for complex correction factors, but at the expense of the computational cost [13, 145 and reference therein]. The FGVT method has also been reported to be more computationally expensive than the VOF approach for LJIC due to its finer grid requirements for the advection of the interface [144], which can cut by half the allowable time-step size [135]. Thus, the VOF approach was selected as the interface capturing method used in this research to assess, validate, and develop higher-fidelity numerical modelling methodologies for turbulent LFJIC. This ensures the numerical methodologies developed can maintain a sharp interface while conserving the volume of liquid in the domain [141, 148], which likely makes them more suitable for cases with high turbulence and/or atomization levels. The governing equations of the VOF and VOF-Lagrangian approach are further described in Chapter 6 and Chapter 5.

The Lagrangian approach allows to model the discrete phase at a much lower cost than the interface-capturing methods by using a statistical method to discretize the spray into multiple groups (i.e. parcels) of identical particles instead of an exponentially larger number of individual and unique particles [132]. However, the savings in computational cost are often made at the expense of accuracy due to the simplified modelling of the dense spray region and particle-particle interactions [132]. Although different names have been used to refer to this method, it is more precisely classified as an Eulerian-Lagrangian approach considering the continuous gas phase is modelled within the Eulerian framework [132]. Unlike the interface-capturing methods, the liquid flow inside the injector can not be modelled. Instead, the parcels are injected at the location of the injector exit with a specified droplet size distribution, cone angle (if applicable) and velocity [130]. The atomization process is then modelled with breakup models that are often deterministic [149, 150, 151, 152, 153] as shown in **Figure 2-10**. Other breakup models such as the Huh [154] and the Linearized Instability Sheet Atomization (LISA) [155] models have been developed to account for the primary breakup process of sprays in coflowing or quiescent air injected from a simple orifice and pressure-swirl injector respectively, but they require exhaustive experimental knowledge of the near-field characteristics [14, 130]. Moreover, they are not deemed likely suitable for modelling the primary breakup processes of LJIC.

A few breakup models have been specifically developed to incorporate the specific features characterizing the primary breakup of LJIC [29, 30, 31, 32], which includes the jet column bending and stripping processes. This is often achieved with the help of the Boundary Layer Stripping (BLS) model [156] or deterministic breakup models (e.g. KH breakup model [30]). Thus, similar to the latter, the LJIC breakup models also rely on empirical constants and correlations to account for the primary and secondary atomization process as described in Chapter 1 and shown in **Figure 2-11**. The Lagrangian approach and the different secondary breakup models that have been used to model LJIC are described in further detail in Chapter 3 and Chapter 4.

The high computational cost of the interface-capturing method and the lower-fidelity nature of the Lagrangian approach motivated the development of hybrid approaches that transform the Eulerian liquid phase into spherical Lagrangian particles based on specific

transition criteria. The most commonly used transition model consists of transforming small spherical droplets into Lagrangian particles [40, 136, 157]. Different criteria can be implemented to identify the liquid phase that will be transitioned, such as the diameter and sphericity [40, 136, 157]. Throughout this work, this type of hybrid transition criteria is referred to as the “resolved” transition model considering it requires resolving the primary breakup process. This implies the need to capture the droplets and ligaments separating from the liquid surface, which inevitably subjects the hybrid approach to the limitations mentioned previously for the interface-capturing methods.

	Jet trajectory	Primary breakup	Secondary breakup	Drop size/velocity for primary breakup	Schematic view
Rachner et al. [31]	One-dimensional theoretical analysis	BLS from a single droplet	BLS	Single-droplet-based correlation SMD empirical correlation	
Madabhushi [30]	Modified the droplet drag coefficient to make the droplets take on a path similar to a LJIC	K-H wave from a single droplet	Local Weber/Ohnesorge number criteria	Single-droplet-based correlation Jet-specific correlations	
Khosla and Crocker [32]	Modified the droplet drag coefficient to make the droplets take on a path similar to a LJIC	BLS from a single droplet	Rayleigh-Taylor	Single-droplet-based correlation	
MIM model [29]	Theoretical analysis by considering: deforming jet, adaptive drag, and mass stripping	Multiple injectors located along two lines parallel to jet and on its sides	TAB	Jet-specific correlations	

Figure 2-11: Description of the breakup models specifically developed for Liquid jet in crossflow (Adapted from [29] with permission from the American Institute of Aeronautics and Astronautics, Inc.).

Recent work has been done to further reduce the computational cost of the hybrid approach for LJIC, such as stripping the Lagrangian droplets from the liquid surface [41, 130] or by coupling the VOF and Lagrangian approach indirectly [38]. In this work, the former will be referred to as the “stripping” transition model and the latter as the “decoupled” VOF-Lagrangian approach. Prior to this research, the stripping transition model was used with empirical correlations to predict the size and position of the transitioned Lagrangian droplets [41]. As for the decoupled VOF-Lagrangian approach,

its implementation needs to be further improved to account for the important blockage effect of the liquid jet column on the spray characteristics [38]. These alternative transition models are further discussed in Chapter 6, where an optimized stripping transition model that does not rely on empirical correlations is proposed.

2.4 Validation Data

This section addresses the choice of datasets and conditions (i.e. specific test points) selected to validate and assess the numerical modelling methodologies presented in the core research chapters. The first step was to conduct a review of the datasets that have been used in the literature to validate the predictive capabilities for liquid jets in crossflow (LJIC) of the different numerical modelling approaches considered in the scope of this work. As mentioned in *section 2.3*, this includes the Lagrangian approach and its direct coupling with the interface capturing method (i.e. hybrid approach). The numerical research gaps identified were then used to inform the selection process along with more general considerations formulated based on the aims, objectives, and scope of this research. The following step consisted of reviewing the existing experimental studies on turbulent liquid fuel jets in crossflow (LFJIC) to identify suitable datasets and down-select them based on the criteria established. The last step was to select specific conditions within the chosen datasets to help fill the gaps in knowledge on the atomization modelling of turbulent LFJIC.

2.4.1 General Considerations

The predictive capabilities of the different atomization modelling approaches are expected to be sensitive to the operating conditions (injector geometry, liquid properties, turbulence levels, etc.) due to their known influence on the spray characteristics [7, 14, 28]. Therefore, general selection criteria were established based on the aim of this research, which was to develop robust numerical tools to hasten the delivery of low-emission gas turbine combustion systems that use liquid fuel injectors. To ensure the validation datasets selected are representative of the intended application, only LJIC datasets using liquid fuels were considered. Moreover, the selection was limited to turbulent jets and crossflows because it is expected to enhance the fuel-air mixing quality to further reduce emissions [7, 9, 10]. Although higher-pressure datasets were prioritized as they are more representative of gas turbine conditions, datasets at ambient pressures

were also included to assess the predictive capabilities of the numerical modelling approaches with and without the added strain of using higher-density ratios. This also ensures the work contributes to fill the gaps in knowledge on the atomization modelling of LFJIC, which are quite numerous even for ambient conditions as presented in the following section.

Furthermore, only datasets at ambient temperatures were considered to ensure the effect of atomization modelling can be assessed independently from those of evaporation modelling. Thereby providing a fair basis for assessing their predictive capabilities. This is also justified by the existing research gaps in the numerical modelling of LJIC at ambient temperatures that still need to be addressed. Indeed, very few validation studies available in the literature have used datasets for LJIC under high-temperature conditions [21, 36]. Moreover, they were limited to water sprays [21, 36]. This can be partially attributed to the experimental research gaps on LJIC at high temperatures, especially for fuels as discussed in *Appendix A.1*. This research limitation and related recommendations for future work are further discussed in Chapter 7.

It is also important to note that very few studies on LJIC have been conducted with an injector type other than the plain orifice atomizer as presented in *section 2.1.1*. This can be partially attributed to the current gaps in knowledge on the fundamental physics and modelling of LJIC that still need to be addressed, especially for fuels and/or higher-pressure conditions as detailed in *Appendix A.1*. This type of fundamental research work can not be done with more complex injectors due to their strong impact on the spray characteristics. Therefore, the datasets considered for the selection process were limited to plain orifice injectors. However, the numerical methodologies developed from this research could still be used to inform the modelling approaches to simulate more complex injectors as discussed in *section 7.5* from Chapter 7.

2.4.2 Literature Review: Numerical Validation Studies

The purpose of this section is to highlight the numerical research gaps in the validation of the Lagrangian and hybrid approach for the stochastic (i.e. SSD) and deterministic breakup models used in state-of-the-art (SOA) CFD and specifically developed for LJIC. Thus, this assessment only takes into account the studies that have reproduced experimental conditions to validate the approaches within the scope of this work. Indeed,

a few numerical studies on LJIC have used boundary conditions that have not yet been experimentally studied as their purpose was to gain a better understanding of the spray characteristics under more extreme conditions [20, 25, 39]. In other words, these studies use boundary conditions that were not derived from any existing datasets due to the current experimental research gaps. As a result, the LJIC spray characteristics were either not validated [e.g. 20, 25, 173] or only for the spray trajectory using empirical correlations either at significantly lower pressures [39] or for a different type of injector [15]. For the studies that include both types of boundary conditions, only those derived from experimental data are considered. This also extends to the numerical work done to model combustion with LFJIC, but that does not include validation of the spray characteristics due to the experimental challenges of measuring them in reacting flows [26, 158, 159].

Furthermore, the datasets selected from this process were used in all the core research chapters to strengthen the conclusions from this research. This procedure ensures the validation and assessment of the different numerical methodologies developed are consistent. Thus, the numerical studies considered in this section to help establish the selection criteria only include those that were publicly available within the first year of this project. However, the studies published recently that were excluded from this subsection (i.e. [20, 26, 27]) are still used in the following sections and chapters for comparison purposes where applicable.

2.4.2.1 Numerical Research Gaps: Liquid Fuels

Considering the model constants of the deterministic breakup models used in SOA CFD were originally derived from experiments on spray in quiescent or coflowing air at atmospheric conditions or using water [24, 25], several research efforts have been made to calibrate and validate their applicability for LJIC as shown in **Figure 2-12**. However, the studies conducted with the lower-cost Lagrangian approach to validate and calibrate their predictive capabilities have been mostly limited to water sprays [16, 17, 18, 19, 21, 22, 23]. Although a recent study has calibrated the Wave breakup model using a liquid fuel dataset, the momentum flux ratio used was limited to low values ($J = 10$) [38]. The studies conducted using a LJIC breakup model have also been mostly validated for liquid fuels [30, 31, 32, 38]. Thus, selecting any LJIC datasets for fuels, especially for $J > 10$,

would help fill the gaps in knowledge on the predictive capabilities of the Lagrangian approach with the SOA breakup models.

Furthermore, the studies conducted to validate the hybrid approach for LJIC were limited to using datasets of water sprays [35, 36, 41] or non-turbulent LFJIC [40]. Although a fuel dataset has been used to assess a methodology that couples the Lagrangian approach with an interface capturing method [38], the VOF-Lagrangian coupling was not direct. Thus, selecting any turbulent LFJIC datasets would provide a better understanding of the standard hybrid approach's predictive capabilities (direct Lagrangian coupling), regardless of the breakup model used.

To the best knowledge of the author, the studies conducted to validate the predictive capabilities of the SSD breakup model for LJIC with the Lagrangian or hybrid approach were also limited to water sprays [35, 36, 37], except for the decoupled VOF-Lagrangian approach [38]. Therefore, selecting any LFJIC datasets would contribute to bridging the research gaps on the predictive capabilities of the SSD breakup model when coupled with the Lagrangian and hybrid approaches

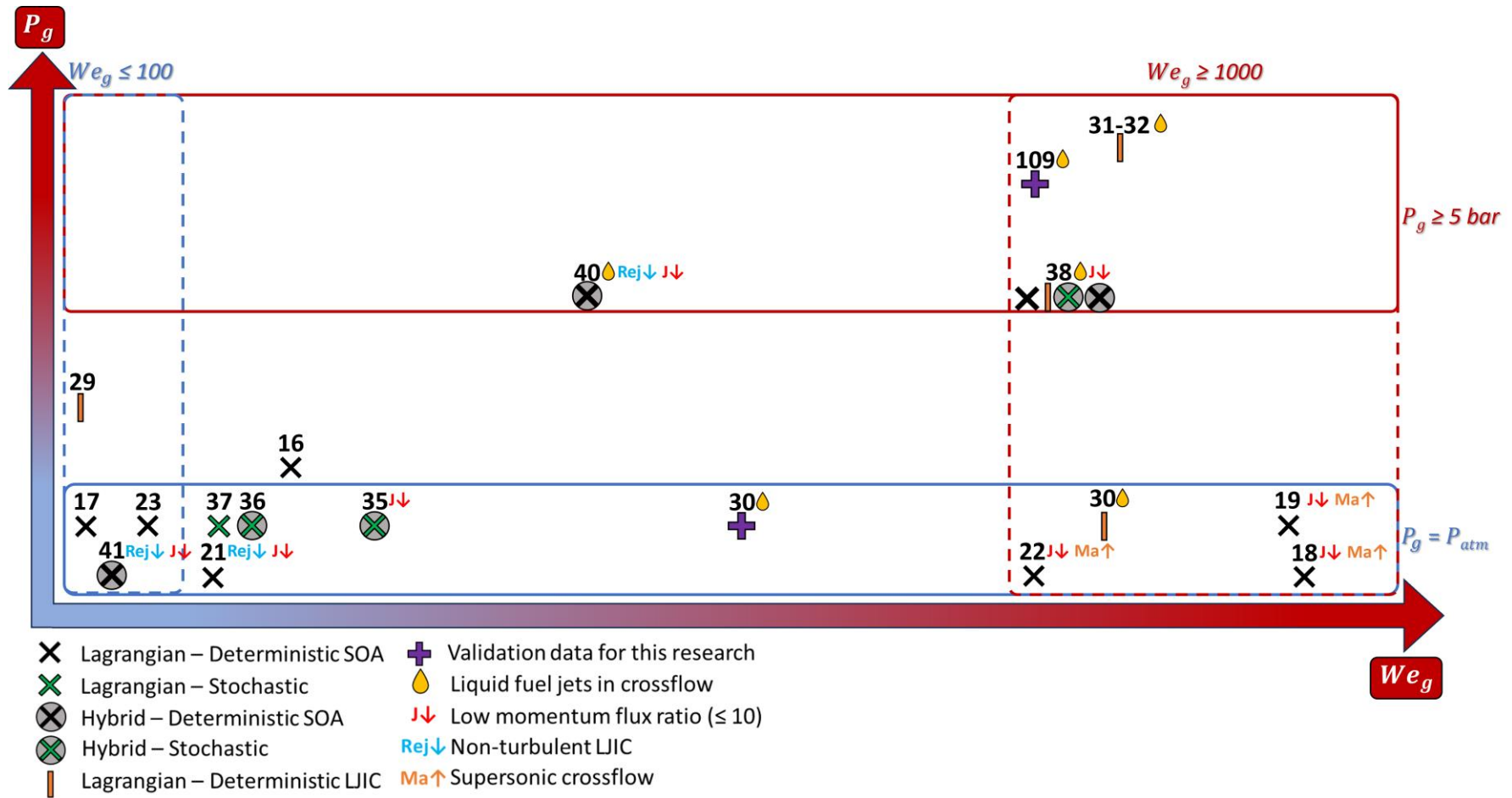


Figure 2-12: Extreme range of conditions used in numerical studies available in the literature (reference number indicated above symbols) to validate different modelling approaches for liquid jets in crossflow compared to this research (dataset reference number indicated above purple crosses)

2.4.2.2 Numerical Research Gaps: Gas Pressure

Figure 2-12 shows the predictive capabilities of the SOA breakup models for LJIC have been mostly assessed using datasets at standard pressure, often at ambient conditions [17, 18, 19, 21, 22, 23, 41] or for pressures lower than 5 bar [15, 16, 38, 40]. Thus, any LJIC dataset with $P_g \geq 5$ bar would help fill the gaps in knowledge on the predictive capabilities of the SOA breakup models with the hybrid or Lagrangian approach.

As for the SSD breakup model, its predictive capabilities for LJIC have only been assessed at ambient pressures [35, 36, 41] with the Lagrangian or hybrid approach, although up to 5 bar with the decoupled VOF-Lagrangian approach [105]. Thus, any LJIC datasets with non-ambient pressures would contribute to bridge the research gaps on the predictive capabilities of the SSD breakup model when coupled with the Lagrangian and hybrid approaches.

While the Madabhushi [30] and Multiple Injector Model (MIM) [29] breakup models specifically developed for LJIC have been validated mostly at lower pressures ($P_g \leq 5$ bar) [29, 30, 38], those using the Boundary Layer Stripping (BLS) model used datasets up to 9 bar [31, 32]. Therefore, it could be relevant to select a LFJIC dataset for similar pressures ($P_g \approx 9$ bar), but it is not a priority considering the LJIC breakup models are not explicitly used in this research (thus not directly compared) as they mostly rely on empirical correlations [29, 31, 32].

2.4.2.3 Numerical Research Gaps: Gas Weber Number

The hybrid approach for LJIC has been validated using datasets with gas Weber numbers inferior to 330 [35, 36, 41] or up to 550 when using non-turbulent liquid fuels [40], except for the decoupled VOF-Lagrangian approach which was validated for $We_g > 1000$ [38]. Thus, any turbulent LFJIC datasets with $We_g > 330$ would help improve the understanding of the standard hybrid approach's predictive capabilities for such applications regardless of the breakup model used.

To the best knowledge of the author, validation of the SSD breakup model with the Lagrangian or hybrid approach for LJIC has also been limited to $We_g \leq 330$ [35, 36, 41], except for the decoupled VOF-Lagrangian approach as mentioned above [38]. Therefore,

any LJIC datasets with $We_g > 330$ would help fill the gaps in knowledge on the predictive capabilities of the SSD breakup model with the Lagrangian and hybrid approaches.

The studies conducted to validate the predictive capabilities of the SOA deterministic breakup models with the Lagrangian approach for LJIC at high gas Weber numbers ($We_g > 1000$) either used datasets for water sprays under supersonic crossflow [18, 19, 22], which is not representative of industrial gas turbine conditions and for stationary or subsonic aircraft operations [8], and/or for low momentum flux ratios ($J \leq 10$) [18, 19, 22, 38]. Moreover, most validation studies conducted with LJIC datasets for subsonic crossflows were limited to $We_g \leq 240$ [16, 17, 21, 23, 37]. Thus, selecting any subsonic LJIC datasets with $We_g > 1000$ and $J > 10$ would contribute to bridge the research gaps on the predictive capabilities of the Lagrangian approach with the SOA breakup models.

The LJIC breakup models have also been mostly validated for $We_g > 1000$ [30, 31, 32, 38] either with low momentum flux ratios ($J \leq 10$) at the highest pressures [31, 32, 38] or with $J \leq 12$ at ambient pressure [30]. Therefore, it could also be interesting to prioritize selecting datasets for high gas Weber numbers ($We_g > 1000$) that also provide higher pressures ($P_g \approx 9$ bar) conditions or slightly higher momentum flux ratios if the pressure is closer to ambient ($J \geq 12$).

2.4.2.4 Numerical Research Gaps: Momentum Flux Ratio

The studies on the SSD or SOA deterministic breakup models that have been conducted using datasets at higher pressures ($P_g \geq 5$ bar) and/or gas Weber numbers ($We_g > 1000$) were limited to low momentum flux ratios ($J \leq 10$) [18, 19, 22, 38, 40]. The studies conducted for $J > 10$ were limited to $We_g \leq 240$ [16, 17, 23, 36, 37]. Thus, LJIC datasets with $We_g > 1000$ and $J > 10$, especially if $P_g \geq 5$ bar, would help fill the gaps in knowledge on the predictive capabilities of the SSD and SOA deterministic breakup models regardless of the approach (Lagrangian or hybrid). This is also true for the datasets at ambient pressure with $We_g > 330$.

The LJIC breakup models that have been validated for high momentum flux ratio ($J \leq 18$) were limited to $P_g \leq 6$ bar [29, 30, 31, 32, 38]. The datasets used for validation with the highest momentum flux ratios ($J \leq 34$) were limited to lower pressures ($P_g \leq 3$ bar) and

$We_g < 720$ [29, 30]. Thus, further consideration should be given to datasets with similar conditions to help fill the gaps in knowledge on the LJIC breakup models. In fact, the high-pressure datasets considered in the following sections are mostly comprised of those used in the studies of LJIC breakup models.

2.4.3 Datasets Selection Criteria

The following selection criteria were formulated based on the general considerations and research gaps:

1. For the reasons detailed in *section 2.4.1*, only datasets for turbulent liquid fuel jets in turbulent crossflow at ambient temperature and obtained using a plain orifice injector are considered for the validation studies.
2. Based on the general considerations detailed in *section 2.4.1*, at least one dataset at standard temperature and pressure (STP) and one at standard temperature and high pressure (STHP) must be selected.
3. Considering the research gaps highlighted in *section 2.4.2*, the datasets selected should have at least $We_g > 330$ regardless of the pressure and momentum flux ratio to help fill the gaps in knowledge on the predictive capabilities of the SSD breakup model.

The following criteria formulated based on the information provided in *section 2.4.2*, which are presented in order of priority, were used to further guide the selection of the STP dataset:

4. The STP dataset selected should be for turbulent LFJIC with $We_g > 330$ and $J > 10$.
5. Considering the research gaps on the LJIC breakup models, the gas Weber number and Momentum flux ratio of the STP dataset selected should ideally be similar to those used by Madabhushi et al. [30] ($J \approx 34$ and $We_g \approx 720$).

The following criteria were used in order of priority to select the STHP datasets to help fill the research gaps discussed in *section 2.4.2*:

6. Considering the research gaps in the validation of the SSD and deterministic SOA breakup models, datasets for high gas Weber numbers ($We_g > 1000$) and high momentum flux ratios ($J > 10$) should be prioritized and ideally for $P_g \geq 5$ bar.
7. Based on the studies done to validate the breakup models specifically developed for LJIC, datasets with $We_g > 1000$ and $P_g \approx 9$ bar should ideally be selected.

2.4.4 Dataset Selection

Table 2-5 compares the experimental conditions and validation data provided by the studies available in the literature for turbulent LFJIC under STP conditions. **Table 2-6** presents the same information but for STHP conditions. The datasets that were ultimately selected are indicated by the gray cells. It should be noted that the studies providing partial details on their specific test conditions were excluded from consideration due to the difficulty of reproducing them numerically [i.e. 27, 160, 161].

In addition to the studies presented in **Table 2-5**, it is worth mentioning those conducted by Sallam et al. [82] and Lee and al. [88] to characterize the primary breakup characteristics of turbulent and non-turbulent LJIC at STP conditions using water sprays as well as glycerol [82], ethanol [82] and ethyl alcohol [88]. However, the studies from this research group were conducted at low gas Weber numbers ($We_g < 300$) and were mainly focused on mapping the non-dimensional spray characteristics to better define the different turbulent breakup regimes. Thus, they are not deemed suitable candidates based on the selection criterion presented in *section 2.4.3*.

Table 2-5: Turbulent Liquid fuel jets in crossflow datasets under standard temperature and pressure conditions available in the literature.

Turbulent LFJIC Study		Shaw and Gutmark [162]	Farvardin et al. [111]	Stenzler et al. [119]		Tambe et al. [81]		Madabhushi et al. [30]
Conditions	Fuel	Jet A (A-2)	Diesel and blends	Acetone	4-Heptanone	Jet A	N-Heptane	Jet A
	J	20	10	18	18	1	1	5
			135	36	36	10	10	34
	We_g	70	29	1.3	12	99	302	180
			82	106	106	1274	1725	1680
	u_g [m/s]	40	35	10	30	173	119	69
			58	90	90	198	215	138
	Re_g	4.5E+05	2.3E+05	1.8E+04	5.5E+04	2.8E+05	1.9E+05	3.1E+05
			3.8E+05	1.6E+05	1.6E+05	3.2E+05	3.5E+05	6.1E+05
	Re_{jet}	4.9E+03	4.7E+03	1.1E+03	1.4E+03	6.3E+02	3.6E+03	4.4E+03
			7.8E+03	1.4E+04	6.0E+03	1.1E+04	2.3E+04	1.7E+04
Validated Spray features	x/d	100	100	100	100	30	30	14
						65		33
	Trajectory		X	X	X	X	X	
	SMD	X	X			X	X	X
	Velocity	X	X			X		X
	Shadowgraph		X	X	X	X	X	
	Droplet Size Distribution		X					
	Fuel Flux	X	X			X		
	Column Breakup		X			X	X	

To the best knowledge of the author, the studies from Madabhushi et al. [30] and Tambe et al. [81] on turbulent LFJIC are the only ones to provide STP datasets for $We_g > 110$. Thus, they are the only ones presented in **Table 2-5** that respect the minimum selection criterion defined in *section 2.4.3*. However, the dataset from Tambe et al. [81] covers a slightly smaller range of Weber numbers and its maximum momentum flux ratio ($J = 10$) is much smaller than the maximum value provided by the dataset from Madabhushi et al. [30] ($J = 34$). Furthermore, the latter covers a much higher and wider range of turbulent Reynolds numbers for the crossflowing gas stream compared to any other STP dataset. Therefore, the dataset provided by Madabhushi et al. [30] was chosen to validate the numerical modelling approaches in this research.

The STHP datasets available in the literature all respect the selection criteria formulated in *section 2.4.3*. Thus, the down-selection process requires a more in-depth comparison of the validated features and operating conditions used. As shown in **Table 2-6**, the experimental studies on LFJIC conducted at the highest pressures ($P_g \geq 10$ bar) [121, 123] tend to cover a lower range of gas Weber numbers and provide measurement data for fewer spray characteristics compared to other STHP datasets. This is also true for the datasets provided by Becker and Hassa [91] considering all spray characteristics were provided for $P_g \leq 9$ bar except for the shadowgraph images. Thus, the STHP datasets that were further considered in the selection process cover a range of pressure from 2 to 9 bar.

Table 2-6: Turbulent Liquid fuel jets in crossflow datasets under standard temperature and high-pressure conditions available in the literature.

Turbulent LFJIC Study			Freitag and Hassa [109]	Song et al. [48]	Becker and Hassa [91]	Lubarsky et al. [124]	Ragucci et al. [121]	Li et al. [123]
Conditions	Fuel		Kerosene	Jet A	Jet A-1	Jet A	Jet A-1	Kerosene
	P_g [bar]	min	2	2.1	1.5	5	10	10
		max	8	9.7	15			20
	J	min	3	5	2	5	11	18
		max	24	25	18	100	74	55
	We_g	min	39	250	90	400	297	400
		max	3281	1000	2120	1600	609	860
	u_g [m/s]	min	25	30	50	66	37	45
		max	150	137	100	140	53	
	Re_g	min	2.5E+05	1.7E+05	1.5E+05	5.9E+05	5.8E+05	1.1E+06
		max	1.5E+06	7.8E+05	1.8E+06	1.3E+06	8.3E+05	2.3E+06
	Re_{jet}	min	7.4E+02	9.6E+03	2.0E+03	2.7E+03	4.5E+03	-
		max	1.0E+04	4.5E+04	9.6E+03	$\approx 2.5E+04$	1.2E+04	-
Validated Spray features	x/d	min	143	50	178	60	12	40
		max						
	Trajectory		X	X	X	X	X	X
	SMD		X	X	X	X		
	Velocity							
	Shadowgraph		X	X	X	X	X	
	Droplet Size Distribution			X	X			
	Fuel Flux		X	X	X			
	Column Breakup					X	X	
	Width				X			

Compared to the remaining STHP datasets under consideration ([48, 91, 124]), the study from Freitag and Hassa [109] covers a much higher and wider range of gas Weber numbers. Compared to the other dataset from the same research group [91], it also offers a higher range of momentum flux ratios and jet Reynolds numbers. Thus, although the dataset from Becker and Hassa [91] provides a wider variety of spray characteristics data, the conditions provided by the more recent study from Freitag and Hassa [109] were preferred. This also applies to the dataset from Lubarsky et al. [124] due to the higher and wider range of pressures covered by the conditions from Freitag and Hassa [109]. As for the dataset from Song et al. [48], it offers a much lower range of gas Weber numbers and gas Reynold numbers. Thus, despite covering a similar range of momentum flux ratios, the dataset from Freitag and Hassa [109] was chosen instead.

The selection process described in this subsection further emphasizes the significant research gaps in knowledge on the physics of turbulent LFJIC under more representative gas turbine conditions, especially at higher pressures. This aspect is further discussed in Appendix A.

2.4.5 Datasets Conditions Selected

For each dataset selected, at least one experimental condition was chosen to validate the predictive capabilities of the numerical methodologies developed using the SSD breakup model and to assess the predictive capabilities of the non-calibrated SOA breakup model.

The STP dataset from Madabhushi et al. [30] provides 4 different conditions. According to the 6th selection criteria in *section 2.4.2*, priority could be given to higher momentum flux ratio conditions ($J \geq 10$) if the gas Weber number is much larger than 330. The highest gas Weber number condition provided by Madabhushi et al. [30] has a momentum flux ratio ($J = 12$) relatively close to the minimum value specified. Meanwhile, the highest momentum flux ratio condition provided ($J = 34$) has a gas Weber number ($We_g = 720$) much larger than the minimum value targeted. Thus, the latter condition was selected to help fill the gaps in knowledge on the SSD breakup model for turbulent LJIC instead of the condition represented in **Figure 2-12**.

The dataset from Freitag and Hassa [109] provides a total of 33 conditions for 3 different injector sizes. The highest-pressure condition ($P_g = 8$ bar) that includes a shadowgraph image of the spray was selected ($d = 0.5$ mm). Despite its lower momentum flux ratio ($J = 6$), it has a high gas Weber number ($We_g \geq 1000$). To assess the effect of pressure on the predictive capabilities of the Lagrangian approach, the data provided for the same momentum flux ratio at a lower pressure of 4 bar was selected. To assess the sensitivity of the predictive capabilities to the momentum flux ratios, the highest momentum flux ratio ($J = 24$) condition provided for the same injector diameter and pressure ($P_g = 4$ bar) was selected.

It is important to note the other STHP datasets considered in *section 2.4.4* for similar pressures ([48, 91]) either limit their highest momentum flux ratio ($J \geq 10$) conditions to $We_g \leq 200$ [48] or their highest gas Weber number conditions ($We_g > 1000$) to $J < 10$ [48, 91]. Thus, the limitations imposed on the momentum flux ratio for the highest-pressure conditions from Freitag and Hassa [109] could not have been avoided by selecting another dataset instead. The numerical studies conducted under similar pressures [31, 32] also face the same limitations considering they used the dataset from Becker and Hassa [91].

The purple crosses included in **Figure 2-12** illustrate how the validation datasets and conditions selected will help fill the gaps in knowledge on the predictive capabilities of the Lagrangian and hybrid approach for turbulent LFJIC, especially for the SSD breakup model. The core research chapters include a more detailed comparison of the datasets selected to those used in the literature. In addition to the numerical research gaps discussed in *section 2.4.4*, the numerical validation work has also been limited by the lack of datasets available in the literature providing a wide variety of measurements in both breakup regions. As a result, many studies have only validated the predictions for the spray trajectory [15, 18, 35, 36, 39], the SMD [17, 19] or a combination of both [21, 23, 40]. Very few studies have assessed the predictive capabilities of the droplet axial velocity [27, 38] or its magnitude [16, 22, 27, 29, 41]. Furthermore, it is less common to find studies validating all three parameters simultaneously (SMD, trajectory and droplet velocity/axial velocity) [16, 22, 27, 29]. Although the accuracy for the volumetric flux is sometimes considered [27, 31, 32, 37], few studies have compared the results to

shadowgraph images of the spray [19, 20, 32]. These limitations seem to affect particularly the numerical work on the direct coupling of the Lagrangian approach with the interface capturing methods (hybrid approach) as seen in **Table 2-7**. It can also be observed that this work compensated for these limitations by selecting two different datasets. Indeed, this strategy allowed to assess the sensitivity of the different numerical modelling approaches to the experimental set-up (different test sections, injector geometries, conditions, etc.), which further strengthened the engineering conclusions of the work. To the best knowledge of the author, no other numerical studies on LFJIC have used more than one dataset.

Table 2-7: Numerical validation studies available in the literature on the hybrid approach for LJIC compared to this research (Chapter 5).

Numerical Study		Herrmann [35]	Bravo et al. [36]	Wen et al. [39]	Heinrich and Schwarze [40]	Fontes et al. [41]	Chapter 5
Interface-Capturing Method		RLSG	VOF	CLSVOF	VOF	VOF	VOF
Breakup Model	Deterministic			N/A	RD	TAB, AB-TAB	
	stochastic	X	X	N/A			X
Validation datasets	# Datasets	1 ([98])	1 ([89])	N/A	1 ([161])	1 ([163])	2 ([30, 109])
	# Conditions	1	4	5	1	2	2 (1 per dataset)
	P_g [bar]	min	1	30	5	1	1
		max					8
	J	min	6	15.9	10	6	6
		max		139.1		12	33.6
	We_g	min	330	100	554	11	720
		max		160		53	1172
	Fuel Data			X	X		X
	Turbulent jet	X	X				X
Validated Spray features	Near-Field	X	X	X	X		X
	Far-Field				X	X	X
	Trajectory	2 External corr.	Exp. curve.	2 External corr.	Exp. curve.		Dataset 1: Exp. maximum centreline profile height [30] and 2 external corr. [111, 81]. Dataset 2: Exp. curve [109]
	SMD				Exp. centreline profile at $x/d=30$ and $x/d=60$ [161].	Exp. mass fraction distribution with droplet diameter [163].	Dataset 1: Exp. centreline profile at $x/d \approx 33$ [30]. Dataset 2: Global SMD value [109].
	Velocity					Exp. droplet velocity evolution with droplet diameter at $x/d=147$ [163].	Dataset 1: Exp. centreline profile at $x/d \approx 33$ [30]. Dataset 2: Validation of the profile's shape based on common measured features for turbulent LJIC (No data available).
	Others						Dataset 2: Shadowgraph images [109].

2.5 Predictive Capabilities of Existing Numerical Approaches

The objective of this section is to help address the 1st research objective by reviewing the current predictive capabilities of the different atomization modelling approaches reported in the literature. As previously mentioned, their accuracy is expected to vary greatly based on their deterministic nature and the conditions simulated. Considering this work focuses on developing a stochastic numerical methodology for turbulent LFJIC, their baseline predictive capabilities should ideally have been validated for similar conditions. However, it was found in *section 2.4.2* that very few studies have been conducted on the stochastic secondary breakup model (SSD) using liquid fuels [38] and one of the deterministic breakup models for LJIC was developed using water datasets [29]. Thus, the current predictive capabilities of the SSD and LJIC breakup models were established in this section by considering all the numerical validation studies available in the literature. For similar reasons, the assessment of the predictive capabilities for LFJIC of the deterministic models used in state-of-the-art (SOA) CFD was expanded to non-turbulent jets without regard to the Weber numbers or momentum flux ratios.

The numerical studies considered in this assessment have used different methods to report the agreement with the experimental data. While most of them describe the predictive capabilities based on the different spray regions (i.e. leeward, spray core and windward) [29, 31, 32, 35, 38, 40] often by comparing the centreline SMD or velocity profiles, others have assessed the global error by comparing the average values at a fixed plane [27]. In addition, few studies provide a quantitative description of the discrepancies with the experimental data [27, 29, 36, 40]. Thus, further post-processing work is needed to evaluate the baseline predictive capabilities of the different modelling approaches. Therefore, the experimental and numerical data presented in the different validation studies were extracted from the tables and figures included. A post-processing methodology was then developed and consistently used to determine the predictive capabilities achieved in each numerical study. Considering the prediction trends (i.e. overpredicted or underpredicted) are expected to vary based on the conditions and breakup model used, the assessment focuses on comparing their general agreement with the experimental data. This was done by using the extracted values to calculate the absolute error, which is also referred to as the absolute relative difference.

To obtain the absolute error in the centreline SMD and droplet axial velocity, the relative difference from each data point was calculated using the numerical value predicted at the same measurement location. The latter was either extracted from the numerical curve provided or interpolated between the numerical data points provided if the closest was not located within $\pm 0.2y/d$ of the experimental data point. The absolute error within each spray region was then calculated by averaging the absolute relative difference from each local data point. Considering the spray penetration varies greatly based on the conditions imposed, the lengths of the leeward and spray core regions were set equal to $1/3$ of the maximum location of the experimental data points (y_{max}). The windward region includes all numerical data points located above the latter ($y \geq (2/3)y_{max}$). Although the length of each region could be determined on a case-to-case basis, using a consistent methodology for all numerical studies ensures their predictive capabilities are impartially and fairly evaluated.

The absolute error in the spray trajectory was extracted similarly to the absolute error in centreline SMD and droplet axial velocity. When the trajectory curves were not reported, the maximum heights reached by the centreline curves (i.e. maximum data points) were used instead to estimate the error in spray penetration. To obtain the absolute error in the average centreline SMD and droplet axial velocity, the experimental and numerical data points located across the entire spray height were separately averaged. If the numerical results were reported as a centreline curve, the average was calculated using numerical points extracted from the curve at a fixed interval of $\approx 0.5d$.

The absolute error was calculated for each condition and/or centreline plane studied, which was then used to calculate the numerical study's average absolute error for each breakup model assessed. The latter corresponds to the value represented by the columns in **Figure 2-13** to **Figure 2-15**. Considering the predictive capabilities of a given numerical model were found to vary significantly based on the centreline plane location and the conditions used, error bars were added at the centre of the column to indicate the minimum and maximum discrepancies achieved.

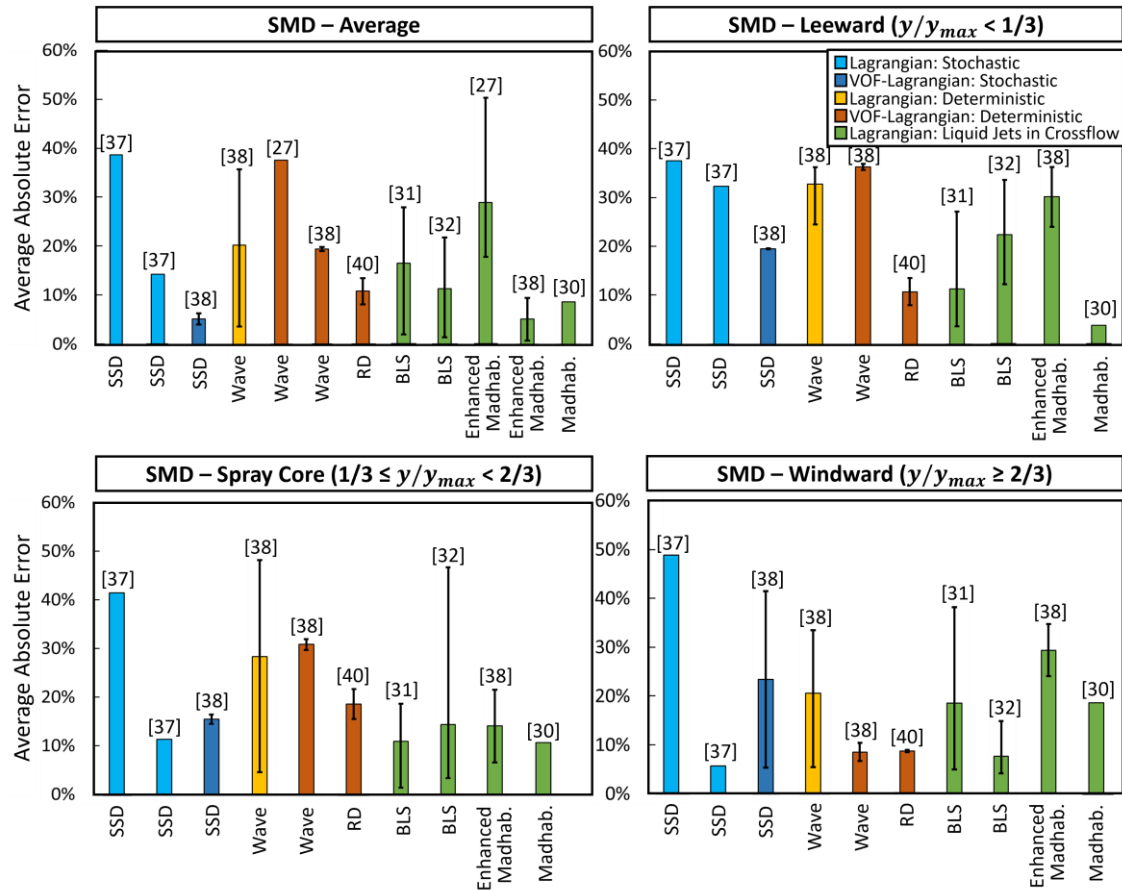


Figure 2-13: Average absolute error in SMD reported in the literature for liquid jets in crossflow using different numerical approaches (reference number indicated above the bar and breakup model used indicated below).

The high values of average absolute error shown in **Figure 2-13** to **Figure 2-15** provide a good insight into how challenging it is to accurately model the complex physics of LJIC even when using higher fidelity approaches or breakup models specifically developed for such applications. Comparing the predictive capabilities of the different Lagrangian breakup models reveals that the accuracy of the SOA deterministic models developed for coaxial and/or quiescent sprays often falls within the absolute error range achieved by those specifically developed for LJIC. This is also true for the SSD breakup model, but more validation work is needed considering the only study done to validate its predictive capabilities when coupled with the Lagrangian approach used a water spray at ambient pressure and low gas Weber number [37]. Moreover, the significant width of the error bars further supports that the accuracy of the deterministic breakup models is quite sensitive to the operating conditions, the location of the measurement plane and the

coupling with other Lagrangian sub-models. In fact, a few studies have reported an absolute error range larger than 30% for the average SMD [27, 38] and larger than 40% within the spray core region for a single breakup model [32, 38]. Thus, while the average predictive capabilities of the Lagrangian approach for the mean SMD can vary between 5% to 39%, the error can be as high as 50%. The discrepancies in SMD were also found to be more important in the spray core and windward regions where the average absolute error locally varies between 11% to 41% and between 6% to 49% respectively. Similar observations can be made regarding the predictions in droplet velocity and spray penetration using the Lagrangian approach. These results suggest that there is room for improving the predictive capabilities of the Lagrangian breakup models.

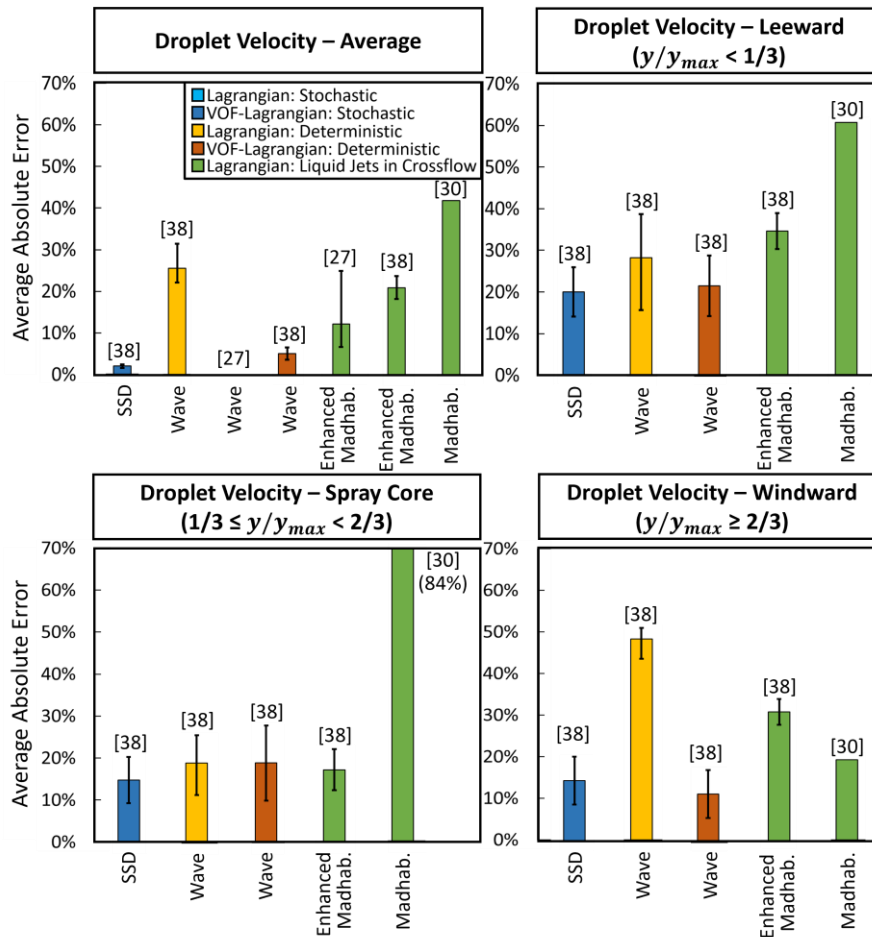


Figure 2-14: Average absolute error in droplet velocity reported in the literature for liquid jets in crossflow using different numerical approaches (reference number indicated above the bar and breakup model used indicated below).

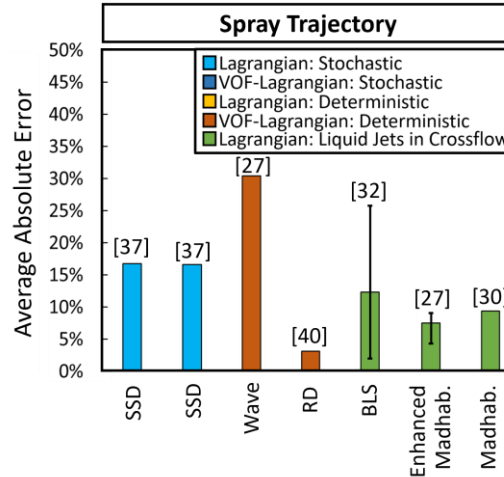


Figure 2-15: Average absolute error in maximum spray penetration reported in the literature for liquid jets in crossflow using different numerical approaches (reference number indicated above the bar and breakup model used indicated below).

The lower limit of the absolute error ranges mentioned in the previous paragraph often comes from the better agreement with the data that can be achieved by the breakup models specifically developed for jets in crossflows. However, their accuracy seems to be more sensitive to the operating conditions, which can be observed by comparing the error ranges from Feiz et al. [27] and Wang et al. [38]. Although both studies use the enhanced Madabhushi breakup model, the absolute error in average SMD reported by the former varies between 18% and 50% while it is 9% at most for the lower pressure conditions from Wang et al. [38]. In addition, the predictive capabilities in SMD of the jets in crossflow breakup models seem to be strongly influenced by the numerical methodology used to implement them. Indeed, the numerical studies conducted by Rachner et al. [31] and Khosla and Crocker [32] using the BLS model were found to have significantly different ranges of absolute error across the entire spray height despite using the same dataset for validation. These conclusions also apply to the predictions for the droplet velocity especially in the leeward and spray core regions where the absolute error can be as high as 60% and 84% respectively. Despite the exhaustive calibration efforts required by these jets in crossflow breakup models as described by Feiz et al. [26, 27], the discrepancies with the experimental data can be quite important. Moreover, it was found that their absolute error can sometimes surpass those achieved using the state-of-the-art and/or non-calibrated SSD breakup models. These findings further support the objectives

of this work as they indicate the SSD breakup model could potentially achieve similar or better accuracy than the models specifically developed for LJIC.

The predictive capabilities in average SMD of the hybrid approach are very similar to the lower-cost Lagrangian breakup models considering the absolute error was found to vary between 5% and 38%. However, it tends to predict more accurately the SMD within the windward region compared to the Lagrangian approach when using the same breakup model. Another advantage of using the higher-fidelity hybrid approach is the improved predictions achieved for the average particle velocity as shown in **Figure 2-14**. Indeed, the average absolute error varies between 12% and 42% with the Lagrangian approach compared to 5% at most with the hybrid approach. Moreover, the results reported by Wang et al. [38] show that even with a decoupled VOF-Lagrangian approach, using a hybrid method with the SSD breakup model often results in better agreement with the data for the droplet velocity compared to using a deterministic breakup model for the same conditions. This further supports that the numerical modelling of LJIC could be further improved by using the hybrid approach. This strategy was implemented to improve the predictive capabilities of the Lagrangian approach for turbulent LFJIC as presented in Chapter 5 and Chapter 6.

3 Validation and Assessment of a Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow

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3.1 Abstract

For lean combustion technology, sufficient mixing between fuel and air helps to move away from stoichiometric combustion, the flame temperature of which enormously promotes the production of harmful pollutants. Good fuel-air mixing is also essential to avoid fuel-rich pockets, where unburnt hydrocarbon and soot are likely to be produced. For low-emission gas turbines using liquid fuels, such as diesel, jet in crossflow is one of the approaches used to achieve efficient liquid jet breakup and evaporation as well as superior mixing characteristics.

In order to develop low-emission fuel spray technologies that use transverse jets, it is important that the current numerical tools have the ability to accurately predict the jet breakup, both primary and secondary, and evaporation mechanisms, to properly assess the performance of an injector design. However, because the numerical tools often use model constants that are calibrated with experimental data mostly only applicable to a specific range of operating conditions, a particular test fluid or injection method, it is very challenging to assess the accuracy of the predicted results without further experimental validation. To the author's best knowledge, the breakup mechanism and the predictive capabilities of the breakup models used to guide the design of novel injectors for fuel transverse jets at elevated pressure and high-speed turbulent crossflow have not been reported in full detail.

Thus, the main focus of this study is to compare and assess the capabilities of the breakup models used in state-of-the-art CFD, including a stochastic approach that relies less on experimental model constants, to predict the spray characteristics of turbulent jets in crossflow at different pressures P_g , Weber numbers and momentum flux ratios J that are more representative of gas turbine applications. This study will be conducted by using

Simcenter STAR-CCM+. The simulated results will be compared to experimental data to validate and calibrate the breakup models through a parametric and sensitivity study.

Keywords: CFD; Lagrangian-Eulerian; Turbulent; liquid fuel; Crossflow; Breakup models; Atomization; Gas Turbine.

3.2 Introduction

Developing more sustainable technologies for stationary and aero gas turbine applications is critical to achieve the environmental targets set by various legislative bodies. Liquid fuel injected in a combustion chamber is subjected to a primary and secondary breakup process that generates small droplets forming a spray which mixes with the air following their evaporation. To reduce emissions of harmful pollutants, in particular CO₂ and NO_x, advanced mixing technologies, such as liquid-fuel jets in crossflow, aim at improving the mixing between fuel and air, which can be further enhanced by the turbulent characteristics of both phases [5, 6, 164]. Robust numerical tools that accurately predict the spray characteristics are needed for the development of such advanced low-emission technologies considering that the combustion process is significantly influenced by the breakup processes as they affect the spray and evaporation characteristics, which impact the mixing quality [5]. To hasten the delivery of novel liquid-fuel injectors, the design work is often facilitated by using Eulerian-Lagrangian approaches as well as Reynolds-Averaged Navier-Stokes (RANS) approaches over Large Eddy Simulations (LES) and interface-capturing methods (e.g. Volume-of-Fluid (VOF)) due to their lower computational cost. Therefore, the purpose of the present study is to validate a numerical methodology for turbulent liquid-fuel jets injected into a crossflowing air stream using the Eulerian-Lagrangian framework for steady and unsteady RANS (URANS) approaches.

The breakup models used in state-of-the-art CFD are not likely suitable for more representative gas turbine conditions due to their heavy dependence on model constants obtained experimentally at atmospheric conditions or using water [24, 25]. In fact, most of them rely on deterministic breakup models based on Kelvin-Helmholtz instabilities (KH model) [149] or on Taylor's analogy between a spring-mass system and an oscillating droplet (Taylor Analogy Breakup (TAB)) [151]. The latter considers droplet distortion due to aerodynamic forces to be analogous to a damped spring-mass system

where breakup occurs at a critical oscillation frequency characterized by experimentally determined non-dimensional constants and critical Weber number [151]. The Wave model considers that droplet breakup is caused by Kelvin-Helmholtz instabilities on the droplet surface that are growing due to the aerodynamic forces caused by the shear motion between the liquid droplet and gas [149], which are characterized by correlations extremely dependent on the experimental conditions.

Multiple secondary breakup models were also developed from them to improve their predictive capabilities, such as the KHRT breakup model [150] which combines the KH and Rayleigh-Taylor (RT) models [152]. The latter improves the predictions in the near-field region by modelling the catastrophic breakup caused by RT instabilities, which arise from the drag-deceleration normal to the liquid-gas interface due to the high relative velocity between the liquid and gas. The KHRT breakup model inherits the strong dependency on experimental data of the KH breakup model and needs to be tuned to produce accurate predictions of the spray characteristics [5, 14]. The Reitz-Diwakar (RD) breakup model, which oversimplifies the breakup process by injecting a droplet whose initial size equals the nozzle diameter, is mostly considered a primary breakup model and has been coupled in the literature with secondary breakup models to form other hybrid breakup models [14]. However, it also relies on empirical model constants [14, 153]. The constants and correlations used by these models must be calibrated with experimental data to predict accurately the spray penetration and droplet size distribution [14].

Considering that CFD is used as a tool to guide the design of novel injectors, the numerical models used to do so should ideally not require prior knowledge of their performance through experimental data and only require minimal calibration. The Stochastic Secondary Droplet (SSD) breakup model allows doing so by considering the nature of the breakup process to be random using Kolmogorov's stochastic theory [33]. Thus, unlike the other models, it has been deemed more suitable for gas turbine applications as it captures the important breakup processes, such as the effects of turbulence and the catastrophic breakup regime that occur at the high gas Weber numbers We_g often used in gas turbine combustion [12, 34]. This model also relies significantly less on experimental data and more on the boundary conditions [33, 34]. Moreover, although the SSD breakup model was not specifically developed for jets in crossflows,

the authors [33] have qualitatively demonstrated its potential for such complex flow applications.

The predictive capabilities of breakup models can also be expected to vary with the injection method and injector characteristics due to their influence on the atomization process [7, 14, 28]. Because these breakup models were mainly developed using liquid jets injected in coflowing or quiescent air, multiple numerical studies have been conducted to validate their use for liquid jets in crossflow applications. The SSD breakup model has mostly been assessed for jets in crossflow at low pressure using water [35, 36, 37]. This is also true for the KHRT breakup model [15, 16, 18] and the Reitz-Diwakar breakup model [16]. Most of these numerical studies were also conducted at low atomization levels [16, 35, 36, 37]. Moreover, some of them used non-turbulent jets [36, 40] and low momentum flux ratios [15, 16, 18, 35, 40]. Many of these studies also focused on hybrid approaches that couple an interface capturing method with the Lagrangian approach, which are more computationally expensive than the latter [35, 36, 40]. Thus, further validation work is required to assess their predictive capabilities for turbulent liquid jets in crossflow under representative gas turbine conditions.

Fewer breakup models have been developed to account for the specific aerodynamic and breakup characteristics of jets in crossflow, such as the jet column bending. For the primary breakup of transverse jets, the models from Rachner et al. [31] and Khosla and Crocker [32] include the column breakup and jet surface stripping through the Boundary-Layer-Stripping (BLS) model [156], which was developed using experimental correlations for transverse jets subjected to shock waves. The Madabhushi breakup model [30] uses the Wave breakup model instead and calculates the breakup characteristics and child droplet velocities through experimental correlations. While the Multiple Injector Model (MIM) [29] does not rely on experimental correlations for the primary breakup, it does for the jet trajectory and for the secondary breakup as it uses the TAB breakup model. The model developed by Kholsa and Crocker [32] also uses a deterministic model for secondary breakup, the RT breakup model. Thus, almost all breakup models developed specifically for jets in crossflow also rely to some level on experimental data. Moreover, their application is mostly limited to the shear breakup regime [29, 31, 32], which is not always representative of the high turbulence levels of gas turbine applications. Thus, even

if some of these models were validated using experimental data for turbulent transverse jets at high pressure and high gas Weber numbers We_g [31, 32], only the Madabhushi breakup model, which was originally validated using experimental data for turbulent jets at high gas and jet Weber numbers We_{jet} , is used in the present study for comparison purposes.

Another important characteristic of jets in crossflow atomization is the distortion of the droplets under the aerodynamic forces, which can be numerically accounted for with the TAB distortion model [165]. This model has been used in numerical studies conducted on liquid jets in crossflow [15, 16, 17, 18, 19, 166] often with the objective of improving the drag force predictions for high-speed crossflows under supersonic conditions [15, 16, 18, 19]. However, only a few of them focused on assessing its impact on the predictive capabilities [16, 17, 18] and they only studied its coupling with the TAB [16, 17] or KHRT [18] breakup models. In addition, all these studies were conducted using water at low pressures and either with low momentum flux ratios [18], low Weber numbers [16, 17] or under supersonic conditions [16, 18], which are not representative of industrial gas turbine conditions and for stationary or subsonic aircraft operations [8]. Moreover, to the best knowledge of the authors, the effect of coupling the SSD breakup model with the TAB distortion model for jets in crossflow has not yet been studied. Thus, there is a need for further validation and assessment of the TAB distortion model for transverse liquid fuel jets applications.

The aim of the present study is to provide accurate and less computationally expensive numerical design tools by further validating the predictive capabilities of the secondary breakup models used in state-of-the-art CFD for turbulent liquid fuel jets in crossflow at more representative gas turbine pressures and atomization levels. To do so, RANS and URANS simulations are performed to assess the accuracy of the KHRT, Reitz-Diwakar and SSD breakup models against the Madabhushi breakup model. The effect of the spray discretization, TAB distortion model and model constants of the SSD breakup model are also assessed.

3.3 Governing Equations

To reduce the computational cost, the Lagrangian-Eulerian approach uses a discrete element type of method and a statistical approach to track inside the computational domain and solve the governing equations for parcels of particles with identical properties [132].

3.3.1 Lagrangian Framework

The two-way coupling model considers the reciprocating effects of the interactions between the continuous and dispersed phases. To do so, the dispersed phase equations are integrated over the cell for each droplet crossing its volume and summed up to obtain the net exchange of mass, momentum, and energy between both phases, which are then applied as source terms to the governing equations of the gas phase [85, 132]. For a steady RANS approach, the resulting transfer rate of mass S_M , momentum S_v and energy S_E to the continuous phase from each computational cell are defined by equation (3-1), equation (3-2) and equation (3-3) respectively. [85, 132]

$$S_M = - \sum_{\pi} \sum_{\delta t_p} \dot{n}_{\pi} \dot{m}_p \delta t_p \quad (3-1)$$

$$S_v = - \sum_{\pi} \sum_{\delta t_p} \dot{n}_{\pi} (F_s + \dot{m}_p u_p) \delta t_p \quad (3-2)$$

$$S_E = - \sum_{\pi} \sum_{\delta t_p} \dot{n}_{\pi} \left(F_s \cdot u_p + Q_t + \frac{1}{2} \dot{m}_p u_p^2 + \dot{m}_p h \right) \delta t_p \quad (3-3)$$

The local parcel time-step δt_p controls the temporal error through an imposed maximum Co_{max} and minimum Co_{min} Lagrangian courant number as shown by [85]

$$\frac{Co_{min} \Delta x_{cell}}{\max(|u|, |u_p|)} \leq \delta t_p \leq \frac{Co_{max} \Delta x_{cell}}{\max(|u|, |u_p|)} \quad (3-4)$$

Where Δx_{cell} is a characteristic length of the cell. For unsteady simulations, the inverse of the physical time-step Δt is multiplied to the transfer rate equations and the particle flow rate $\dot{n}_{\pi}$ is replaced by the number of particles per parcel n_{π} .

In the present work, heat and mass transfers between phases are not modelled considering the gas is at ambient temperature and close to the liquid's temperature as presented in *section 3.4*. Thus, the mass transfer rate $\dot{m}_p$, droplet convective heat transfer Q_t and corresponding enthalpy h are neglected in the above equations and the net exchange of

momentum and energy are dictated by the surface force F_s , which is the sum of the drag force F_d and pressure gradient force F_p acting on the droplet surface. The latter accounts for the effects of pressure changes within the continuous phase and is calculated as [85, 132]

$$F_p = -V_p \nabla P_{static} \quad (3-5)$$

Where V_p is the particle's volume and ∇P_{static} the static pressure gradient. The aerodynamic effects are characterized by the momentum-relaxation time scale τ_v and the drag coefficient C_D , as shown in equation (3-6). [85, 132]

$$F_d = \frac{1}{2} C_D \rho A_p |u_s| u_s = \frac{m_p u_s}{\tau_v} \quad (3-6)$$

Where m_p is the particle mass, A_p is the particle's projected area and u_s the particle's slip velocity, which is calculated as the difference between the continuous phase velocity u and droplet velocity u_p . The latter is obtained by integrating over time the equation of the conservation of linear momentum defined in equation (3-7), which prescribes the droplet's motion as a function of the forces acting on its surface. [85, 132]

$$m_p \frac{du_p}{dt} = F_s \quad (3-7)$$

The particle's trajectory is obtained by integrating over time the particle's instantaneous position, which is obtained by integrating the particle's instantaneous velocity [85].

3.3.2 Drag Force and TAB Distortion

To account for the droplet's deformation under aerodynamic forces, the Liu Dynamic drag coefficient, which uses the TAB distortion model, is defined as [165].

$$C_D = C_{D_{sphere}} (1 + 2.632 y_{TAB}) \quad (3-8)$$

The normalized droplet distortion y_{TAB} is prescribed by the TAB model and is obtained by analytically solving a second-order ODE. Its value varies between 0 and 1, with the former representing a perfectly spherical droplet, and strongly depends on the Weber number defined as [151]

$$We = \frac{\rho |u_s|^2 D_p}{\sigma} \quad (3-9)$$

The drag coefficient of the undistorted droplets $C_{D_{sphere}}$ defined by equation (3-10) is a function of the droplet's Reynolds number Re_p , which is calculated with the slip velocity. [165]

$$C_{D_{sphere}} = \begin{cases} \frac{24}{Re_p} \left(1 + \frac{1}{6} Re_p^{\frac{2}{3}}\right) & Re_p \leq 1000 \\ 0.424 & Re_p > 1000 \end{cases} \quad (3-10)$$

The Schiller-Naumann drag coefficient [167] is a common alternative to the Liu drag coefficient due to its reduced complexity and lower computational cost. Despite not accounting for the droplet's distortion through sub-models, it is deemed suitable for liquid droplets and is defined as [85]

$$C_D = \begin{cases} \frac{24}{Re_p} (1 + 0.15 Re_p^{0.687}) & Re_p \leq 1000 \\ 0.44 & Re_p > 1000 \end{cases} \quad (3-11)$$

3.3.3 Rietz-Diwakar Breakup Model

The Reitz-Diwakar breakup model considers atomization to occur in the bag or stripping breakup regime. This model does not generate child parcels. The parent droplet size D_p decreases according to equation (3-12), hence its low computational cost. [149, 153]

$$\frac{dD_p}{dt} = \frac{D_s - D_p}{\tau_{bu}} \quad (3-12)$$

Bag Breakup occurs if the Weber number We is superior to a critical Weber number We_{crit} , which has a default value of 12 [85]. The breakup time τ_{bu} and stable droplet diameter D_s are then calculated using equation (3-13) and equation (3-14) respectively. [153]

$$\tau_{bu \text{ Bag}} = \frac{C_{b2} D_p}{4} \sqrt{\frac{\rho_p D_p}{\sigma}} \quad (3-13)$$

Where C_{b2} is the bag breakup time-scale coefficient with a default value equal to 3.1415 [153].

$$D_{s \text{ Bag}} = \frac{\sigma}{\rho |u_s|^2} We_{crit} \quad (3-14)$$

Stripping breakup occurs if the Weber number is also superior to another critical value calculated using equation (3-15). [153]

$$We > \max(2C_{s1}\sqrt{Re_p}, We_{crit}) \quad (3-15)$$

If the above criterion is met, the breakup time and stable droplet diameter are calculated using equation (3-16) and equation (3-17) respectively [153].

$$\tau_{bu \text{ stripping}} = \frac{C_{s2}D_p}{2} \sqrt{\frac{\rho_p}{\rho}} \frac{1}{|u_s|} \quad (3-16)$$

Where C_{s1} and C_{s2} are model constants for the stripping breakup regime with default values equal to 0.5 and 20. [153]

$$D_{s \text{ stripping}} = \frac{\sigma}{\rho|u_s|^2} \max(2C_{s1}\sqrt{Re_p}, We_{crit}) \quad (3-17)$$

If both breakup regimes are predicted to occur due to both critical Weber number criteria being satisfied, the smallest breakup time dictates the dominant breakup regime. [85]

3.3.4 KHRT Breakup Model

The growth of KH and RT instabilities can occur simultaneously and compete against each other. The KHRT model determines which one dominates by considering their lifetime, which depends on their growth rate Ω and wavelength Λ , and the parent droplet size D_p . Catastrophic breakup due to RT instabilities occur when their lifetime τ_Λ reaches the RT breakup time given by equation (3-18). [150]

$$\tau_{bu \text{ RT}} = \frac{C_\tau}{\Omega_{RT}} \quad (3-18)$$

But only if the parent droplet diameter is simultaneously larger than a critical droplet size $D_{crit \text{ RT}}$ defined as [150]

$$D_{crit \text{ RT}} = C_3\Lambda_{RT} \quad (3-19)$$

Where C_τ and C_3 are the RT time and length coefficients with default values of 1 and 0.1. If the above conditions are not met, KH breakup will occur when the parent droplets are bigger than a critical KH droplet size defined as [150]

$$D_{crit \text{ KH}} = 2B_0\Lambda_{KH} \quad (3-20)$$

Over the KH breakup time defined by equation (3-21), the parent droplet sheds mass that accumulates within the parent parcel until an imposed proportion of their initial mass is reached [85].

$$\tau_{bu\ KH} = \frac{1.894B_{01}D_P}{\Lambda_{KH}\Omega_{KH}} \quad (3-21)$$

Where B_0 and B_{01} are the KH length and time coefficients which have a default value of 0.61 and 10. [85, 150] The new parcels created contain the child droplets which gain a velocity component normal to the parent droplet's initial velocity, as defined by equation (3-22). [150]

$$u_{p,c\ KH} = A_1\Lambda_{KH}\Omega_{KH} \quad (3-22)$$

The normal velocity coefficient A_1 , which has a default value of 0.188, dictates the spray angle. Following KH or RT breakup, the diameter of the child droplets is equal to the corresponding critical droplet size. [85, 150]

3.3.5 SSD Breakup Model

The SSD model considers atomization to occur when the droplet's surface is unstable due to aerodynamic and surface tension forces. Thus, the breakup process is governed by the local flow characteristics. In fact, the breakup conditions of the SSD model depend on the flow properties, droplet slip velocity and Weber number We . For breakup to occur, the latter must be bigger than an empirically defined critical value of 6 [33, 85] and the droplet must reach a size superior to a critical radius defined as [33, 34]

$$r_{crit} = \frac{We_{crit}\sigma}{\rho|u_s|^2} \quad (3-23)$$

The resulting droplet breakup time defined by equation (3-24) also depends on a model constant B_1 , which has a default value of $\sqrt{3}$ [85, 168].

$$\tau_{bu} = B_1 \sqrt{\frac{\rho_p}{\rho}} \frac{r_p}{|u_s|} \quad (3-24)$$

The radius of the child droplets $r_{p,c}$ follows the log-normal distribution defined by equation (3-25) and is obtained by solving analytically the probability density function of the droplet diameter through a Fokker-Planck differential equation. [33, 34]

$$\Phi(r_{p,c}) = \frac{1}{2} \left(1 + \operatorname{erf} \left[\frac{\log\left(\frac{r_{p,c}}{r_p}\right) - \langle \xi \rangle}{\sqrt{2\langle \xi^2 \rangle}} \right] \right) \quad (3-25)$$

As seen in equation (3-26), the mean value of the breakup distribution function $\langle \xi \rangle$ is a model constant K_0 which has a default value of -0.1 [85].

$$\langle \xi \rangle = K_0 \quad (3-26)$$

The variance of the droplet diameter distribution function $\langle \xi^2 \rangle$ is proportional to a model constant K_1 , which has a default value of 0.1 [85], and is also a function of the local flow characteristics, as seen in equation (3-27).

$$\langle \xi^2 \rangle = K_1 \ln \left(\frac{We}{We_{crit}} \right) \quad (3-27)$$

The child droplet velocity $u_{p,c}$ as defined by equation (3-28) is calculated to account for the momentum gained in the direction normal to the slip velocity vector by scaling the parent droplet's velocity with a multiplication factor $|W_{bu}|$. [33, 34]

$$u_{p,c} = |W_{bu}|u_p = \left(\frac{K_3 r_{p,c}}{\tau_{bu}} \right) u_p \quad (3-28)$$

The spray angle is influenced by the normal velocity coefficient K_3 , which can take a value between 0 and 1. [85]

3.4 Methodology

An assessment of the predictive capabilities of the numerical models available in Simcenter STAR-CCM+ 2020.2 was conducted for RANS and URANS simulations. Experimental data available in the literature for turbulent jets in crossflow at high gas Weber number We_g and only at standard temperature were selected as further explained in *section 2.4.1*. The datasets used are presented in **Table 3-1**. To validate the SMD predictions at high momentum flux ratio and jet Reynolds number, the dataset at standard pressure conditions using Jet A fuel from Madabhushi et al. [30] was used. To validate the trajectory predictions at high-pressure conditions, the dataset at high gas Reynolds numbers and gas Weber numbers using Kerosene fuel from Freitag and Hassa [109] was used. The results obtained in the present study using the conditions from Madabhushi et al. [30] are also compared to their predictions made using the Madabhushi breakup model [30].

The numerical domains and meshes used to reproduce numerically the experimental conditions from Madabhushi et al. [30] and Freitag and Hassa [109] are presented in **Figure 3-1** and **Figure 3-2** respectively. The lengths of the numerical domains were made longer upstream and downstream of the droplet injection point compared to their respective experimental test sections in order to improve convergence and to have an

established gas flow field before the phases interact together. Their cross-section dimensions correspond to the ones used experimentally and the droplets are injected at their centre. Considering that both experiments use plain orifice injectors, the point injector method was selected to inject parcel streams containing droplets with an initial size equal to the nozzle diameter.

Table 3-1: Datasets used for the numerical assessment.

Dataset reference	Madabhushi et al. [30]	Freitag and Hassa [109]
d [mm]	0.762	0.5
P_g [bar]	1.01325	8.0
u_g [m/s]	138	75
u_{jet} [m/s]	31	19.7
J	33.6	6
We_g	720	1172
We_{jet}	24 711	7032
$Re_{g,d}$	7.8E+03	1.8E+04
Re_g	6.1E+05	1.5E+06
Re_{jet}	1.2E+04	5.2E+03

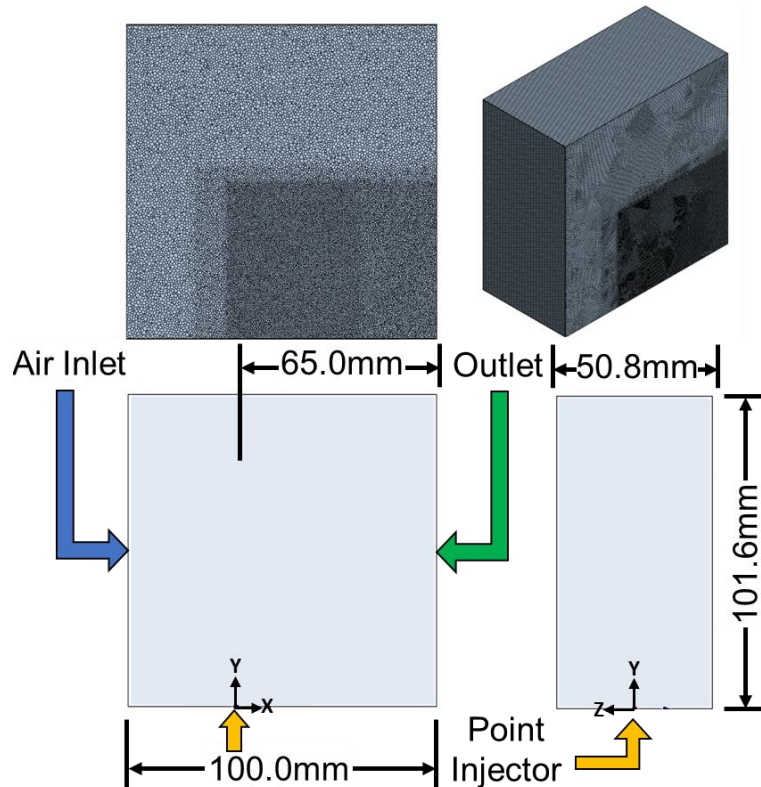


Figure 3-1: Numerical domain and mesh used with the dataset from Madabhushi et al. [30] (Lengths based on existing work with Wave breakup model [169]).

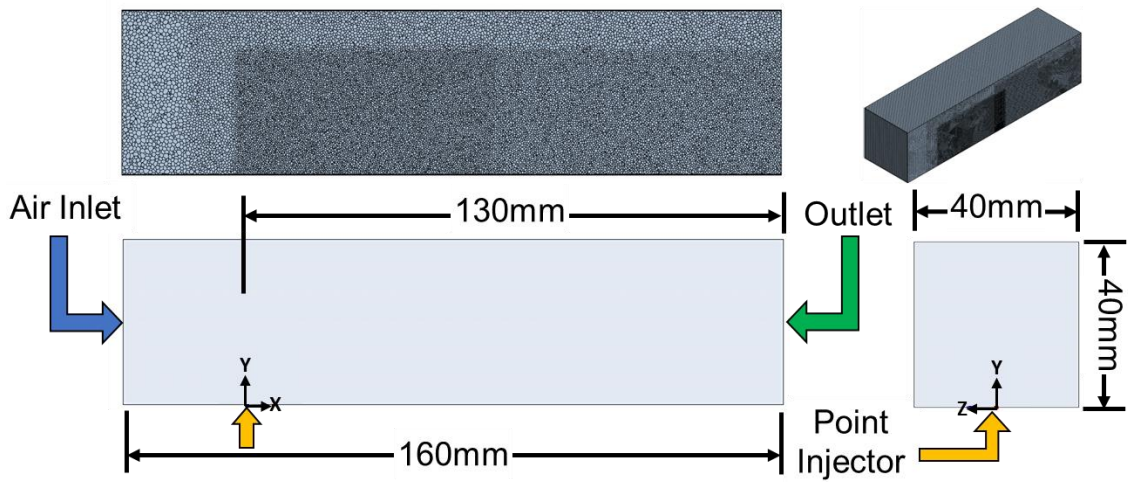


Figure 3-2: Numerical domain and mesh used with the dataset from Freitag and Hassa [109].

The polyhedral mesh parameters used for all simulations were selected following a RANS mesh refinement study using the dataset from Madabhushi et al. [30] with different breakup models. It was found that increasing the number of cells increases the volume fraction in the jet column region, which impacts the stability of the solution as the Lagrangian approach limits the volume fraction to 0.75 in an increased number of cells. The maximum cell size was set to 0.8mm with a base size of 1mm and a volume growth rate of 1.1. The volume mesh in the spray far-field and near-field regions were refined respectively to 0.45mm and 0.4mm. These parameters allow to obtain a courant number near or below unity for unsteady simulations and a wall y^+ value below 2. The resulting mesh for the numerical domain used with the datasets from Madabhushi et al. [30] has 3.37 million elements and 2.79 million elements for the one used with the datasets from Freitag and Hassa [109].

All simulations are three-dimensional, turbulent, and adiabatic and use the coupled energy and flow models with a second-order discretization scheme to improve the phase coupling. The CFL of the coupled solver was adjusted to improve the stability and convergence of the simulations. Turbulence was modelled using the Realizable k-epsilon Two-Layer model with a two-layer all y^+ wall treatment. For the Lagrangian phase, the two-way coupling and turbulent dispersion models, which accounts for the interaction between the droplets and the turbulent eddies contained within the turbulent flow field [85], are used. Where it is not specified that the TAB distortion model is used, the Schiller-

Naumann drag coefficient is used. Considering the objective is to compare the basic predictive capabilities of the breakup models, their parameters, such as the model constants, were kept to the default values unless otherwise specified. For the SSD breakup model, the maximum number of child parcels was set to 2 for the RANS simulations and to 10 for the URANS simulations. Moreover, the normal velocity coefficient K_3 was set to 1 to increase the radial diffusion in the spray unless otherwise specified.

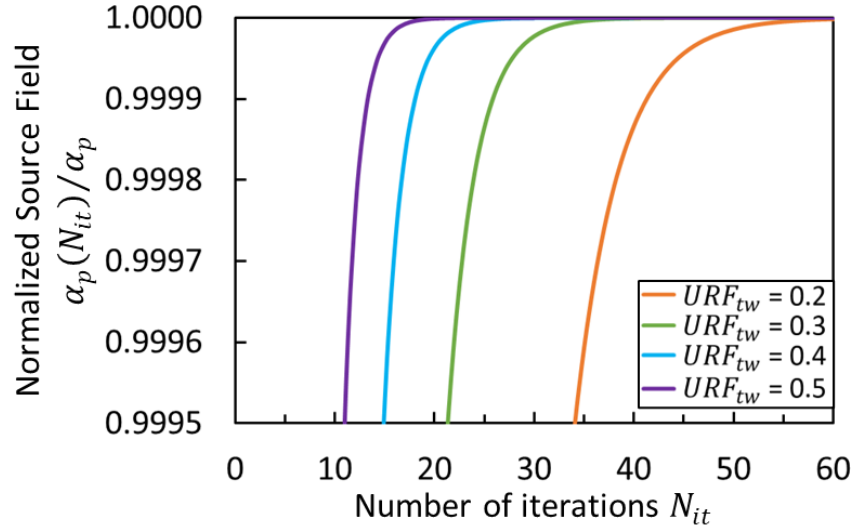


Figure 3-3: Update frequency required for a given URF of the two-way coupling solver to fully apply the source terms (Represented as the normalized source field $\alpha_p(N_{it})/\alpha_p$ assuming $\alpha_p(0)=0$).

For the RANS simulations, the flow was incompressible. The number of iterations N_{it} required to fully apply the Lagrangian source terms to the continuous phase equations varies with the two-way coupling under-relaxation factor (URF) URF_{tw} , which stabilizes the particle volume fraction α_p as shown in equation (3-29) [85]

$$\alpha_p(N_{it}) = [1 - URF_{tw}]\alpha_p(N_{it-1}) + URF_{tw}\alpha_p \quad (3-29)$$

Figure 3-3 shows that decreasing URF_{tw} increases the number of iterations N_{it} required between each Lagrangian update ($\alpha_p(N_{it})/\alpha_p = 1$), which increases the accuracy of the solution at the expense of the computational cost [85]. Preliminary RANS studies were conducted with the SSD model coupled with the TAB distortion model using the datasets from Madabhushi et al. [30] to assess the effect of those parameters. The two-way coupling URF was set to 0.3 with an update frequency of 50 iterations and to 0.5 with an update frequency of 20 iterations, which is the approximative value recommended [85],

and 28 iterations, which is the minimum value required. The results were compared to the ones obtained using a URF of 1 with a conservative update frequency of 20 iterations. Considering that no significant differences in SMD, particle axial velocity or droplet trajectory were observed, the two-way coupling URF was set to 1 with a Lagrangian update frequency of 20 iterations for all RANS simulations to reduce the computational cost.

For URANS simulations, the flow was compressible using ideal gas. To ensure the solution converges at least to the second or third order of magnitude, the solution time-step was set to $1\mu\text{s}$ and the number of inner iterations to 20 for the standard pressure conditions and 65 for the higher-pressure conditions.

The maximum and minimum courant numbers of the Lagrangian phase were selected to ensure that the local parcel time-step remained inferior to the physical time-step. Once this restriction is incorporated into equation (3-4), the resulting expression can be manipulated to yield the following condition

$$Co_{max} \leq \Delta t \frac{\max(|u|, |u_p|)}{\Delta x_{cell}} \quad (3-30)$$

The maximum Lagrangian courant number Co_{max} to impose can be calculated conservatively with equation (3-30) by using the initial jet and gas velocities and the maximum cell size in the refined spray region. As a result, Co_{max} was set inferior to 0.25 and Co_{min} to 0.1, which is much less than Co_{max} .

Preliminary URANS simulations were also conducted with the SSD model coupled with the TAB distortion model using the dataset from Madabhushi et al. [30] to assess the effect of the number of parcel streams (PS) and target number of child particles per parcel. To do so, the number of parcel streams was varied from 30 to 100 for a constant target number of child particles per parcel of 100, and the latter from 100 to 500 for 30 parcel streams. No significant differences were observed for the SMD and particle velocity, which confirmed that they do not affect the droplet characteristics predicted by the SSD model. However, slight differences were observed in terms of spray trajectory and spray width. Thus, to be conservative, the number of parcel streams was set to 100 for all URANS simulations conducted using the datasets from Madabhushi et al. [30]. For those conducted with the datasets from Freitag and Hassa [109], the number of parcel streams

was increased to 200 to achieve a better discretization of the spray considering that the numerical results are validated against experimental data for the particle trajectory.

3.5 Results

All RANS simulations were conducted using the dataset from Madabhushi et al. [30]. The experimental and numerical results presented for the centreline SMD and particle axial velocity are taken at 25.4mm downstream of the injector for the latter and at 30mm for the dataset from Freitag and Hassa [109]. For the URANS simulations, the data and contours presented are time-averaged values.

3.5.1 RANS Results

Reducing the number of droplets in the numerical domain allows to reduce the computational cost. However, this must not be done at the expense of the spray discretization. RANS simulations using the datasets from Madabhushi et al. [30] were performed to study the sensitivity of the KHRT breakup model to the number of child parcels imposed by setting it to 50, 1000, 2000 and 4000 child parcels.

As seen in **Figure 3-4**, increasing the number of child parcels from 50 to 4000 increases the spray width and reduces the spray trajectory as it is 3.9% lower with 1000 child parcels and 6.8% lower with more than 2000. However, no significant differences in SMD nor droplet axial velocity could be observed. The discrepancies between the centreline profiles for the droplet axial velocity that occur at a higher transverse distance most likely indicate that the spray physics is oscillating between two solutions due to its unsteady nature. This conclusion is drawn from the two different centreline profiles that can be observed without any relation to the number of child parcels. Indeed, the centreline profile for the droplet axial velocity predicted with 50 and 4000 child parcels are very similar and different from the ones obtained using 1000 and 2000 child parcels, which are also very similar together. Thus, using unsteady simulations should be considered. Moreover, increasing the number of child parcels does not improve the predictions, which shows the accuracy of the KHRT model for jets in crossflow can't be compensated by a higher spray discretization.

RANS simulations were also performed to compare the predictive capabilities of the KHRT, Reitz-Diwakar and SSD breakup models. Based on the previous results, the

number of child parcels for the KHRT breakup model was set to a conservative value of 4000 as the spray maximum trajectory doesn't change beyond 2000 child parcels. A similar spray discretization is obtained for the SSD breakup model by setting the average target count of child particles per parcel to 1000, which gives a number of particles in the same order of magnitude for both breakup models. The only exception is for the Reitz-Diwakar model as it does not generate child parcels.

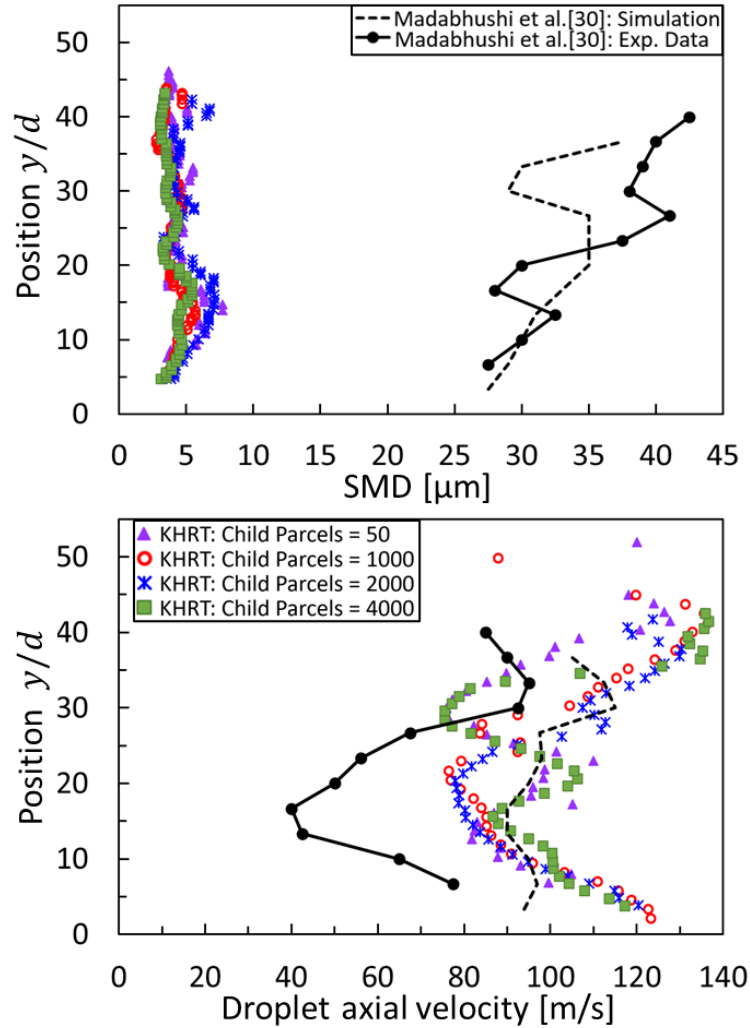


Figure 3-4: Effect of the number of child parcels on the centreline SMD (top) and droplet axial velocity (bottom) predicted by the KHRT breakup model.

As shown in **Figure 3-5** and **Figure 3-6**, the Reitz-Diwakar breakup model does not generate a physical spray compared to the other breakup models, which was expected as it's similar to a primary breakup model. Despite this, it should predict the main breakup characteristics considering it is offered in Simcenter STAR-CCM+ as a secondary breakup model with its purpose presented as giving a first approximation [85]. However,

this is not the case as the SMD is significantly overpredicted by approximately more than 210% while the droplet axial velocity is significantly underpredicted compared to the experimental data and other breakup models. As seen in **Figure 3-6**, the Reitz-Diwakar model also significantly overpredicts the spray trajectory by more than 39% compared to the other breakup models due to its underprediction of the droplet axial velocity, which indicates the aerodynamic effects on the jet bending are not well captured. It was also observed that the Reitz-Diwakar model struggles to predict the breakup process as the distance from the nozzle injection point increases. Indeed, it significantly underpredicts the Weber number in the secondary breakup region as the values vary between no breakup (under 6) and stripping breakup (under 100). This might be due to the Reitz-Diwakar model being more suitable as a primary breakup model.

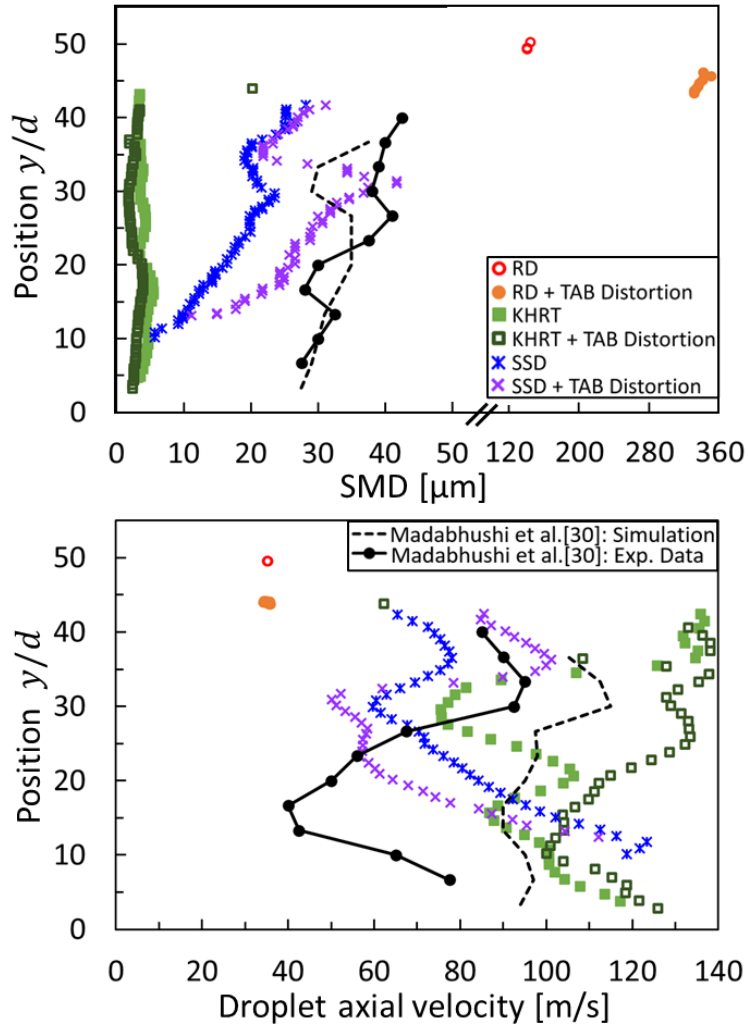


Figure 3-5: Centreline SMD (top) and droplet axial velocity (bottom) predicted by different breakup models with and without the TAB distortion model.

Unlike the Reitz-Diwakar model, the predictions made by the KHRT and SSD breakup models agree more together as they both tend to overpredict the axial droplet velocity at lower transverse distances, underpredict the SMD overall and predict similar spray trajectories. However, the droplet axial velocity predicted by the SSD breakup model tends to agree more with the experimental data as the transverse distance increases. Moreover, unlike the SSD model, the KHRT breakup model significantly underpredicts the SMD and its variance with the transverse distance, hence its worse agreement with the data.

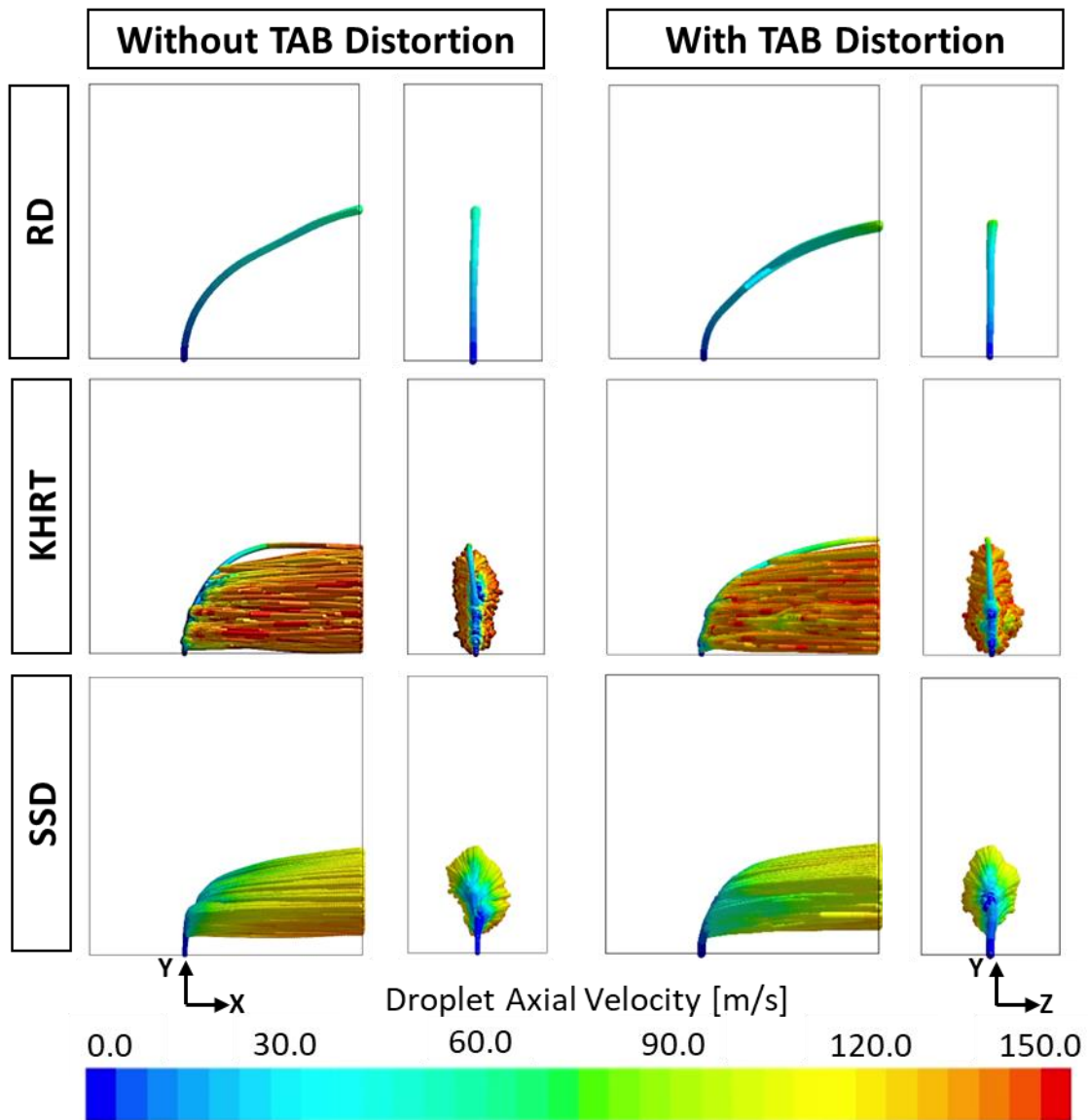


Figure 3-6: Droplet axial velocity predicted by different breakup models with and without the TAB distortion model.

The effect on the accuracy of the numerical predictions of accounting for the droplet distortion was studied by coupling the breakup models with the TAB distortion model. For the KHRT and SSD breakup models, it does not significantly impact the spray trajectory. However, it tends to predict a higher SMD for the latter. For the Reitz-Diwakar model, the TAB distortion model also significantly increases the predicted SMD, which increases the discrepancies with the experimental data as seen in **Figure 3-6**. Despite not having any significant impact on the droplet axial velocity, it tends to better capture the jet bending under the aerodynamic forces as the maximum spray penetration decreases by 10.9%, which reduces the overprediction of the latter compared to the other breakup models from 39% to 25.3%.

For the KHRT breakup model, the TAB distortion model increases the droplet axial velocity predicted in the windward region, but has no significant impact on the SMD. Once again, this shows how much its model constants dictate the physics of the spray, which agrees well with what has previously been reported in the literature for coflowing sprays [5, 14, 85, 150, 153].

As for the SSD model, the TAB distortion model allows to better capture the aerodynamic effects in the windward region as the droplet axial velocity increases and agrees significantly more with the experimental data as seen in **Figure 3-6**. The predictions in droplet axial velocity also tend to improve in the spray core region, especially at lower transverse distances, but the difference with the data remains important. As for the leeward region ($y/d \leq 10$), the impact on the droplet axial velocity is not as important and it remains significantly overpredicted. It can be observed in **Figure 3-6** that the SMD is also less sensitive to the effect of the TAB distortion model at lower transverse distances. The SMD predictions also tend to improve in the spray core region and close to the leeward region as the value predicted increases. However, unlike the predictions for the droplet axial velocity, the TAB distortion model has no significant impact on the SMD in the spray windward region and it remains underpredicted compared to the data. Therefore, while the TAB distortion model tends to significantly improve the accuracy for the droplet axial velocity with an increasing transverse distance, it tends to have the opposite effect on the SMD. It is important to note that the SSD model considers the breakup process to be more independent of the parent droplet size. This along with the

choice of model constants could explain why the SMD predictions do not agree well with the experimental data in some regions of the spray where the opposite is true for the droplet axial velocity. This is further investigated through a parametric study.

3.5.2 URANS Results

Finally, an unsteady parametric study was conducted using both datasets to assess the effect of the SSD model constants when coupled with the TAB distortion model. The breakup parameter B_1 in equation (3-24) is mostly reported in the literature equal to $\sqrt{1/3}$ [33, 34, 151], but other sources suggest using a value of $\sqrt{3}$ instead to obtain more accurate results [85, 168]. Thus, the effects of both values on the predictions are assessed at standard and high pressure. The effect of the normal velocity coefficient K_3 in equation (3-28) on the spray radial diffusion is also assessed by comparing the suggested default value of 0.1 to the maximum possible value of 1.

Regardless of the experimental conditions, increasing the breakup parameter B_1 increases the spray penetration on average by 15% for the dataset from Freitag and Hassa [109] and by 10% for the dataset from Madabhushi et al. [30] as seen in **Figure 3-7** and **Figure 3-8**. For the latter, the difference in spray trajectory tends to increase with the axial distance. This is also true for the dataset from Freitag and Hassa [109] but only in the near-field region ($x/d < 30$) where the relative difference increases up to 27%. Moreover, it also results in a smaller spray width as it decreases on average by 21% for the dataset from Freitag and Hassa [109] and 28% for the dataset from Madabhushi et al. [30]. It is possible to notice that the average difference in spray penetration is greater at the higher pressure and gas Weber number conditions of Freitag and Hassa [109] while the average difference in spray width is greater at the lower pressure and higher momentum flux ratio conditions of Madabhushi et al. [30]. This could indicate that the effect of the breakup parameter B_1 on the droplet radial dispersion and penetration is sensitive to the experimental conditions. The dependence of the breakup parameter on those properties should be further investigated.

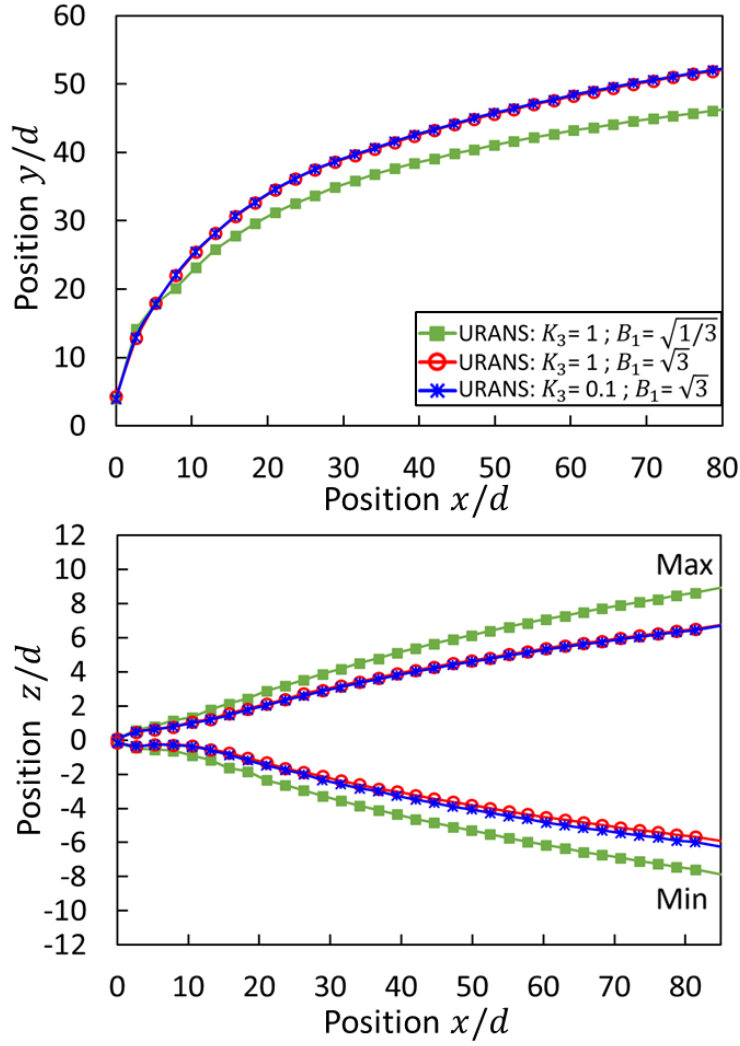


Figure 3-7: Maximum spray trajectory (top) and spray width (bottom) predicted by the SSD breakup model with TAB distortion model using the dataset from Madabhushi et al. [30].

Compared to the experimental correlation from Freitag and Hassa [109], which is shown over the shadowgraph image in **Figure 3-9**, a higher breakup parameter B_1 increases the discrepancies in the secondary breakup region. Although the maximum trajectory becomes significantly overpredicted with the axial distance, a better agreement with the data is achieved in the primary breakup region. Indeed, as seen in **Figure 3-8**, the average relative error in the far-field region increases from 5% to 14%, but decreases in the near-field region from 18% to 6%. Despite improving the predictions in the near-field region, a higher breakup parameter B_1 reduces the overall accuracy of the spray trajectory considering the relative error across the entire spray rises from 7% to 13%.

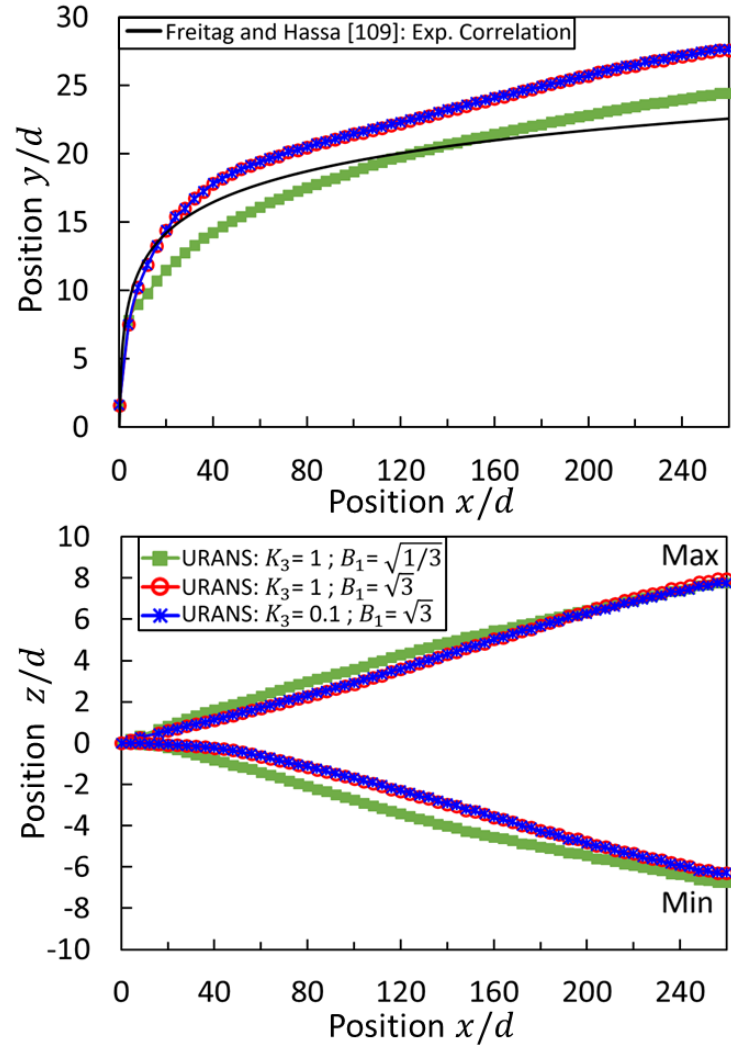


Figure 3-8: Maximum spray trajectory (top) and spray width (bottom) predicted by the SSD breakup model with TAB distortion model using the dataset from Freitag and Hassa [109].

As seen in **Figure 3-10**, increasing the breakup parameter B_1 also increases the SMD in the core and windward regions of the spray for the conditions from Madabhushi et al. [30], but it has no significant impact in the leeward region where the SMD remains significantly underpredicted. Although it improves the overall accuracy of the SMD predictions, it also significantly overpredicts the SMD at the maximum windward interface between the phases. Moreover, a lower breakup parameter B_1 allows to better capture the vertical spread of the spray, but at the expense of the agreement with the experimental data for the SMD in the windward and spray core regions. **Figure 3-11** shows that similar conclusions for the SMD can be made for the dataset from Freitag and

Hassa [109], but the impact of the breakup parameter B_1 on the SMD predictions in the windward region is less important. Again, this could be due to the effects of the breakup parameter B_1 being sensitive to the experimental conditions and should be further investigated.

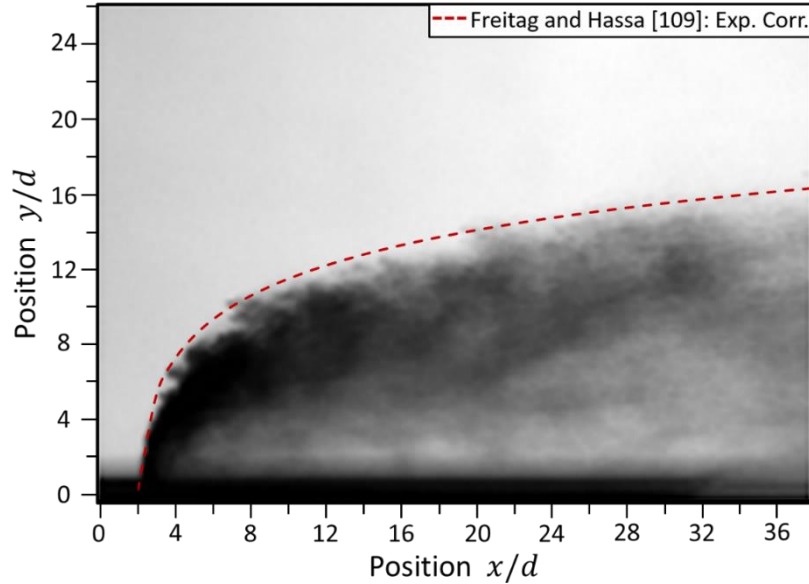


Figure 3-9: Experimental correlation for the maximum spray trajectory compared to the shadowgraph picture taken for the dataset selected from Freitag and Hassa [109].
(Adapted from [109] with authorization from ILASS Europe).

It can be observed in **Figure 3-12** and **Figure 3-13** that increasing the breakup parameter B_1 produces bigger child droplets across the entire spray. This was expected considering that the SSD model breakup time τ_{bu} varies proportionally with it as shown in equation (3-24). Thus, decreasing its value enhances the breakup process and results in smaller droplets. This explains why the SMD predicted in the spray core and windward regions tends to increase with the breakup parameter B_1 for both datasets. The present work highlights the reduced influence of the breakup parameter B_1 on the SMD in the leeward spray region compared to its influence on the droplet velocity. This could indicate that the breakup process in the leeward region is governed by other phenomena over which the breakup time has lesser influence or that the SSD breakup model tends to overpredict breakup in that region. The latter conclusion would agree with what has been reported in the literature regarding the underprediction of the SMD by the SSD breakup model [33, 34, 170]. Further studies should be conducted to determine the influence on the SMD

predictions of the model constants that act directly on the droplet size distribution function.

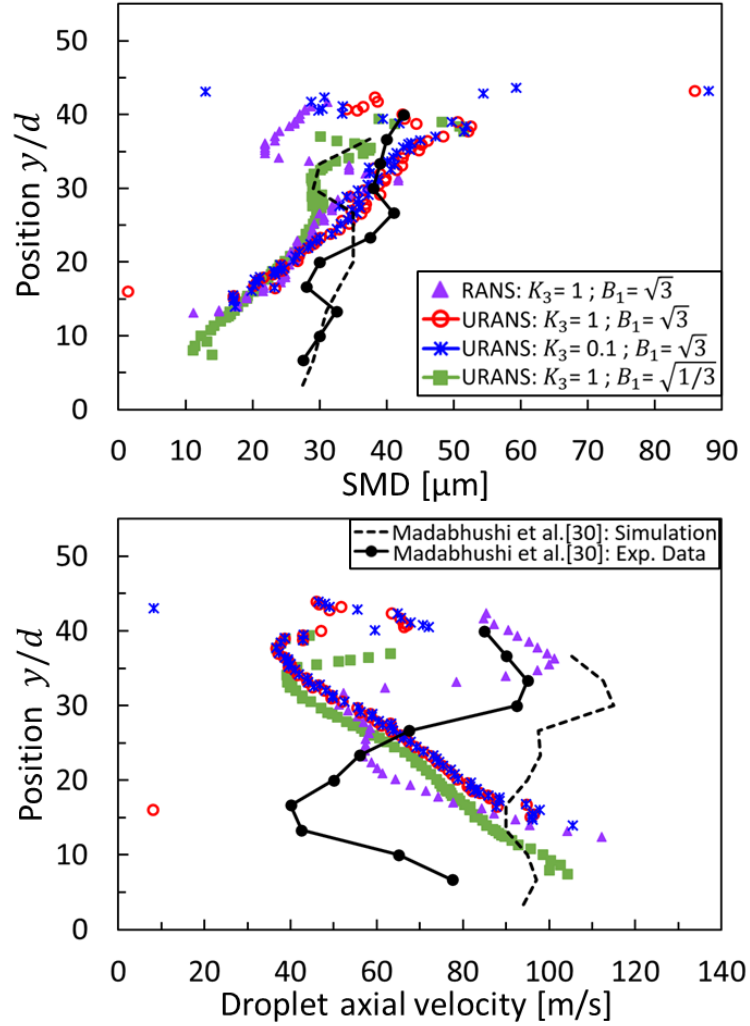


Figure 3-10: Centreline SMD (top) and droplet axial velocity (bottom) predicted by the SSD breakup model with TAB distortion model using the dataset from Madabhushi et al. [30].

In addition, a higher breakup parameter B_1 causes the droplet axial velocity to decrease in the spray windward region and to increase in the spray core and leeward regions. As shown in equation (3-28), the child droplet velocity is inversely proportional to the breakup time and directly proportional to the child droplet size. Thus, the droplet velocity is predicted to decrease for an increasing breakup time if the effect of the latter on the momentum transfer is more important than the impact of bigger droplet sizes. This explains the trends observed in the windward spray region for both datasets. A higher breakup parameter B_1 has the opposite effects in the spray core and leeward regions as

reported. As seen in **Figure 3-10**, it also increases the discrepancies in the leeward and windward regions of the spray and does not significantly improve them in the core region.

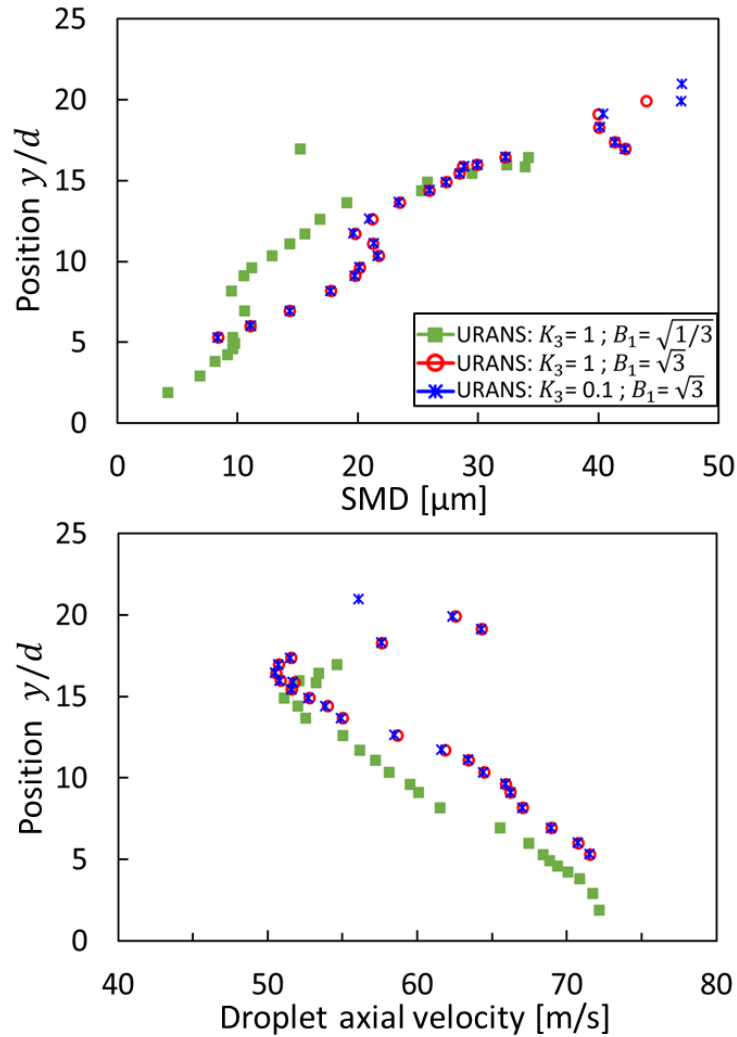


Figure 3-11: Centreline SMD (top) and droplet axial velocity (bottom) predicted by the SSD breakup model with TAB distortion model using the dataset from Freitag and Hassa [109].

As for the normal velocity coefficient K_3 , it has no significant impact on predictions, except in the windward interface between the phases as a smaller value tends to predict a slightly higher SMD.

Another important observation is that while using the unsteady solver improves the SMD predictions in the spray core and windward regions, it significantly worsens them for the droplet axial velocity in the same areas. Moreover, it has no significant impact on the

predictions in the spray leeward region as the droplet axial velocity remains significantly overpredicted and the SMD significantly underpredicted.

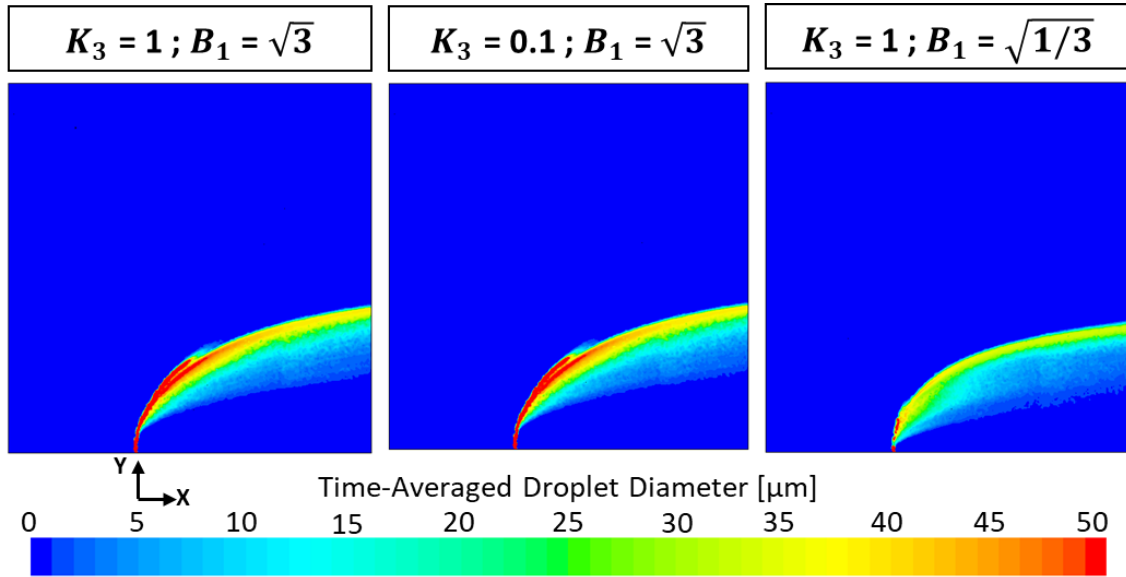


Figure 3-12: Droplet diameter in the XY cross-section plane ($z/d=0$) predicted by the SSD breakup model with TAB distortion model using the dataset from Madabhushi et al. [30].

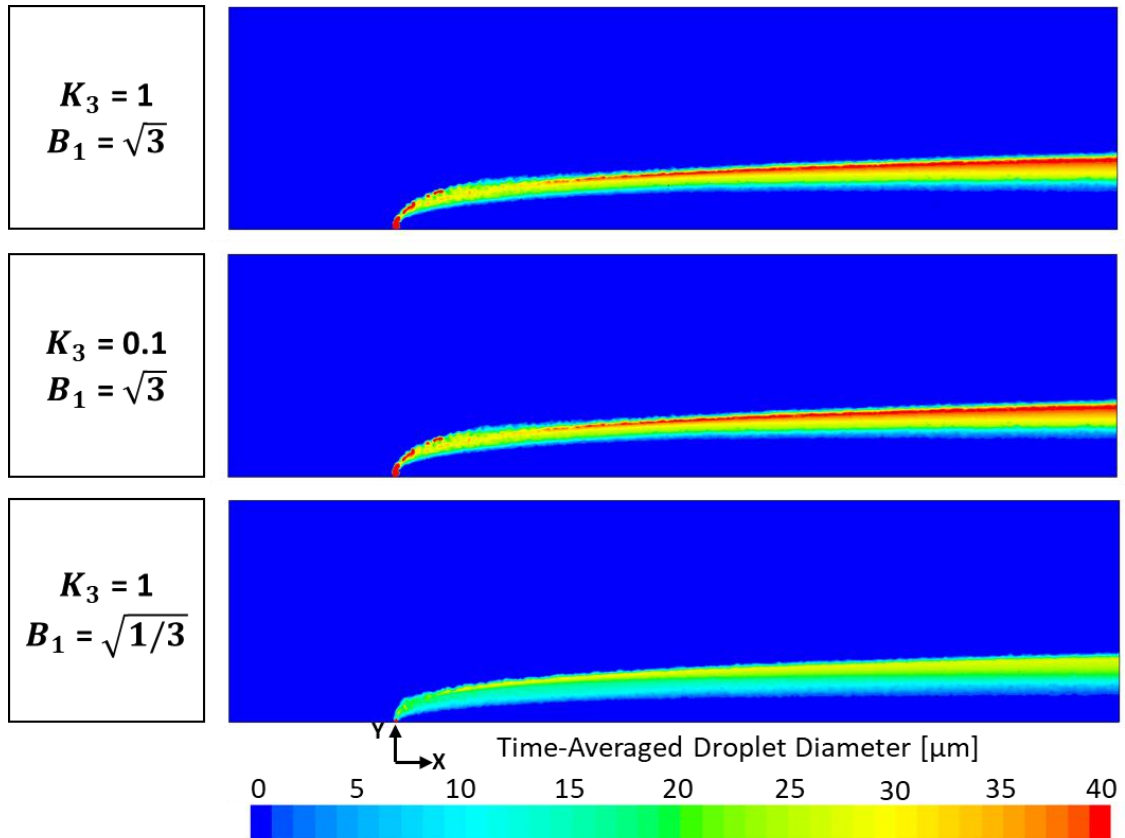


Figure 3-13: Droplet diameter in the XY cross-section plane ($z/d=0$) predicted by the SSD breakup model with TAB distortion model using the dataset from Freitag and Hassa [109].

3.6 Conclusion

In conclusion, this work contributed to assess the predictive capabilities of different breakup models used in state-of-the-art CFD against experimental data at standard and high-pressure conditions for turbulent liquid fuel jets in crossflow for RANS and URANS simulations to provide accurate and less expensive computational tools for design purposes.

The present study concludes that the Reitz-Diwakar breakup model should not be used as a secondary breakup model for transverse jets nor as a first approximation because it significantly overpredicts the spray trajectory and SMD as well as underpredicts the droplet velocity even when coupled with the TAB distortion model. It was also shown that the accuracy of the KHRT breakup model can't be improved by increasing the discretization of the spray or by using the TAB distortion model and it is not deemed likely to improve with an unsteady solver. Thus, even for transverse jets, its accuracy can't be compensated as it relies too strongly on tuning the empirical constants to the experimental conditions. This is a problem for design exploration purposes considering the lack of data available when developing new designs and the associated time constraints. The SSD breakup model is the recommended choice to guide the design of novel jets in crossflow injectors due to its superior predictive capabilities even without tuning its model constants. To achieve even greater accuracy, it is recommended to couple it with the TAB distortion model. The parametric study of the SSD breakup model concluded that the normal velocity coefficient K_3 has no significant impact on the spray characteristics for jets in crossflow regardless of the experimental conditions. Moreover, it was found that increasing the breakup parameter B_1 value from $\sqrt{1/3}$ to $\sqrt{3}$ improves the solution accuracy for the SMD, but at the expense of the accuracy for the droplet axial velocity and the spray trajectory as it significantly overpredicts it with the axial distance. It is recommended to further investigate the dependence of this model constant on the flow properties. To improve the droplet size predictions in the spray leeward region, future work should be done to assess the effect of the SSD model's constants used to dictate the mean and variance of the droplet-size distribution function. The present work also concludes that the unsteady solver increases the overall accuracy for the SMD, but at the expense of the predictions for the droplet axial velocity.

The numerical methodology developed from this study was used to guide the design of an experimental test rig on visualizing and measuring diesel jet breakup at representative gas turbine conditions, which is presented in Appendix A. The high-pressure and high-temperature datasets produced will be used to further assess the predictive capabilities for jets in crossflow of the SSD breakup model coupled with the TAB distortion model and to develop numerical modelling approaches for this application.

3.7 Acknowledgment

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4 Validation of a Stochastic Breakup Model for Turbulent Jets in High-Speed Crossflow: Assessment of Turbulent Interactions and Sensitivity to Boundary Conditions

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4.1 Abstract

Improving the mixing of fuel and air by injecting a turbulent liquid fuel jet into a high-speed crossflowing gas can reduce the emissions of gas turbine applications. To facilitate and hasten the development of such low-emission technologies, accurate predictions of the spray characteristics are needed. The objective of the present study is to validate the predictive capabilities of a stochastic breakup model for turbulent transverse jets over a wide range of representative pressures and atomization characteristics. The effect of turbulence modelling is also assessed to provide accurate and computationally less expensive Eulerian-Lagrangian transient approaches. To do so, the predictions made with the Large Eddy Simulation (LES) approach for different subgrid-scale (SGS) models and with the Synthetic Eddy Method (SEM) are compared to the ones made using the unsteady Reynolds-Averaged Navier-Stokes (RANS) approach with and without a turbulent dispersion model. The sensitivity of the numerical methodology to the upstream velocity profile, pressure and momentum flux ratio were also assessed. Properly accounting for the upstream gas velocity profile was found to be critical to ensure accurate predictions of the spray characteristics. The unsteady RANS (URANS) turbulent approach coupled with the turbulent dispersion model showed good agreement with experimental data, but the LES approach tends to overpredict the spray penetration and underpredict the Sauter Mean Diameter (SMD). This could be due to the lower turbulent interactions it predicts, which may lead to lower momentum transfer between the phases.

Keywords: Liquid jet, Crossflow, High pressure, Secondary Breakup, Stochastic, Turbulent dispersion, Simulations, CFD, LES, Unsteady RANS.

4.2 Introduction

To address the growing environmental concerns, highly ambitious targets have been set by various legislative bodies to reduce emissions from both stationary and aero gas turbine applications. It is critical to develop more sustainable technologies, such as advanced mixing technologies that reduce emissions by improving the mixing of liquid-fuel sprays with air [5]. Once injected into the combustor, the liquid jet is divided into small droplets by going through a primary and secondary breakup process to form a spray that evaporates and mixes with the air. The breakup processes influence the spray characteristics, which significantly influence the combustion process and emissions [5]. Mixing can be improved by injecting the liquid fuel transversely into a crossflowing air stream and can be further enhanced by the turbulent characteristics of the liquid jet and air stream [6, 9, 164]. To facilitate the design work and hasten the delivery of new sustainable technologies, the Lagrangian approach is preferred over the computationally expensive interface-capturing methods, such as the Volume-of-Fluid (VOF) approach. Thus, this study focuses on validating a numerical methodology for turbulent liquid jets in crossflow using a Lagrangian approach.

However, the breakup models used in state-of-the-art CFD are deemed unlikely to be suitable at representative conditions because they are often based on Kelvin-Helmholtz (KH) instabilities growing on the droplet surface (Wave/KH model) [149], such as the KHRT breakup model [150], or on Taylor's analogy (TAB model) [151], such as the ETAB breakup model [171]. These use correlations or model constants experimentally determined mainly at atmospheric conditions or without fuel [24, 25]. Thus, they need to be calibrated to accurately predict the spray penetration and droplet size distribution [5, 14]. Other breakup models developed to improve the predictions in the primary region also require knowledge of the near-field characteristics [14].

The need to generate experimental data to obtain accurate results is counterproductive considering that CFD is used as a tool to guide the design. Thus, numerical models should ideally require minimal calibration. To the best knowledge of the authors, the Madabhushi et al. [30] breakup model is the only one used in state-of-the-art CFD that has been developed for turbulent jets in crossflow to account for their distinctive characteristics, such as the column bending under aerodynamic forces. However, it also relies on

experimental data as it uses the Wave breakup model to account for the primary breakup and other experimental correlations.

The Stochastic Secondary Droplet (SSD) breakup model [33] was developed to rely less on experimental data as it considers droplet breakup to be random in nature and to depend more on the boundary conditions by using Kolmogorov's stochastic theory [33, 34]. Thus, the breakup is not limited to a single scale and the important processes that occur at the high gas Weber numbers often used in gas turbine applications are captured, such as the effect of turbulence and catastrophic breakup [33, 34]. Therefore, the current work studies the predictive capabilities of the SSD model for turbulent jets in crossflow.

Previous studies conducted with the LES and URANS approach showed good agreement between the SSD model and experimental data for different types of coflowing atomizers over a wide range of conditions. However, they noted the SMD tends to be underpredicted regardless of the pressure [33, 34, 170] and despite the use of a primary breakup model [170, 172]. To the best knowledge of the authors, previous studies coupling the Lagrangian or hybrid approach (e.g. VOF-Lagrangian) with the SSD breakup model for a jet in crossflow configuration were limited to ambient pressure and low gas Weber numbers [35, 37], used water [35, 36, 37] or used either non-turbulent jets [36] or a very low momentum flux ratio [35]. Moreover, they mostly focused on assessing the predictive capabilities in the primary breakup region with a hybrid approach [35, 36], which is not where the SSD model dominates. Regarding turbulence modelling, Apte et al. [34] obtained good agreement for coflowing sprays between URANS and LES with a dynamic subgrid-scale model but recommended the use of additional models for the RANS turbulence approach due to disparities observed in the far-field region. Heide et al. [173] concluded that such additional turbulence models were necessary for coflowing sprays to obtain accurate trajectory predictions in the near-field region. Blanchard and Shi [37] explored reducing the computational cost by using RANS simulations with a turbulent dispersion model, but did not focus on assessing the effects of the latter on the predictive capabilities.

Furthermore, most numerical studies on jets in crossflow assume a constant gas velocity profile as they consider the difference between the mean and peak velocity to be negligible [39, 174]. Many experimental studies [e.g. 75, 108, 111, 119, 124] interpret the

velocity profile as flat despite a thick boundary layer measured or the use of a long flow straightening channel since achieving it used to be a popular design criterion. Meanwhile, other research reporting similar velocity profiles [e.g. 91, 84, 116, 117, 123] have a different interpretation despite the similar experimental setup and often use the mean velocity to extract an experimental correlation. However, the experimental test sections commonly used are usually small (a few millimetres) and only one order of magnitude higher than the boundary layer thickness. Thus, the effect of the latter on the flow field could be important. To the best knowledge of the authors, the effect of assuming a constant gas velocity profile on the spray predictions has not been assessed yet.

Therefore, the objective of this study is to answer the need to validate the predictive capabilities of the SSD breakup model at more representative gas turbine conditions for turbulent liquid jets in crossflow. The effect of additional turbulence modelling on less computationally expensive Eulerian-Lagrangian transient approaches is also assessed to provide fast and accurate design tools. To do so, the effects on the LES predictions of different subgrid-scale models and of using turbulent boundary conditions through the Synthetic Eddy Method (SEM) are compared to the effect on the URANS predictions of using a turbulent dispersion model. The results are validated against experimental data available in the literature over a wide range of conditions. The sensitivities of the numerical approach to the velocity profile, pressure and momentum flux ratio are also studied.

4.3 Governing Equations

With the Lagrangian-Eulerian approach, a discrete element type of method is used to track clusters of particles with identical properties inside the computational domain and to solve governing equations for their instantaneous state as described by Crowe [132]. Using a statistical approach by solving the Lagrangian equations for parcels of particles reduces the computational cost.

4.3.1 Lagrangian Approach

The interactions between the dispersed and continuous phases are modelled through two-way coupling, which considers the influence of the gas on the droplets as well as the opposite. In the present work, heat and mass transfer were neglected due to the negligible

temperature differential as presented in *section 4.4*. Therefore, the interactions are modelled by only considering the transfer of momentum and energy by applying as a source term the resulting net exchanges to the corresponding governing equation of the continuous phase. For each cell, the net exchange of all particles crossing its volume is obtained by summing-up the change of each particle. These are calculated by integrating the dispersed phase equations over the cell. The resulting transfer rates of momentum S_v and energy S_E to the continuous phase are defined as [85, 132]

$$S_v = -\frac{1}{\Delta t} \sum_{\pi} \sum_{\delta t_p} n_{\pi}(F_s) \delta t_p \quad (4-1)$$

$$S_E = -\frac{1}{\Delta t} \sum_{\pi} \sum_{\delta t_p} n_{\pi}(F_s \cdot u_p) \delta t_p \quad (4-2)$$

Where n_{π} is the number of particles within a parcel, Δt the physical time-step, δt_p the local parcel time-step and u_p the particle velocity. The surface force applied to the droplets F_s represents the aerodynamic effects and pressure changes in the continuous phase and is calculated as [85, 132]

$$F_s = F_d + F_p \quad (4-3)$$

Where F_d is the drag force and F_p the pressure gradient force, which is defined as [85, 132]

$$F_p = -V_p \nabla P_{static} = -\left(m_p / \rho_p\right) \nabla P_{static} \quad (4-4)$$

Where m_p is the particle mass, V_p the particle's volume, ρ_p the particle's density and ∇P_{static} the static pressure gradient of the continuous phase. The drag force in equation (4-3) is defined as [85, 132]

$$F_d = \frac{1}{2} C_D \rho A_p |u_s| u_s = (m_p u_s) / \tau_v \quad (4-5)$$

Where C_D is the drag force coefficient, ρ the continuous phase's density, A_p the particle's projected area, τ_v the momentum-relaxation time scale and u_s the particle's slip velocity calculated as [85, 132]

$$u_s = u - u_p \quad (4-6)$$

Where u is the velocity of the continuous phase. The motion of the particle due to the forces acting on its surface is defined by the equation of the conservation of the translational momentum [85, 132]

$$m_p \frac{du_p}{dt} = F_s \quad (4-7)$$

Integrating over time the particle's equation of motion described in equation (4-7) gives the particle's instantaneous velocity u_p . Integrating the latter over time gives the particle's instantaneous position vector R_p , which once integrated over time gives the particle's trajectory. Within a time-step Δt of the unsteady solver, the solution of each parcel is time-marched every inner iteration by the Lagrangian solver through an adaptive local parcel time-step δt_p . The temporal error is controlled through the latter by restricting its value to [85]

$$\frac{Co_{min}\Delta x_{cell}}{\max(|u|, |u_p|)} \leq \delta t_p \leq \frac{Co_{max}\Delta x_{cell}}{\max(|u|, |u_p|)} \quad \text{where } \delta t_p \leq \Delta t \quad (4-8)$$

Where Co_{max} and Co_{min} are the maximum and minimum Lagrangian phase courant numbers and Δx_{cell} is a characteristic length of the cell. A smaller time-step and Lagrangian courant numbers increase the accuracy of the solution at the expense of computational time.

4.3.2 Drag Force and Tab Distortion

The Liu Dynamic drag coefficient C_D defined in equation (4-9) accounts for the droplet's deformation due to the surrounding aerodynamic forces [165] through the TAB distortion model, which considers it to be analogous to a damped spring-mass system where breakup occurs at a critical oscillation frequency characterized by a critical Weber number [151].

$$C_D = C_{D_{Sphere}}(1 + 2.632y_{TAB}) \quad (4-9)$$

Where $C_{D_{Sphere}}$ is the drag coefficient of an undistorted droplet defined by [175]

$$C_{D_{Sphere}} = \begin{cases} \frac{24}{Re_p} \left(1 + \frac{1}{6} Re_p^{2/3}\right) & Re_p \leq 1000 \\ 0.424 & Re_p > 1000 \end{cases} \quad (4-10)$$

Where Re_p is the particle's Reynolds number as calculated by

$$Re_p = \frac{\rho |u_s| D_p}{\mu} \quad (4-11)$$

Where μ is the continuous phase's dynamic viscosity and D_p the particle diameter. The normalized droplet distortion y_{TAB} is calculated by analytically solving a second-order ODE function of the Weber number calculated as

$$We = \frac{\rho |u_s|^2 D_p}{\sigma} \quad (4-12)$$

Where σ is the surface tension. The value of the normalized distortion y_{TAB} is 0 when the droplet is spherical, and 1 when the droplet is completely distorted.

4.3.3 SSD Breakup Model

The Stochastic Secondary Droplet (SSD) breakup model [33] is based on the stochastic Lagrangian breakup model first proposed by Gorokhovski and Saveliev [176]. It considers the secondary breakup process to be a discrete random occurrence independent of the parent droplet diameter. To do so, it uses a reformulation of Kolmogorov's stochastic theory where the breakup process is asymptotically reduced to the Fokker-Planck differential equation [33, 176]. Within each parcel where breakup is predicted to occur, the diameters of the child droplets are sampled according to the log-normal distribution obtained by analytically solving the Fokker-Planck differential equation for the droplet diameter probability density function [33, 176]. The SSD model considers that the secondary breakup process depends on the aerodynamic and surface tension forces acting on the droplet's surface. Hence, the temporal evolution of the distribution function is governed by the local flow characteristics and its parameters are given as a function of the Weber number defined in equation (4-12) [34]. With the SSD model, two criteria must be met for secondary droplet breakup to occur. The droplet surface must first be unstable, which occurs when the parent droplet radius is bigger than a critical radius defined as

$$r_{crit} = \frac{We_{crit} \sigma}{\rho |u_s|^2} \quad (4-13)$$

When the droplet radius is equal to the critical droplet radius r_{crit} , the SSD model considers that the hydrodynamic forces are balancing the capillary forces, which makes the droplet on the verge of becoming unstable [33]. Thus, a droplet with a larger radius is considered subjected to a force imbalance, which causes the droplet's surface to become unstable and makes it prone to breakup. The Weber number must also be bigger than a critical value, which was assumed equal to 6 based on the linear stability analyses of the related experimental correlation [86]. Secondly, the local residence time in the computational domain of an unstable droplet must be larger than its breakup time, which is calculated as [85]

$$\tau_{bu} = B_1 \sqrt{\frac{\rho_p}{\rho} \left(\frac{r_p}{u_s} \right)} \quad (4-14)$$

Decreasing the model constant B_1 increases droplet breakup because it reduces the breakup time. When both droplet breakup conditions are met, the parent droplet is replaced by child droplets. For the statistical approach of the Lagrangian framework, breakup occurs when the identical droplets contained within a parcel meet the breakup conditions of the SSD model. The parent parcel disappears after it breaks up into a number of child parcels each containing identical child droplets that can cause further breakup if they meet the breakup conditions. The diameter of the child droplets contained within the child parcels is obtained by sampling the log-normal size-distribution function

$$\Phi(r_{p,c}) = \frac{1}{2} \left(1 + \operatorname{erf} \left[\frac{\log(r_{p,c}/r_p) - \langle \xi \rangle}{\sqrt{2\langle \xi^2 \rangle}} \right] \right) \quad (4-15)$$

Where $r_{p,c}$ is the radius of the child particle, r_p is the radius of the parent particle, $\langle \xi \rangle$ is the first logarithmic moment of the breakup spectrum function and $\langle \xi^2 \rangle$ is the second logarithmic moment, which can be interpreted as indicators of its mean value and variance respectively. Further details on the equations and effects of the parameters from the SSD breakup model can be found in Apte et al. [33, 34] and references therein. Although the SSD model considers the droplet size distribution function to be independent of the parent droplet diameter, it is included as a parameter in equation (4-15) to set the upper limit of the child droplet diameter range. The lower limit corresponds to half the critical diameter. The mean value of the breakup distribution function is defined as

$$\langle \xi \rangle = K_0 \quad (4-16)$$

Where K_0 is a model constant of default value -0.1. Increasing its value increases the mean diameter of the child parcels. The variance of the droplet diameter distribution is defined as

$$\langle \xi^2 \rangle = K_1 \ln(We/We_{crit}) \quad (4-17)$$

Where K_1 is a model constant imposed to the recommended baseline value of 0.1. Increasing its value or the Weber number increases the variance of the size-distribution, causing the child droplet diameters to deviate more from the mean value of the distribution. Due to the nature of the breakup process, the child droplets are assumed to gain momentum in the direction normal to the slip velocity vector, which is accounted for

by applying a multiplication factor $|W_{bu}|$ to the inherited parent droplet velocity. Since this multiplication factor considers the child droplet sizes, their velocity $u_{p,c}$ can only be calculated once their diameter is obtained from equation (4-15) and is then defined as

$$u_{p,c} = |W_{bu}|u_p = (K_3 r_{p,c} / \tau_{bu})u_p \quad (4-18)$$

Where K_3 is a normal velocity coefficient impacting the spray angle with a value limited between 0 and 1. Increasing its value increases the radial diffusion of the spray.

4.3.4 Turbulent Dispersion

Particles travelling through a turbulent flow field are assumed to interact with turbulent eddies, which subjects them to a randomly fluctuating flow field that modifies their respective trajectories following the principle of inertia. To capture the resulting higher level of droplet dispersion, the effect of the turbulent eddies must be included along with the aerodynamics effects. For many flow applications, the LES approach accounts for the turbulent interactions more accurately than the RANS approach [177, 178]. However, as further discussed in *section 4.5.1.4*, this is not the case when unresolved small-scale motions could have a significant impact on the physical process modelled [177, 179]. In the present study, the baseline predictive capabilities of LES for turbulent jets in high-speed crossflow are compared to the unsteady RANS approach with and without the use of a stochastic model that better accounts for turbulent interactions.

The Turbulent Dispersion model adapted from Gosman and Ioannides [180] can be added to the Eulerian-Lagrangian Framework to improve the turbulence modelling of the unsteady RANS approach. With the latter, turbulence is modelled through a turbulent eddy viscosity applied to a time-averaged flow field. A stochastic method based on the phase interaction model developed by Dukowicz [181] is used to include the effect of the instantaneous velocity field fluctuating under the disruptions caused by turbulent eddies, which is calculated as

$$u = \bar{u} + u' \quad (4-19)$$

Where $\bar{u}$ is the local Reynolds-averaged velocity and u' is the fluctuating eddy velocity, which is calculated using a normal Gaussian. The fluctuating eddy velocity is applied to the Reynolds-Averaged flow while the droplet interacts with the eddy, which ends when

the lifetime of the eddy is reached, or when the distance between both of them exceeds the eddy length scale. This eddy interaction time τ_l is defined as [182]

$$\tau_l = \min(\tau_e, \tau_c) \quad (4-20)$$

Where τ_c is the eddy transit time and τ_e the eddy time scale representing its lifetime given by

$$\tau_e = \frac{2\mu_t}{\rho u_e^2} = \frac{3\mu_t}{\rho k} \quad (4-21)$$

Where μ_t is the turbulent eddy viscosity, k the turbulent kinetic energy and u_e the eddy velocity scale. The eddy transit time, which represents the time it takes for the droplet to be separated from the eddy by a distance larger than its length, depends on the aerodynamic forces and is defined as

$$\tau_c = \begin{cases} \infty & \tau_v \leq l_e/|u_s| \\ -\tau_v \ln\left(1 - \frac{l_e}{\tau_v|u_s|}\right) & \tau_v > l_e/|u_s| \end{cases} \quad (4-22)$$

Where τ_v is the momentum relaxation time scale in equation (4-5) and l_e the eddy length scale defined as

$$l_e = u_e \tau_e = \left(2\mu_t/\rho\right) \sqrt{3/(2k)} \quad (4-23)$$

The eddy velocity scale, which represents the standard deviation of the eddy velocity fluctuation, is calculated as

$$u_e = \left(l_t/\tau_t\right) \sqrt{2/3} = \sqrt{(2k)/3} \quad (4-24)$$

Where l_t is the turbulent length scale and τ_t the turbulent time scale. The definition of the turbulent time scale, velocity scale, kinetic energy and viscosity depend on the turbulence model used.

4.3.5 RANS Turbulence Modelling

For the URANS simulations, turbulence is modeled using the Realizable k-epsilon Two-Layer model, which applies the two-layer approach [183] to the Realizable k-epsilon model and allows to use an all y^+ wall treatment. The turbulent length and time scales are calculated as

$$\tau_t = k/\varepsilon \quad (4-25)$$

$$l_t = \tau_t \sqrt{k} \quad (4-26)$$

The dissipation rate ε and the turbulent kinetic energy k are obtained through the Realizable k-epsilon transport equation [133]. With the Two-Layer model, the turbulent dissipation rate and turbulent viscosity near the wall are prescribed by the Wolfshtein [184] formulations. The turbulent viscosity is calculated considering the applicability limit of the two-layer formulation through a wall-proximity indicator [185], which blends the turbulent viscosities of the Two-Layer model and Realizable k-epsilon model. The formulation of the latter is similar to the standard k-epsilon model, but it applies a damping factor that is a function of the mean strain rate and vorticity tensors. The turbulent viscosity is used to compute the viscous stress tensor, which is added to the stress tensor used in the RANS transport equations to effectively close them.

4.3.6 LES Turbulence Modelling

For LES, the smaller scales are implicitly filtered by accounting for the subgrid-scale (SGS) interactions through a stress tensor described by the Boussinesq approximation. It is then added to the stress tensor used in the filtered transport equations to effectively close them. In the present work, the WALE SGS model with a length scale limit applied [134] and the Smagorinsky [186] SGS model with a standard Van Driest [187] damping function are used with their standard model constant. Once the turbulent SGS viscosity is obtained, the LES approach prescribes an algebraic formulation to compute the related SGS turbulent kinetic energy and dissipation rate, which are defined as [188]

$$k_{SGS} = C_t S(\mu_t/\rho) = C_t S(\Delta^2 S_{SGS}) \quad (4-27)$$

$$\varepsilon_{SGS} = S^2(\mu_t/\rho) = S^2(\Delta^2 S_{SGS}) \quad (4-28)$$

Where C_t is a model constant equal to 3.5 and Δ is the grid-filtered width. For the WALE SGS model, S_{SGS} is a deformation parameter computed from the resolved velocity and the modulus of mean strain rate tensor S . For the Smagorinsky SGS model, it corresponds to the latter. The SGS values are used in equation (4-25) and equation (4-26) to obtain the SGS turbulent time and length scales.

4.4 Computational Set-Up

4.4.1 Numerical Domain, Mesh and Boundary Conditions

Experimental datasets at standard temperature and high-pressure using Kerosene fuel from Freitag and Hassa [109] were used to validate the predictions in jet trajectory at high pressure (case 1-2 $P_g=4$ bar, case 3 $P_g=8$ bar), high gas Weber number (case 1-2 $We_g=586$, case 3 $We_g=1172$) and high droplet gas Reynolds number (case 1-2 $Re_{g,d}=9.2E+03$, case 3 $Re_{g,d}=1.8E+04$). The datasets at standard temperature and pressure using Jet A fuel from Madabhushi et al. [30] ($We_g=720$, $Re_{g,d}=7.8E+03$) were used to assess the predictions for the Sauter Mean Diameter (SMD) at high jet Weber number We_{jet} and jet Reynolds number Re_{jet} , which are compared in **Table 4-1**. Madabhushi et al. [30] also developed a breakup model specifically for jets in crossflow and their numerical predictions will be compared. These datasets can also be characterized by their momentum flux ratio J , which is initially calculated as

$$J = (\rho_{jet}u_{jet}^2)/(\rho_g u_g^2) \quad (4-29)$$

Where u_{jet} is the initial jet velocity at the nozzle exit, u_g the crossflow gas velocity upstream of the injector, and ρ_{jet} and ρ_g the initial jet and gas density. A higher value of J results in a higher spray trajectory [9]. A previous parametric study of the SSD breakup model using similar datasets was conducted by the authors [42]. The numerical domain lengths and mesh settings used are imposed in the present study. The experimental cross-section dimensions were used to define the numerical domains shown in **Figure 4-1**.

Table 4-1: Experimental flow properties used for the numerical operating conditions.

Datasets	Madabhushi et al. [30]	Freitag and Hassa [109]		
	Dataset 1	Dataset 2		
		case 1	case 2	case 3
u_{jet} [m/s]	31	13.9	27.9	19.7
u_{jet}/u_g	0.22	0.19	0.37	0.26
J	33.6	6	24	6
We_{jet}	2.47E+04	3.52E+03	1.41E+04	7.03E+03
Re_{jet}	1.18E+04	3.70E+03	7.39E+03	5.23E+03

For the boundary conditions, an inlet velocity profile is imposed, and adiabatic no-slip walls are used. For the dataset of Freitag and Hassa [109], an unsteady non-reflecting condition is imposed at the pressure outlet to prevent non-physical acoustic reflections.

The injection is done in the middle, downstream of the air inlet to achieve an established flow field in the spray region. Because both experiments used plain orifice injectors, the parcel streams were injected with droplets initially at the size of the nozzle diameter d , which corresponds to 0.762 mm and 0.5 mm for the dataset from Madabhushi et al. [30] and Freitag and Hassa [109] respectively.

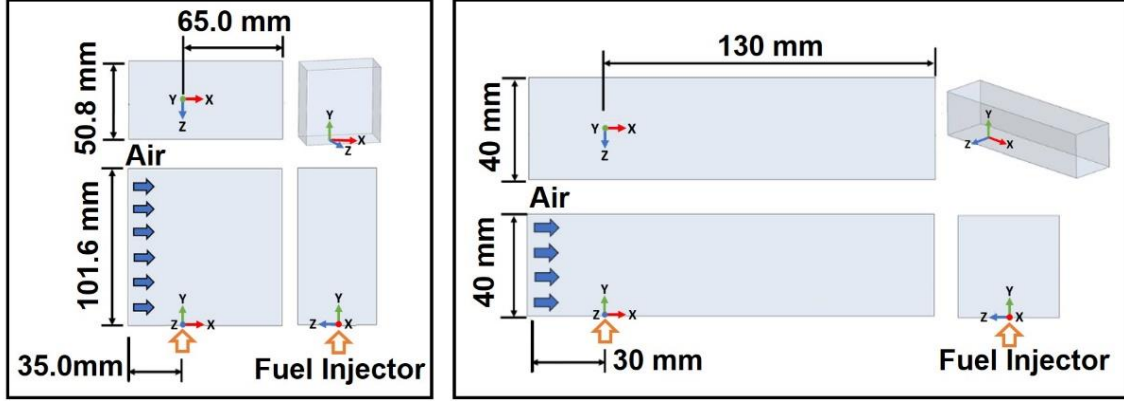


Figure 4-1: Numerical domain used for the assessment done using the datasets from Madabhushi et al. [30] (left) and Freitag and Hassa [109] (right).

For all simulations, the mesh is made of polyhedral cells with the same parameters, which were selected following a mesh refinement study using the dataset from Madabhushi et al. [30]. The volume mesh was refined to 0.4 mm in the near-field region and to 0.45 mm in the far-field region. The resulting mesh has 3.4 million elements for the numerical domain of Madabhushi et al. [30] and 2.8 million elements for Freitag and Hassa [109]. The mesh was made fine enough for LES to obtain a courant number near or below unity in the spray and wall y^+ values below 2.

4.4.2 Fully Developed Turbulent Velocity Profile Correlation

Using a correlation to predict the turbulent gas velocity profile would reduce the computation time from having to obtain it numerically. The empirical power-law velocity profile correlation for fully developed turbulent flow in circular pipes was adapted for rectangular ducts by Peszyński [189]

$$u_g(y, z) = u_{g,c} \left(1 - (z/0.5W)\right)^{1/n} \left(1 - (y/0.5H)\right)^{1/n} \quad (4-30)$$

Where z and y are the horizontal and vertical coordinates on the rectangular cross-section, W the width, H the height, n a model constant function of the hydraulic Reynolds number and $u_{g,c}$ the centreline velocity calculated as [79]

$$u_{g,c} = u_g(n + 1)(2n + 1)/2n^2 \quad (4-31)$$

The correlation was validated for both datasets by performing URANS simulations with the turbulent dispersion model. The calculated fully developed turbulent velocity profile was imposed at the inlet of the domain in **Figure 4-1** by using equation (4-30) with over 3000 (y, z) coordinates. For the conditions of Freitag and Hassa [109], the constant n was set to 7, which is also the standard value used by the power-law velocity profile that gives reasonable results for many flow applications [79]. For the conditions of Madabhushi et al. [30], a value of 9 was found to agree well with the experimental one, which is more flat-shaped. The resulting predictions were compared to those obtained with a numerically fully developed turbulent velocity profile. To obtain the latter, RANS simulations of the numerical domains elongated to a length superior to a calculated entrance length were performed with a constant inlet velocity profile. The resulting outlet velocity profile was then imposed at the inlet of the shorter domain for the URANS study. The spray characteristics obtained using both velocity profiles were found to agree well together and with the experimental data. Indeed, they did not predict any significant differences in SMD or maximum spray trajectory for the conditions of Freitag and Hassa [109] case 1 and Madabhushi et al. [30]. Thus, equation (4-30) was used to assess the sensitivity of the numerical methodology to the inlet velocity profile.

Preliminary studies were conducted using these results to determine which profile to use for the baseline assessments of the turbulence approaches. For the dataset from Madabhushi et al. [30], a constant velocity profile ($u_g=138\text{m/s}$) is imposed due to the better agreement with the experimental one. For the dataset from Freitag and Hassa [109], a fully developed velocity profile is imposed due to the better agreement with the experimental maximum jet trajectory compared to a constant velocity profile ($u_g=75\text{m/s}$) as further discussed in *section 4.5.4* and *section 4.5.6*.

4.4.3 Physics Model

The simulations conducted using Simcenter STAR-CCM+ 2020.3 are three-dimensional, adiabatic, compressible using ideal gas, turbulent and use the implicit unsteady solver with a second-order temporal discretization. For URANS, the coupled energy and flow models with a second-order discretization scheme are used to improve the phase coupling.

The Realizable k-epsilon Two-Layer turbulence model is used with a Two-Layer All y^+ wall treatment. For LES, the segregated energy solver with a bounded-central convection scheme and the segregated fluid temperature model with second-order convection are used with an all y^+ wall treatment. The Smagorinsky and WALE SGS models are compared, and the impact of turbulent boundary conditions is studied using the Synthetic Eddy Method (SEM) with an assumption of isotropy. For the Lagrangian phase, a two-way coupling approach is used with the SSD breakup model coupled with the TAB distortion model for the drag coefficient. The model constants B_1 and K_3 were respectively imposed equal to $\sqrt{3}$ and 1, which have been shown to improve the SMD predictions and enhance the spray radial diffusion [42].

A preliminary parametric study using the URANS approach was done with the datasets from Madabhushi et al. [30] to assess the effect of the target number of particles per parcel and the number of parcels. Increasing their values can reduce the statistical error by improving the spray discretization, but at the expense of increasing the computational cost [85]. It confirmed that these parameters do not affect the droplet characteristics but tend to impact the spray width and jet trajectory. Because the datasets from Freitag and Hassa [109] are used to assess the latter, the target number of particles per parcel and number of parcel streams are imposed to higher values of 200 and 500 respectively. For the datasets of Madabhushi et al. [30], they are both set to 100. The maximum number of child parcels is set to 10.

The Lagrangian Courant numbers are imposed to respect the restrictions on the local parcel time-step δt_p defined in equation (4-8) and its maximum is limited by the solution time-step according to

$$Co_{max} \leq \max(|u|, |u_p|) \Delta t / \Delta x_{cell} \quad (4-32)$$

To determine the smallest value of Co_{max} required to be suitable for the entire spray, u_p was set equal to u_{jet} , u to the minimum value between the volume average and maximum velocity in the domain prior to any injection and Δx_{cell} to the maximum cell size in the spray region. Co_{min} was then set to a smaller value. The values of Co_{max} and Co_{min} were inferior to 0.25 and 0.1 respectively.

For URANS, the constant CFL number was selected to ensure stable convergence. The time-step Δt was set to $1\mu s$ and the numbers of inner iterations were selected to ensure a minimum convergence to the 2nd or 3rd order of magnitude. For LES, more than 80% of the turbulent kinetic energy spectrum was resolved in the spray.

4.4.4 Post-Processing Methodology

All values presented (axial evolutions, centreline profiles, contours, etc.) are time-averaged over at least twice the residence time. The properties of the continuous phase (u, ρ, k, μ_t) and parameters that depend only on them (τ_e, u_e, l_e) are volume-averaged unless otherwise specified. The properties of the dispersed phase (u_p, ρ_p, m_p) and related parameters (u_s, τ_v) are particle-averaged unless otherwise specified. The parameters depending on both phases (J_{local}, τ_c) are calculated using a combination of volume-averaged and particle-averaged values. They are assessed within the spray region by using a volume threshold of the droplets. Their axial evolution is obtained by dividing the latter into sections of equal width ($\Delta x=2mm$) and evaluating their values within each section.

To assess the turbulent interactions, the eddy time and length scales, eddy transit and interaction times are calculated using the expressions of the turbulent dispersion model defined in *section 4.3.4*. For LES, the resolved turbulent kinetic energy is obtained by summing up half of the velocity components variance. To assess the phase interactions, the net momentum transfer rate is obtained from equation (4-1) through a volume-summation as described in *section 4.3.1*. The cumulative curves are then obtained by successively summing up the net momentum transfer rate within each volume section. The local momentum flux ratio J_{local} across the spray is also analyzed using equation (4-29) by replacing u_{jet} with the vertical component of the droplet velocity u_{p_y} and u_g by the local value u . It is then normalized by the imposed momentum flux ratio J presented in **Table 4-1**.

The spray trajectories predicted are obtained by evaluating the droplets' maximum vertical position within each volume section. For the datasets from Freitag and Hassa [109], they are compared to those obtained with their empirical correlation derived from the same experiments as presented in **Table 4-2**. For the dataset from Madabhushi et al. [30], empirical correlations available in the literature obtained using similar datasets of

liquid-fuel jets in crossflow inside a rectangular channel under standard pressure and temperature are used. The correlations from Becker and Hassa [91] and Farvardin et al. [111] were selected as their ranges of momentum flux ratios cover its conditions. The correlation from Tambe et al. [81] was selected due to its range of nozzle diameters, Re_{jet} and We_g . The latter is also true for Becker and Hassa [91].

Table 4-2: Empirical correlations for the maximum spray trajectory.

Reference	Liquid	Y/d
Freitag and Hassa [109]	Kerosene	$1.6\ln(3.81(x/d) + 1)J^{0.4}$
Tambe et al. [81]	Jet A, Water, N-Heptane	$1.55\ln(1.66(x/d) + 1)J^{0.53}$
Becker and Hassa [91]	Jet A-1	$1.48\ln(3.56(x/d) + 1)J^{0.42}$
Farvardin et al. [111]	Diesel, Diesel blends	$3.688J^{0.430}(x/d)^{0.384}We_g^{-0.085}(\mu_{jet}/\mu_{H2O})^{-0.222}$

The contours presented are on a middle ($z/d=0$) XY cross-section plane and the spray characteristics shown are mapped on the continuous phase. The centreline profile ($z/d=0$) for the SMD, gas velocity and droplet velocity are assessed at a YZ cross-section plane where there are discrepancies in spray trajectories between URANS and LES. The normalized position of $x/d \approx 33$ was selected for both datasets as it enables comparing the predicted SMD with the data from Madabhushi et al. [30]. The SMD is calculated as [28]

$$SMD = \left(\sum n_{\pi} D_p^3 \right) / \left(\sum n_{\pi} D_p^2 \right) \quad (4-33)$$

4.5 Results

An assessment of the turbulence approaches (LES, URANS, turbulent dispersion) is first carried out using case 1 from Freitag and Hassa [109] and the dataset from Madabhushi et al. [30] with a fully developed and constant velocity profile respectively. The sensitivity to the inlet velocity profile is then studied by imposing the opposite velocity profile. The sensitivity to the boundary conditions and velocity profile is further analyzed with the datasets from Freitag and Hassa [109].

4.5.1 URANS Compared to LES: Effect on Predictions

The predictive capabilities of URANS and LES for different SGS models and SEM are compared. The discrepancies are explained by analyzing the momentum transfer and turbulent interactions.

4.5.1.1 URANS Compared to LES: Trajectory Predictions

For the datasets of Freitag and Hassa [109], LES tends to predict a higher maximum spray trajectory compared to the experimental correlation and to URANS after the primary breakup region ($x/d \geq 10$) as seen in **Figure 4-2**. Indeed, it predicts a spray trajectory on average 17% higher than URANS and an average relative error with the data of 25% compared to 7% for URANS. Moreover, URANS yields better agreement with the data on a longer axial distance ($x/d \leq 50$).

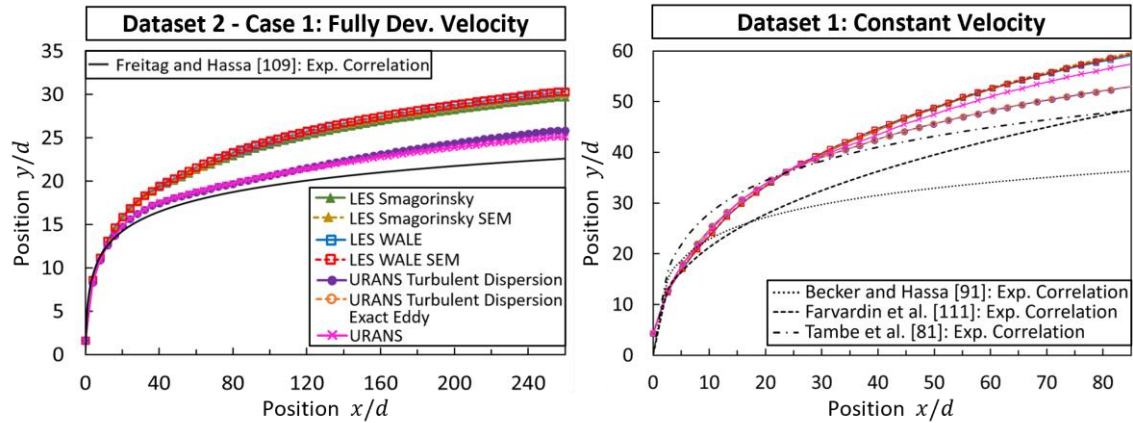


Figure 4-2: Maximum spray trajectory predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

The predictions obtained with the dataset from Madabhushi et al. [30] indicate that LES tends to overpredict the trajectory regardless of the conditions. Indeed, it predicts an average relative error of 40%, 20.5% and 13% with the experimental correlation of Becker and Hassa [91], Farvardin et al. [111] and Tambe et al. [81] respectively, compared to 37%, 19% and 11% for URANS. However, the difference with URANS is less significant as LES predicts it is higher by 3.5% at most. Moreover, the predictions are similar on a longer axial distance ($x/d \leq 30$) compared to the dataset of Freitag and Hassa [109] ($x/d \leq 10$). This could indicate that the trajectory predicted by URANS is sensitive to the boundary conditions. To determine if this is caused by the lower pressure or higher

momentum flux ratio used, further studies were done with the datasets from Freitag and Hassa [109] as discussed in *section 4.5.6*.

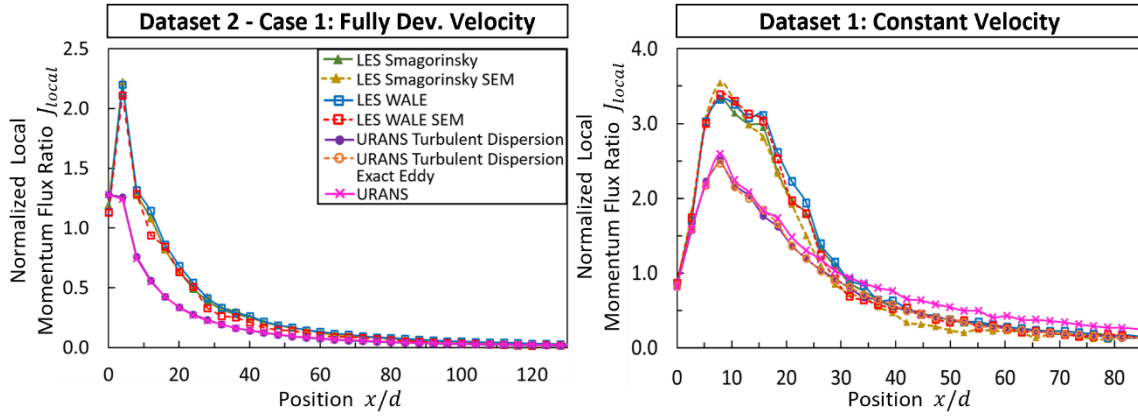


Figure 4-3: Normalized local Momentum flux ratio predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

The local momentum flux ratio is expected to decrease from its imposed value presented in **Table 4-1** as the droplets travel through the domain and exchange their vertical momentum. **Figure 4-3** shows that all simulations captured the imposed value at the injection point ($x/d=0$), but only URANS with the datasets of Freitag and Hassa [109] captured the expected axial evolution trend. Indeed, LES tends to predict that it increases in the near-field region until it reaches a peak value far superior to the one imposed. This is also the case for URANS with the datasets of Madabhushi et al. [30], but the peak values remain significantly inferior to LES. Thus, URANS tends to capture more accurately the axial evolution trends of the local momentum flux ratio.

The higher jet trajectory predicted by LES is reflected by its significantly overpredicted local momentum flux ratio regardless of the conditions, especially in the near-field region as seen in **Figure 4-3**. In the near field region ($x/d \leq 30$), LES predicts J_{local} on average higher by 35% and 72% for the dataset of Madabhushi et al. [30] and Freitag and Hassa [109] respectively. In addition, the higher relative difference with the latter agrees with the higher discrepancies observed in maximum spray trajectory compared to the conditions of Madabhushi et al. [30]. This indicates that URANS might be sensitive to the boundary conditions.

For all simulations, the continuous phase velocity u drives the change in J_{local} as its influence is more important compared to the vertical droplet velocity ($u_{p_y}/u \ll 0.45$). Moreover, since u increases with the axial distance while u_{p_y} decreases, its influence over the latter also increases axially. Thus, the higher momentum flux ratio locally predicted by LES results from its average underprediction of the axial gas velocity. Indeed, **Figure 4-4** shows that regardless of the condition, LES tends to predict a significantly lower gas velocity in the windward spray region, which is where the phase interaction is initially at its highest due to the jet penetrating the gas flow field.

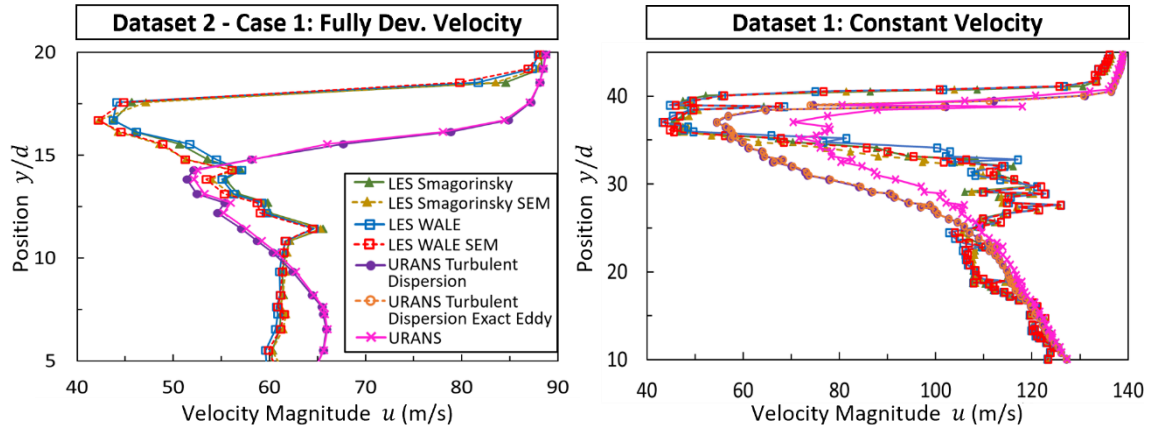


Figure 4-4: Centreline gas velocity profile at $x/d = 33$ predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

For liquid jets in crossflow, the vertical component of the droplet velocity dominates its axial component u_{p_x} near the injection point ($u_{p_y}/u_{p_x} > 1$), which helps the jet penetrate the crossflowing gas flow field. LES predicts that the droplets conserve their vertical velocity on a longer axial distance ($x/d \leq 15$) for the higher jet velocity u_{jet} conditions of Madabhushi et al. [30], which enhances their vertical penetration. While the droplets exchange momentum with the continuous phase, u_{p_x} increases and becomes more important than the vertical component ($u_{p_y}/u_{p_x} < 1$). Regardless of the conditions, LES tends to predict a reduced influence of u_{p_x} especially in the near-field region, which also facilitates the vertical penetration of the droplets. This is due to LES underpredicting the droplet axial velocity in the region where the phases interact most together. Indeed, it can

be observed in **Figure 4-5** that LES predicts u_{p_x} to decrease significantly in the spray core and windward region at transverse distances where URANS predicts the opposite.

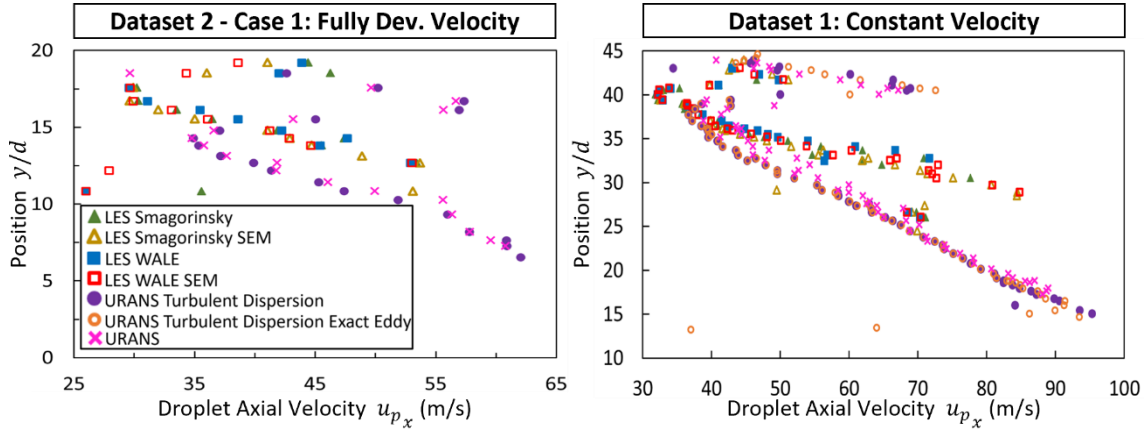


Figure 4-5: Centreline droplet axial velocity profile at $x/d = 33$ predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

4.5.1.2 URANS Compared to LES: SMD Predictions

Regardless of the experimental conditions, **Figure 4-6** shows that LES tends to predict a smaller SMD than URANS in the leeward and spray core regions because of its local overprediction of the continuous phase velocity presented in **Figure 4-4**. This is due to the flow field adapting itself to compensate for the significant decrease in velocity occurring at the higher transverse distance. Although this causes the local particle axial velocity to also increase as shown in **Figure 4-5**, the change is not as important. Thus, LES tends to predict a higher particle slip velocity in the leeward and spray core regions, which locally enhances the breakup process and reduces the SMD.

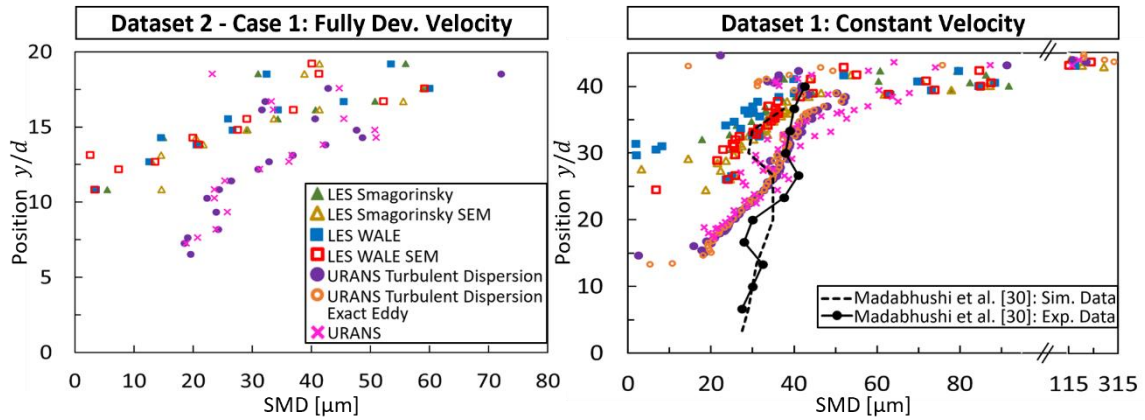


Figure 4-6: Centreline SMD at $x/d = 33$ predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

In addition, LES tends to predict a higher SMD in the windward region due to its local underprediction of the continuous phase velocity. This causes the droplet axial velocity to decrease to values close to those of the gas velocity. As a result, LES tends to predict a locally lower slip velocity that reduces the breakup process, hence the higher SMD observed.

Regarding the accuracy of the predictions, it is possible to observe that LES and URANS tend to underpredict the SMD in the leeward region compared to the data from Madabhushi et al. [30]. LES also tends to underpredict it in the spray core region, which agrees with what has been reported in the literature regarding the SSD model [33, 34, 172]. However, the current methodology combined with the URANS turbulence approach achieves better agreement with the data in the spray core region as the average error is less than 4%. Moreover, as the transverse distance increases, the Madabhushi breakup model underpredicts the SMD which agrees with the current LES predictions. Further studies should be done on the effect of coupling a collision and coalescence model with the presented numerical methodology to improve the SMD predictions in the wake region behind the jet.

The current numerical methodology also tends to predict a higher maximum and minimum droplet transverse location compared to the experimental data of Madabhushi et al. [30]. This agrees with the previously described overpredicted maximum trajectory compared to the experimental correlation from Freitag and Hassa [109]. Thus, it is possible to conclude that the SSD breakup model tends to overpredict the spray trajectory and underpredict the vertical dispersion for jets in crossflow. This could be due to an overall underestimation of the aerodynamics effects on the jet column bending, the turbulent interactions or the momentum transfer. Considering that most of these processes occur in the near-field region, future work should be done to study the effect of coupling the current approach with a locally higher fidelity model for turbulent jets in crossflow.

4.5.1.3 URANS Compared to LES: Effect of Momentum Exchange on Predictions

As previously discussed, the higher jet trajectory and lower SMD predicted by LES are both related to lower velocity predictions. Regardless of the conditions, LES underpredicts the droplet axial velocity because it tends to predict a lower net exchange of axial momentum as seen in **Figure 4-7**. Thus, the droplets receive less axial momentum

from the continuous phase, which could be caused by the locally lower axial velocity of the latter compared to URANS, as shown in **Figure 4-4**.

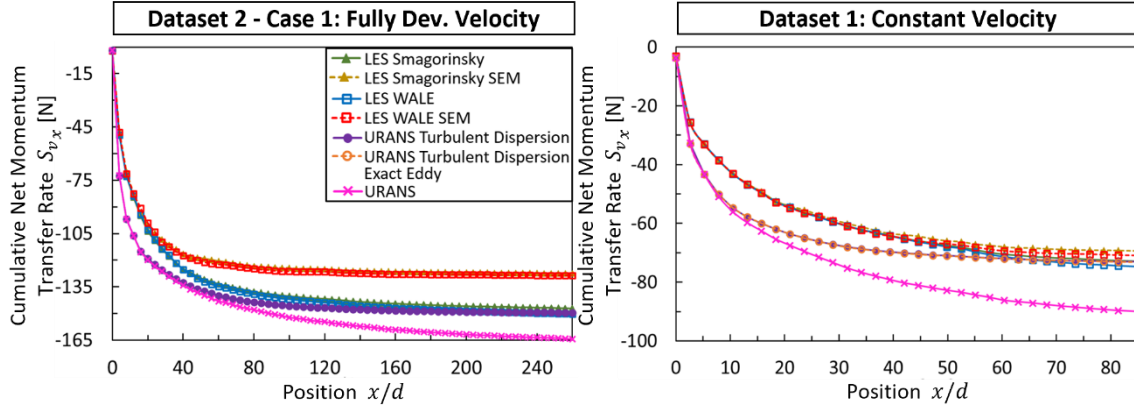


Figure 4-7: Cumulative net transfer rate of axial momentum predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

Figure 4-8 shows that LES also tends to underpredict the net exchange of vertical momentum S_{vy} transferred from the droplets to the continuous phase. This explains why LES tends to predict that they conserve their vertical velocity component on a longer axial distance. For the conditions of Freitag and Hassa [109], this causes LES to overpredict u_{py} , which contributes to enhancing its local momentum flux ratio and maintaining it higher than the one predicted by URANS along the domain.

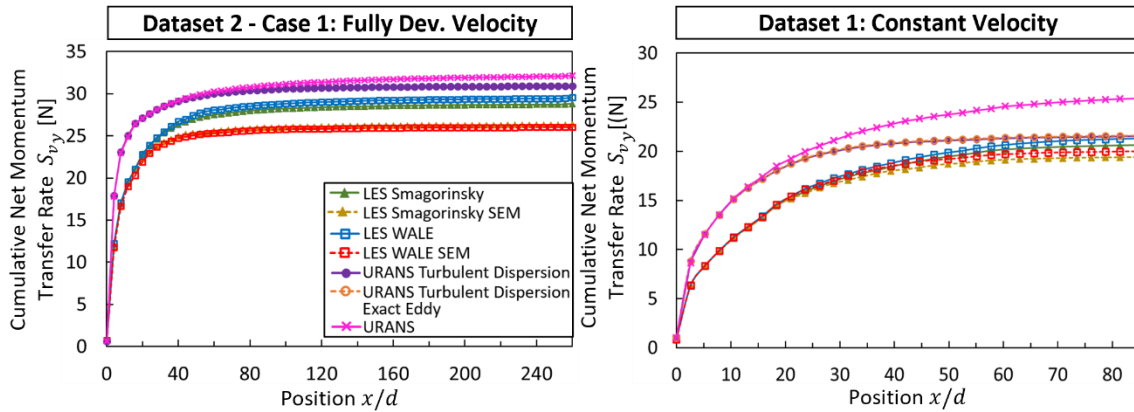


Figure 4-8: Cumulative net transfer rate of vertical momentum predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

It is also possible to observe that the total net momentum transfer for URANS and LES mostly occurs in the near-field region as 80% of it is exchanged before $x/d = 30$.

Afterwards, the exchange of axial momentum is mostly governed by the turbulent characteristics of the flow field. Thus, it is possible that LES tends to underpredict the net exchange of axial momentum because of an underprediction of the turbulent interactions. The continuous phase would then have less axial momentum to transfer due to its resulting lower axial velocity, as previously shown in **Figure 4-4**.

4.5.1.4 URANS Compared to LES: Effect of Turbulent Interactions on Predictions

Regardless of the experimental conditions, LES tends to predict significantly smaller turbulent interaction times across the entire spray as seen in **Figure 4-9**. In the near-field region, they are in the same order of magnitude as URANS up to $x/d = 10$ and $x/d = 30$ for the conditions of Freitag and Hassa [109] and Madabhushi et al. [30] respectively. As previously discussed, there are no significant differences in maximum spray trajectories in these regions. As the droplets travel through the turbulent flow field, URANS predicts that the turbulent interactions increase as expected. This is not the case for LES as there are no comparable changes in τ_l . As a result, LES tends to predict τ_l values multiple orders of magnitude lower than URANS. Thus, it is possible to conclude that the maximum spray trajectory increases when the turbulent interactions decrease as it allows the droplets to further penetrate the turbulent flow field downstream of the injection point.

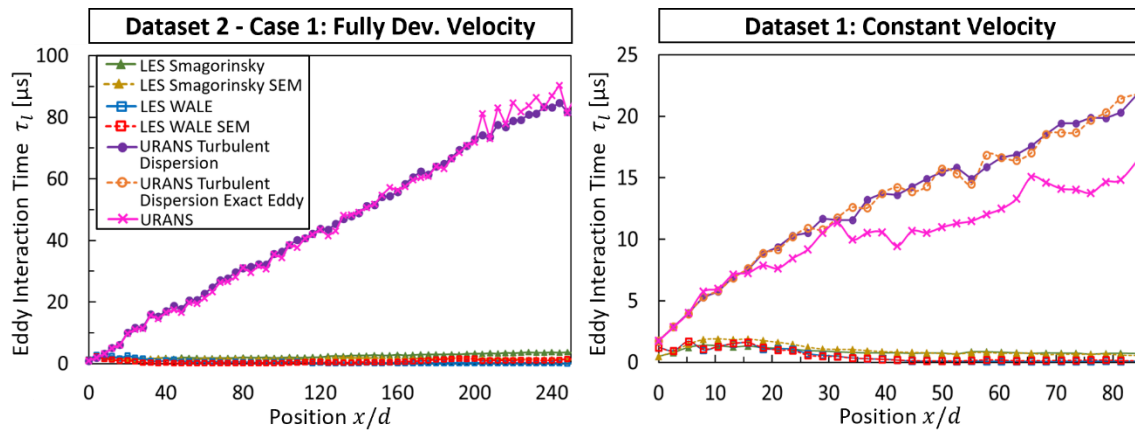


Figure 4-9: Eddy Interaction Time predicted by different turbulence modelling approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

The lower turbulent interactions predicted by LES could also be facilitating the radial dispersion of the droplets. This might explain why the spray width tends to be larger on average by 19% and 226% compared to URANS for the conditions of Madabhushi et al.

[30] and Freitag and Hassa [109] respectively. The higher relative difference for the latter further supports the previous observations regarding the sensitivity of the URANS approach to the boundary conditions.

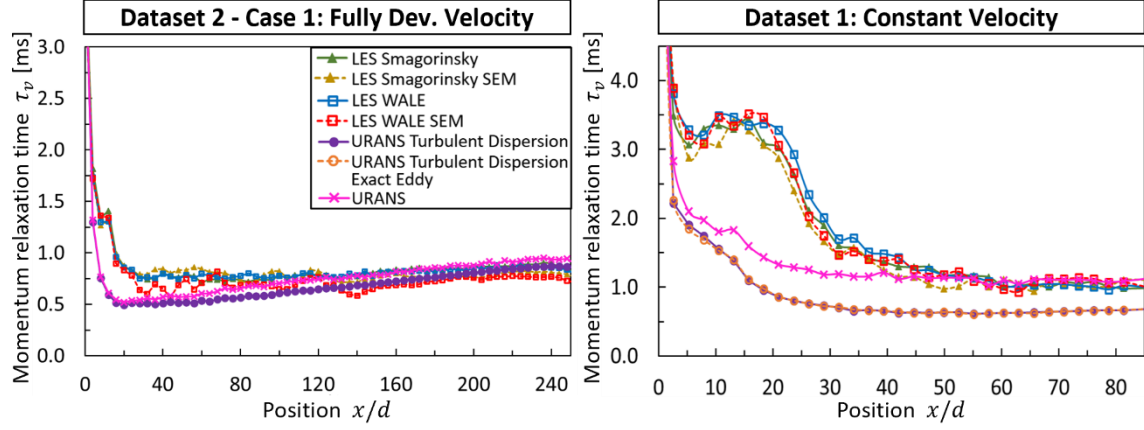


Figure 4-10: Momentum relaxation time predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

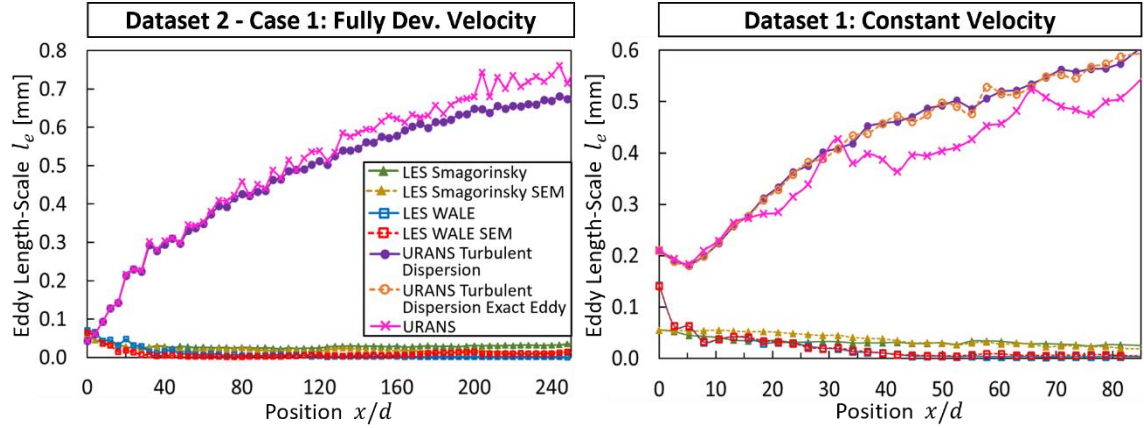


Figure 4-11: Eddy Length-scale predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

For all the simulations, the turbulent interactions are predicted to be governed by the eddy transit time τ_c . This means that the droplets are predicted to have a slip velocity strong enough to pass through the turbulent eddies [180]. As presented in equation (4-22), τ_c decreases with a decreasing eddy length scale and with an increasing momentum relaxation time and particle slip velocity. As seen in **Figure 4-10**, LES tends to predict a higher momentum relaxation time in the primary breakup region, but no significant differences are predicted in the far-field region. Regarding the average particle slip velocity, although LES tends to predict it higher by 8% compared to URANS in the

secondary breakup region for the dataset of Madabhushi et al. [30], it predicts it lower by 13% in the near-field region. Moreover, there are no significant differences predicted in u_s for the dataset of Freitag and Hassa [109] in the far-field region and LES also tends to predict it lower by 15% in the near-field region. Thus, the lower eddy length scale predicted by LES is likely the main factor behind its lower eddy transit time, as shown in **Figure 4-11**. This is even more plausible considering that l_e is also underpredicted by multiple orders of magnitudes except in the primary breakup region, similar to τ_l .

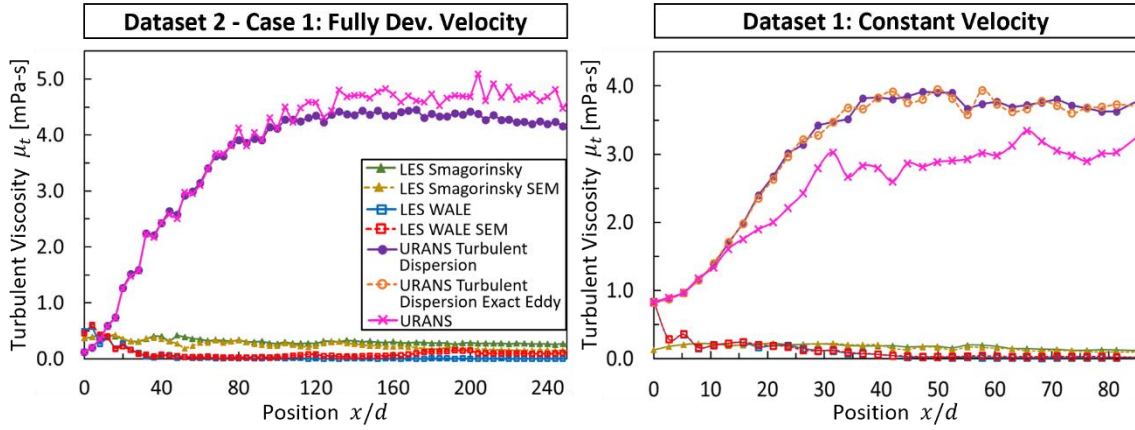


Figure 4-12: Turbulent viscosity predicted by different turbulence approaches using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

As presented in equation (4-23), the eddy length scale decreases proportionally with the turbulent viscosity and for an increasing turbulent kinetic energy. For the conditions of Freitag and Hassa [109], the latter predicted by LES contributes to reducing l_e as it is on average almost 2.5 times the values predicted by URANS. However, it's the opposite for the conditions of Madabhushi et al. [30] as LES tends to predict the turbulent kinetic energy smaller by 23% on average. As seen in **Figure 4-12**, regardless of the conditions, LES tends to predict a significantly smaller μ_t values, especially in the secondary breakup region as it becomes multiple orders of magnitude lower than URANS. Indeed, LES predicts μ_t to be on average smaller by 83% and 91% compared to URANS for the conditions of Freitag and Hassa [109] and Madabhushi et al. [30] respectively. Moreover, URANS is able to capture the expected axial evolution of μ_t as it increases until its value stabilizes with the turbulent length scale. Therefore, it is possible to conclude that the lower turbulent viscosity field that LES tends to predict may result in less turbulent kinetic energy being transferred to the discrete phase, allowing the droplets to penetrate further into the domain. This would also explain the trends observed in SMD predictions.

Moreover, the lower axial velocity of the continuous phase predicted by LES could be due to an underprediction of the filtered stress tensor applied to its filtered momentum and energy transport equations since it's proportional to μ_t .

The LES approach resolves directly on the numerical grid the turbulent large-scale motions and accounts for the effects of the subgrid-scale motions on the large scale through a SGS model [177, 190]. The filtering of the small scales means that the effects of the associated velocity fluctuations are not accounted for in the computation of the continuous phase velocity [179, 190, 191]. The LES approach alone can be considered sufficient to capture the turbulent dispersion if the portion caused by the unresolved smaller-scale motions is negligible [178]. However, this does not apply when the local flow conditions of the physical processes modelled are strongly influenced by the velocity gradient tensor or when large Reynolds numbers are used, such as with turbulent liquid jets [177, 179, 190, 191]. In fact, neglecting the contribution of the unresolved velocity field when using LES with the Lagrangian approach has been reported to underpredict the droplet turbulent dispersion [177, 190, 191]. Thus, the conclusions of the present study regarding LES agree with what has been reported in the literature for coflowing sprays. Indeed, other studies have also observed that it results in lower exchange rates between the phases, an overprediction of the liquid penetration length, a smaller gas entrainment and an overall increase in discrepancies with the experimental data [177, 192, 193]. To improve the accuracy of the predictions of the LES approach for turbulent liquid jets in high-speed crossflow, additional modelling is recommended to account for the subgrid-scale Lagrangian velocity field as suggested by other studies conducted for coflowing sprays [177, 190, 191].

4.5.2 LES: Effect of SGS and SEM

It is possible to observe in the previous section that the SGS models and SEM predict similar droplet and gas velocities, SMD and spray trajectory regardless of the conditions. This is due to their similar predictions of turbulent interactions and net exchange of momentum. However, for the dataset of Freitag and Hassa [109], although the spray widths predicted using both SGS models also tend to agree together when coupled with the SEM, using the latter results in a 31% increase. This indicates that the effect of the SEM on the spray characteristics is sensitive to the conditions.

4.5.3 URANS: Effect of Turbulent Dispersion Model

The effect of the turbulent dispersion model is assessed by comparing the URANS predictions with and without it, which are included in the Figures of *section 4.5.1*. For the conditions of Freitag and Hassa [109], it does not have a significant impact on most spray characteristics as it predicts a similar droplet and gas velocity, SMD and spray trajectory. This is due to its insignificant impact on the net exchange of momentum and turbulent interactions.

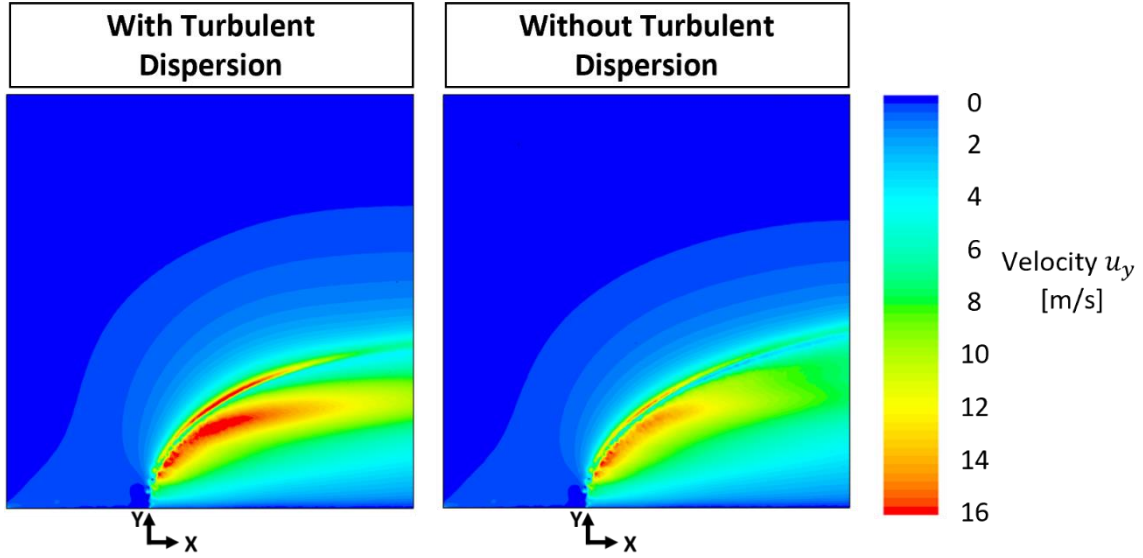


Figure 4-13: Continuous phase vertical velocity predicted by URANS with (left) and without (right) the turbulent dispersion model using the dataset from Madabhushi et al. [30].

For the low pressure and high moment flux ratio conditions of Madabhushi et al. [30], the turbulent dispersion model has a significant impact on the spray characteristics predicted in the far-field region. As seen in **Figure 4-2**, it locally reduces the overpredicted spray trajectory by at least 8% due to a 28% average decrease in the local momentum flux ratio. As seen in **Figure 4-7** and **Figure 4-8**, using the turbulent dispersion model increases the rate at which the total net momentum is exchanged since 80% of it occurs before $x/d = 15$. This indicates that the particles transfer most of their vertical momentum to the continuous phase earlier in the domain. This is illustrated in **Figure 4-13** by the higher gas vertical velocity u_y predicted when using the turbulent dispersion model. Thus, u_{p_y} tends to be smaller in the secondary breakup region and leads to lower J_{local} .

The differences in spray characteristics observed in the secondary breakup region for the conditions of Madabhushi et al. [30] can be attributed to the lower turbulent interactions predicted when the turbulent dispersion is not accounted for. Indeed, **Figure 4-9** shows that it results on average in a 21% decrease in turbulent interaction time above $x/d = 15$. This can be attributed to the local 20% average decrease in turbulent viscosity shown in **Figure 4-12**. Similar to LES, the lower turbulent interactions predicted without the turbulent dispersion model locally increase the discrepancies in spray trajectory compared to the experimental data. Considering that this does not occur for the conditions of Freitag and Hassa [109], not accounting for the turbulent dispersion might cause the URANS turbulence approach to be more sensitive to the boundary conditions.

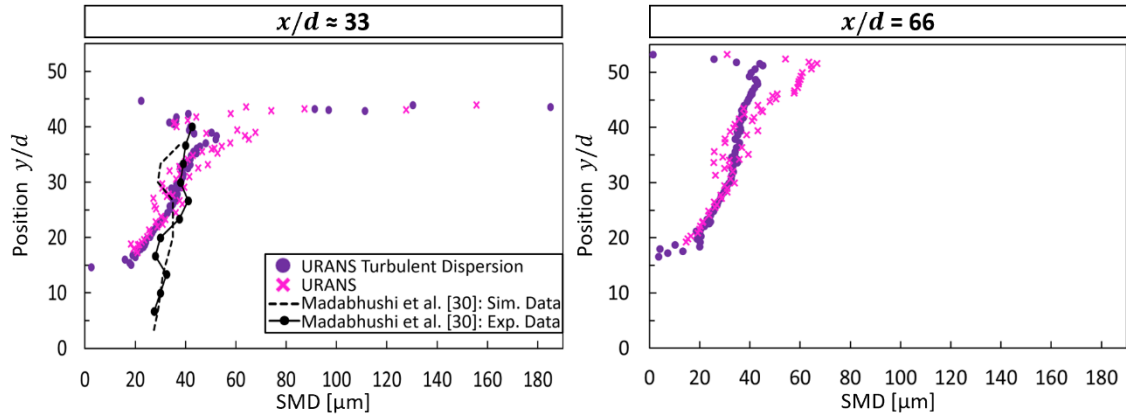


Figure 4-14: Centreline SMD at $x/d = 33$ (right) and $x/d = 66$ (left) predicted by URANS with and without the turbulent dispersion model using the dataset from Madabhushi et al. [30].

Regardless of the conditions, the turbulent dispersion model does not have a significant impact on the SMD in the leeward and spray core region as seen in **Figure 4-6**. The underprediction of the SMD in the leeward region agrees with what has been reported by other URANS numerical studies conducted on the SSD model [170]. However, using the turbulent dispersion model for the conditions of Madabhushi et al. [30] tends to improve the accuracy in the windward region as it reduces the SMD. For all the simulations conducted, the SMD increases with the transverse distance, which indicates that the breakup process is concentrated in the leeward and spray core region. As the droplets travel through the domain, the SMD tends to change less in those regions due to their sizes no longer meeting the critical radius r_{crit} required for breakup imposed by the SSD model. Thus, the secondary breakup process is predicted to mostly occur in the windward

region. Because the rate of momentum exchange in the secondary breakup region decreases significantly without the turbulent dispersion model, the breakup process in the windward region takes a longer axial distance to be completed. Indeed, **Figure 4-14** shows that the discrepancies in the windward region increase with the axial distance due to the SMD still being significantly overpredicted without the turbulent dispersion model.

Regardless of the conditions, using the turbulent dispersion model increases the spray width. For the high-pressure conditions of Freitag and Hassa [109], it enhances the radial diffusion to levels comparable to LES without the SEM. For the lower pressure conditions of Madabhushi et al. [30], it predicts the largest spray width as it increases on average by 45% compared to LES. Additional experimental studies on the radial diffusion of turbulent jets in crossflow at high pressures and momentum flux ratios are needed to evaluate the accuracy of the spray widths predicted.

The effect limiting the parcel time-step δt_p to sum up to the exact eddy interaction time when using the turbulent dispersion model was assessed with the dataset from Madabhushi et al. [30]. As shown in **Figure 4-7**, **Figure 4-8** and **Figure 4-9**, it does not have any significant impact on the net exchange of momentum or turbulent interactions. This explains why no significant differences could be observed in terms of droplet and gas velocities, SMD, spray trajectory and width. This indicates that the strategy used to limit δt_p allows to capture the turbulent interactions that affect the spray characteristics the most. Considering the higher computational cost of using the exact eddy interaction time sub-model, it is recommended to estimate the Lagrangian courant numbers with the strategy described in *section 4.4.3* and to impose a Co_{min} value as small as possible.

4.5.4 Velocity Profile Sensitivity: LES

The sensitivity of the LES approach to the inlet velocity profile was assessed using case 1 from Freitag and Hassa [109] with a constant velocity profile. It is possible to conclude from **Figure 4-15** that the tendency of LES to overpredict the spray trajectory is independent of the velocity profile. Indeed, using a constant velocity profile increases the average relative error to 33%.

The tendency of LES to predict a lower SMD in the spray leeward and core regions is also independent of the velocity profile. This is also true for the local SMD values predicted. However, LES tends to predict a significant increase in SMD at the highest transverse distance when using a constant velocity profile. This agrees with the predictions made by URANS and LES for the conditions of Madabhushi et al. [30] as seen in **Figure 4-6**. Considering they both use a constant velocity profile, it could indicate that the accuracy of the near-field region breakup process predicted by LES at the highest interface is more sensitive to changes in the local velocity field.

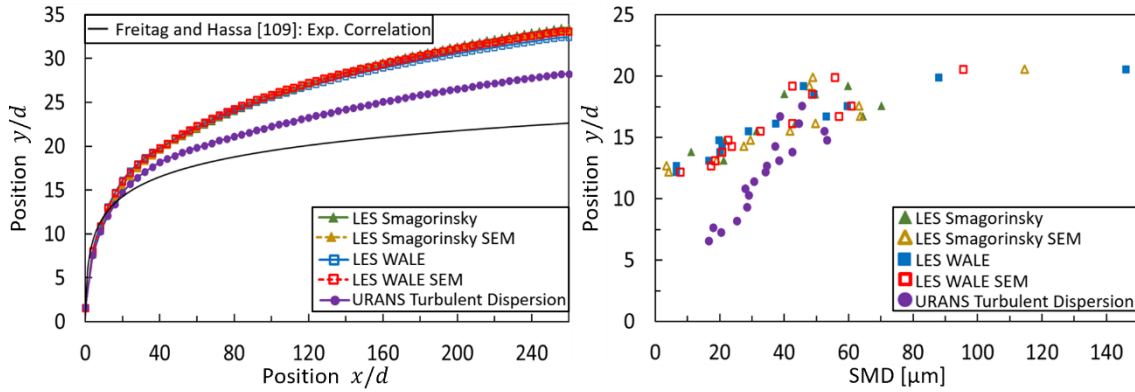


Figure 4-15: Maximum spray trajectory and centreline SMD at $x/d = 33$ predicted by different turbulence approaches using case 1 from Freitag and Hassa [109] for a constant velocity profile.

These results can be explained by the same factors previously described for the dataset of Madabhushi et al. [30] and Freitag and Hassa [109] with a fully developed velocity profile. Indeed, the eddy interaction time and total net transfer rate of momentum across the entire spray predicted by LES are also lower, on average by 84% and 16% respectively compared to URANS with the turbulent dispersion model. Thus, it can be concluded that LES tends to underpredict these important parameters of the phase interactions regardless of the velocity profile.

It is also possible to conclude that regardless of the velocity profile, the SEM and the SGS model do not have a significant impact on the spray characteristics, except for the spray width at the higher-pressure conditions of Freitag and Hassa [109]. Indeed, the SEM tends to predict larger spray widths that agree together regardless of the velocity profile. Moreover, using a constant velocity profile tends to increase the spray width predicted except for the Smagorinsky SGS model used without the SEM where the opposite occurs.

As a result, the latter tends to predict a spray width on average 41% smaller than the WALE SGS model. Thus, the spray widths predicted without the SEM do not agree together when using a constant velocity profile. This indicates that the radial dispersion predicted by the Smagorinsky SGS model might be sensitive to the continuous velocity field for turbulent jets in crossflows, which corroborates previous findings available in the literature for coflowing sprays [33, 34].

4.5.5 Velocity Profile Sensitivity: URANS

The sensitivity of the URANS turbulence approach to the inlet velocity profile was only studied with the turbulent dispersion model as it showed the best agreement with the data as discussed in *section 4.5.3*. Regardless of the conditions or turbulence approach, assuming a constant velocity profile tends to increase the spray jet trajectory. Indeed, the error with the experimental data from Freitag and Hassa [109] in the far-field region increases to 25% as seen in **Figure 4-15**. The difference is less significant for the dataset from Madabhushi et al. [30] as it only increases the trajectory by a maximum of 4%. This indicates that the numerical approach might be less sensitive to higher jet velocities if the gas velocity is also high. Therefore, it can be concluded that the dispersed phase is sensitive to small changes in the gas velocity field regardless of the turbulence approach, but the importance of the resulting discrepancies might depend on the boundary conditions. These results emphasize the importance of accounting for the gas velocity profile.

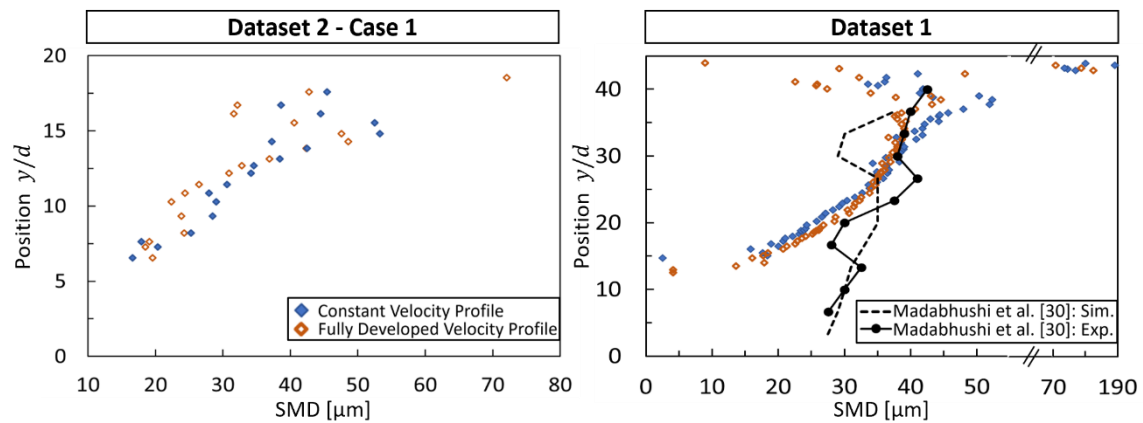


Figure 4-16: Centreline SMD at $x/d = 33$ predicted with the turbulent dispersion model obtained using the dataset from Freitag and Hassa [109] case 1 and Madabhushi et al. [30].

Regardless of the conditions or turbulence approach, using a constant velocity profile tends to increase the SMD predicted in the windward region as seen in **Figure 4-16**. This is due to the higher gas velocity field that the droplets in the windward region are subjected to when using a fully developed velocity profile. Indeed, this results in a higher u_s which locally enhances the breakup process. For the conditions of Freitag and Hassa [109], this effect can also be observed in the leeward and spray core regions. Thus, the sensitivity of the SMD to the velocity profile might also depend on the boundary conditions. This aspect is further studied in *section 4.5.6*. Further studies could be done to improve the SMD predictions by coupling some aspects of the SSD model, such as the particle-size distribution, with the Madabhushi breakup model, which uses a root-normal distribution dependant on the parent droplet size [30].

4.5.6 Boundary Conditions Sensitivity: URANS

The sensitivity of the numerical methodology developed to the boundary conditions was further assessed with both velocity profiles using the datasets from Freitag and Hassa [109]. This study was limited to the turbulent dispersion model for the same reasons stated in *section 4.5.5*. Regardless of the velocity profile, increasing the pressure does not tend to have a significant impact on the predictions as seen in **Figure 4-17**. Indeed, increasing P_g from 4 to 8 bar with a constant J of 6 causes a 3% absolute decrease in the relative error with the experimental data for both velocity profiles. Thus, the lower discrepancies observed previously with the dataset of Madabhushi et al. [30] are more likely caused by its higher momentum flux ratio.

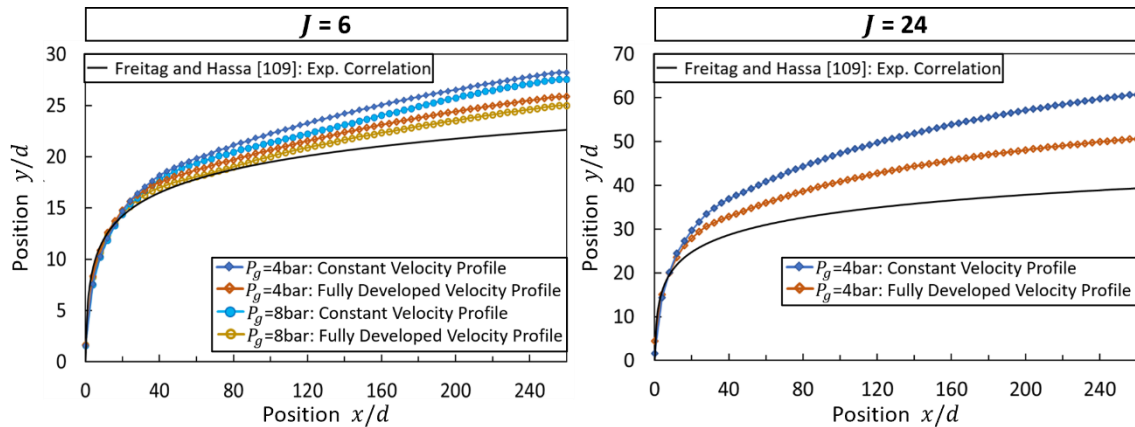


Figure 4-17: Maximum trajectory predicted with the turbulent dispersion model obtained for constant and fully developed velocity profile using the datasets from Freitag and Hassa [109].

Moreover, the slightly lower trajectories predicted at the higher-pressure conditions indicate that the numerical methodology accounts for the pressure effects on the spray characteristics. Although some experimental correlations for jets in crossflow at standard temperature and high-pressure consider the trajectory to be independent of P_g [e.g. 109, 121], others consider that it decreases with an increasing pressure [e.g. 48, 99]. The ability of the numerical methodology to capture the pressure effects was expected since the SSD model has been validated for pressures up to 50 bar although for coflowing gas [33, 34]. Thus, the present work suggests that the SSD model is also suitable for predicting the trajectory of jets in crossflow under high-pressure conditions up to 8 bar.

Regardless of the velocity profile, the numerical methodology tends to be sensitive to higher jet velocities. Indeed, increasing J from 6 to 24 with a constant P_g of 4 bar causes the average relative error to increase from 8% to 21% and from 16% to 40% with a fully developed and constant velocity profile respectively. However, this does not indicate that the numerical methodology studied is not suitable for high momentum flux ratios. In fact, the momentum flux ratios from the datasets of Freitag and Hassa [109] are lower than the one from Madabhushi et al. [30] as shown in **Table 4-1**. Despite this, the SMD predicted tends to agree well with the data and the jet trajectory is less sensitive to local changes in velocity. The main difference between both datasets lies in the imposed jet to crossflow gas velocity ratio, which is significantly lower for Madabhushi et al. [30] ($u_{jet}/u_g \approx 0.22$) compared to the highest momentum flux ratio condition (case 2) from Freitag and Hassa [109] ($u_{jet}/u_g \approx 0.37$) as seen in **Table 4-1**. A higher u_{jet}/u_g ratio indicates that the droplets conserve their vertical momentum on a longer axial distance, which enhances their ability to penetrate the continuous phase due to the resulting higher droplet velocity ratio u_{p_y}/u_{p_x} .

Figure 4-18 shows that the discrepancies in spray trajectory with the experimental correlation tend to increase with the imposed u_{jet}/u_g ratio. Indeed, case 2 has the highest u_{jet}/u_g ratio imposed and highest relative error, followed by case 1. The behaviour of case 3 indicates that high-pressure conditions reduce the sensitivity to the imposed u_{jet}/u_g ratio. Moreover, for a given u_{jet}/u_g ratio, the droplet velocity ratio remains high on a longer axial distance with a constant velocity profile which reduces the accuracy. Thus, the numerical methodology seems to be more sensitive to the imposed jet to gas

velocity ratio than to the momentum flux ratio. This corroborates the findings of Nihasigaye et al. [170] that the predictive capabilities of the SSD model with the URANS approach tend to be sensitive to an increase in maximum droplet velocity. Future work should be done to reduce the sensitivity of the SSD model's predictive capabilities to the imposed velocities.

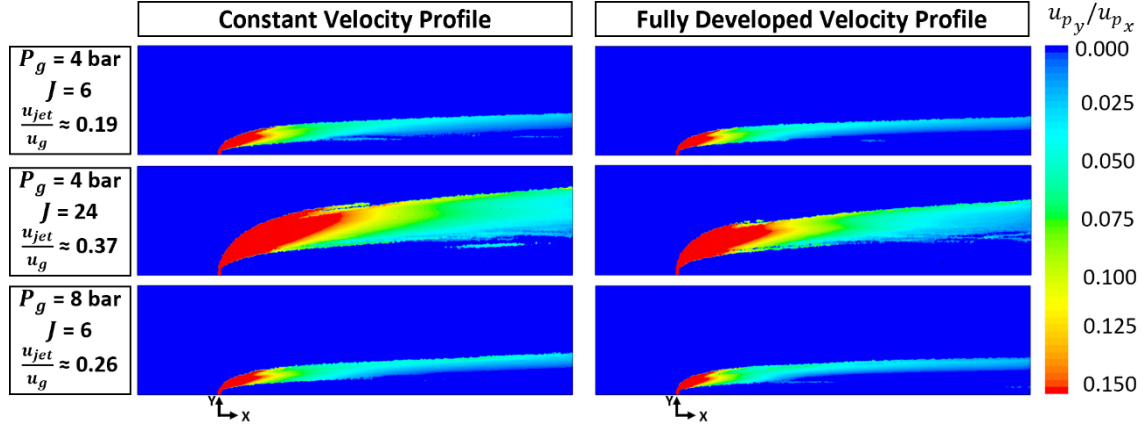


Figure 4-18: Droplet velocity ratio predicted with the turbulent dispersion model obtained using the datasets from Freitag and Hassa [109] case 1 (top), case 2 (middle), case 3 (low).

4.6 Conclusion

In summary, an unsteady numerical methodology using the SSD breakup model combined with TAB distortion model was validated and the effects of different turbulence approaches were assessed for turbulent liquid fuel jets in high-speed crossflow. Good agreement with the experimental data was achieved with URANS for the SMD and spray trajectory at standard and high pressures over a wide range of momentum flux ratios and gas Weber numbers. Coupling the methodology with the turbulent dispersion model is recommended as it was shown to improve the predictions regardless of the conditions or inlet velocity profile. The strategy used to determine the values of the Lagrangian courant numbers is also recommended as it captures the turbulent interactions to a level similar to the Exact Eddy Time sub-model but at a lower computational cost. To improve the predictions, future work should be done on coupling the SSD model with higher fidelity models in the primary breakup region.

Regardless of the experimental conditions or inlet velocity profile, LES used with the standard subgrid-scale models tends to predict higher discrepancies with the experimental data. Indeed, it was shown to overpredict significantly the spray trajectory as well as

underpredict the SMD in the leeward and spray core regions. This might be caused by its tendency to predict a lower turbulent viscosity field, which results in lower turbulent interactions and lower momentum exchanges. In addition, the Synthetic Eddy Method is not deemed worth the extra computational cost due to its insignificant impact on the predictions. The present study recommends using the WALE SGS model over the Smagorinsky SGS model since the latter was shown to be more sensitive to local changes in the velocity field. However, in order to use LES as a robust numerical tool to hasten the delivery of new sustainable technologies, its coupling with the Lagrangian approach needs to be improved. Future work should be done on assessing the impact of coupling LES with a stochastic turbulent dispersion model and of using a SGS model that accounts for the droplets' sub-filtered acceleration as described in Gorokhovski and Oruganti [179] and references therein.

This study also concludes that regardless of the turbulence approach used, proper consideration of the upstream gas velocity profile is essential to accurately predict the spray characteristics for turbulent jets in crossflow. This is especially important when trying to validate and calibrate numerical models as the predictions were shown to be sensitive to changes in the velocity field.

4.7 Acknowledgments

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5 Validation And Assessment of a Hybrid VOF-Lagrangian Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow

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5.1 Abstract

For gas turbine combustors, injecting liquid fuel in crossflow can achieve superior mixing characteristics to improve performance and reduce emissions. Robust numerical design tools are needed to accelerate the development of low-emission technologies. Atomization modelling is often facilitated by using the Lagrangian approach rather than the more complex and computationally expensive Volume-of-Fluid (VOF) approach. However, most Lagrangian breakup models rely on empirical constants that must be fully calibrated for jets in crossflow and representative conditions. A hybrid approach could deliver a better compromise between accuracy and computational cost.

This study proposes and validates a novel numerical methodology for coupling the VOF and Lagrangian approaches using a stochastic breakup model with Adaptive Mesh Refinements (AMR) for turbulent liquid fuel jets in crossflow under more representative gas turbine conditions. The predictions were validated in the near and far-field regions using datasets at high pressures (1-8 bar), gas Weber numbers (720-1172) and momentum flux ratios (6-33). The predictive capabilities and computational cost were also compared to the Lagrangian approach coupled with LES and with the unsteady RANS methodology previously developed and validated by the authors. The effect of different VOF-Lagrangian transition criteria on the computational cost were also assessed and recommendations were provided for further improvements. The overall LES predictions were significantly improved by the proposed hybrid methodology. Although it tends to underpredict the spray trajectory and Sauter Mean Diameter (SMD) compared to the URANS methodology, it better captures the diameter in the wake region and the droplet velocities.

Keywords: CFD; Lagrangian; Volume of Fluid; Turbulent; Liquid fuel; Crossflow; Atomization; Gas Turbine.

5.2 Introduction

Environmental concerns have been addressed by various legislative bodies by setting highly ambitious targets to reduce emissions, in particular CO, CO₂ and NO_x, for both stationary and aero gas turbines. This implies the need to develop more sustainable combustion technologies that allow better control of the combustion process. Advanced mixing technologies improve the uniformity of the fuel-air mixture to reduce emissions. For low-emission gas turbine combustion systems with liquid fuel sprays, superior mixing characteristics can be achieved by using a crossflow configuration to enhance the spray breakup and evaporation processes as well as through the turbulent flow characteristics [5, 6]. Considering the significant influence of the spray characteristics on the combustion process [5], their accurate predictions are needed to facilitate the development and hasten the delivery of such advanced low-emission technologies. The VOF approach has the ability to capture the important breakup characteristics of jets in crossflow, such as the jet column bending and column stripping. Due to its high computational cost, the lower-fidelity Lagrangian approach, which uses breakup models, is often preferred instead to guide the design of novel injectors.

The breakup models' accuracy is expected to depend on the injector properties as they impact the atomization process [14, 28]. To the best knowledge of the authors, only a few breakup models were specifically developed to account for the particularities of jets in crossflow [29]. However, they use empirical correlations or deterministic breakup models. Indeed, to predict surface stripping, the Madabhushi breakup model [30] uses the Kelvin-Helmholtz (KH) breakup model [149]. Although many others [29, 31, 32] use the Boundary-Layer-Stripping (BLS) model [156] instead, they all rely on empirical correlations to predict the column breakup and the characteristics of the droplets being shed [29, 30, 31, 32]. They also rely on deterministic breakup models for the secondary breakup process, either based on Rayleigh-Taylor instabilities (RT model [152]) [30, 32] or on Taylor's Analogy Breakup model (TAB model [151]) [29] associating an oscillating droplet to a damped spring-mass system. Therefore, to the best knowledge of the authors, the models currently available in state-of-the-art Computational Fluid Dynamics (CFD)

to model jets in crossflow all possess empirical constants and correlations that need to be calibrated using experimental data to yield accurate predictions [5, 14]. Moreover, most of these models were not developed for flow conditions beyond the shear breakup regime [29, 31, 32]. Thus, they are also not deemed likely suitable for the higher turbulence levels of gas turbines even if some of them were validated at representative pressures and Weber numbers [31, 32].

To optimally use CFD as a design tool, the accuracy of the numerical models should ideally not depend on having prior knowledge of the injector's performance through experimental data. Therefore, the present study focuses on developing a numerical methodology that requires minimal calibration and that is suitable for representative gas turbine conditions. This could potentially be achieved by using the VOF approach to model the primary breakup coupled with the Lagrangian approach for the secondary breakup to reduce the computational cost. The Stochastic Secondary Droplet (SSD) breakup model is selected for the Lagrangian approach because its predictive capabilities depend more on the local flow conditions and less on empirical model constants [33, 34]. Another advantage of the SSD breakup model comes from its use of Kolmogorov's stochastic theory [33], which allows capturing the turbulent effects and catastrophic breakup regime. Because these processes play an important role in the atomization of sprays under high gas Weber numbers [33, 34], the SSD model is deemed more suitable for gas turbine applications compared to those previously described. Although a few studies have assessed its suitability for jets in crossflow, more validation work is needed as they were mostly conducted using water at low pressures and low Weber numbers [35, 36, 37]. A recent parametric study conducted by the authors showed its good predictive capabilities for turbulent liquid fuel jets in crossflow under more representative conditions [42], but improvements are still needed for the overall droplet velocities and Sauter Mean Diameter (SMD) in the leeward spray region.

Most studies conducted with a hybrid approach for jets in crossflow focused on investigating the primary atomization process [25, 36, 39], where it is challenging to obtain good measurements due to the locally higher density and droplet concentration [25, 39, 49, 50]. Thus, some of them did not include any secondary atomization models [25, 39] considering the numerical modelling in the region of interest is mostly governed

by the interface-capturing method. They most likely used the hybrid approach as a lower-cost alternative to gain more insight into the primary breakup process instead of modelling the entire spray with the higher-fidelity approach, such as VOF. Among the few studies that focused on assessing its predictions, the validation was mainly limited to the near-field region ($x/d < 10$) [35, 36, 39, 40] and often only for the spray trajectory [35, 39] due to the reasons previously mentioned. Although a few studies validated its predictions in the secondary breakup region [40, 41], they used deterministic breakup models relying on empirical constants such as the Reitz-Diwakar model (RD model [153]) [40] and the TAB model [41]. Those conducted with the SSD breakup model [35, 36] only validated the predictions in the near-field region where the higher-fidelity approach dominates, as previously explained.

In addition to being limited to the near-field region, the spray trajectories were mostly validated for low gas Weber numbers ($We_g=10-554$) [35, 36, 39, 40] using either water at ambient pressure [35, 36] or non-turbulent jets [39, 40]. Moreover, the predictive capabilities in SMD were only assessed for non-turbulent jets ($Re_{jet}=22-3400$) at relatively low atomization levels ($We_g=11-554$, $J=6-12$) using either water or low pressures ($P_g=1-5$ bar) [40, 41]. Validation of the droplet velocity has also been limited to non-turbulent water jets at low atomization levels ($We_g=11-53$, $J=6-12$) under ambient conditions [41]. Thus, there is a need for further validation of the hybrid approach, especially in the far-field region, for turbulent jets in crossflow at more representative gas turbine conditions. There is also a need to better understand the impact on the far-field predictions of modelling the important jets in crossflow characteristics with the VOF approach.

The objective of this study is to provide accurate and computationally efficient design tools by assessing the predictive capabilities and computational cost of using a VOF-Lagrangian approach with a stochastic breakup model. To do so, high-fidelity Large Eddy Simulations (LES) using the Lagrangian approach with the SSD breakup model are performed with and without the VOF approach. Adaptive Mesh Refinements (AMR) is used to further reduce the computational cost of the proposed hybrid methodology for industrial research and development purposes. The predictions are compared to those obtained using the computationally less expensive numerical methodology previously

developed and validated by the authors [42, 43], which uses the Lagrangian approach with the unsteady Reynolds-Averaged Navier-Stokes (URANS) turbulence approach. The results are further compared to those obtained by Madabhushi et al. [30] using their developed breakup model as it was validated for turbulent fuel jets and high Weber numbers. Moreover, the effect on the computational cost of using different VOF-Lagrangian transition criteria is assessed.

This research also contributes to fill the gaps in knowledge on atomization modelling for jets in crossflow as the datasets selected allow to validate the predictive capabilities in SMD and droplet velocities at higher pressures, turbulence levels and atomization levels. The spray trajectories are also validated in both breakup regions under more representative conditions.

5.3 Governing Equations

The VOF approach [11] is a high-fidelity interface-capturing Eulerian method that resolves the large-scale interfaces between immiscible phases. Its high computational cost results from the fine mesh and small time-step sizes required to accurately resolve the interface. The lower cost of the Lagrangian approach is due to the discrete and statistical methods used to solve the governing equations for groups of particles with identical properties instead of tracking individual particles with unique properties [132]. The Lagrangian approach and related sub-models used in the present methodology have been described in detail in previous work [42, 43].

5.3.1 VOF Approach

The VOF approach uses the phase volume fraction α_i to capture the distribution and position of the interface. The following transport equation is solved to obtain the volume fraction of a single-phase. [11, 130]

$$\frac{\partial \alpha_i}{\partial t} + \nabla(\alpha_i u) = -\alpha_i \frac{D\rho_i}{Dt} - \frac{1}{\rho_i} \nabla(\alpha_i \rho_i u_{d,i}) \quad (5-1)$$

Where u is the mass-averaged velocity of the mixture, ρ_i is the density of phase i and $u_{d,i}$ is the difference between the phase and mixture velocities. The volume fractions from other phases are then calculated to ensure the total cell value sums up to 1. If $0 < \alpha_i < 1$,

the cell contains an interface and its density ρ and dynamic viscosity μ are obtained by weighting each phase properties with its volume fraction as seen below. [11, 130]

$$\rho = \rho_G \alpha_G + \rho_L \alpha_L \quad (5-2)$$

$$\mu = \mu_G \alpha_G + \mu_L \alpha_L \quad (5-3)$$

The incompressible Navier-Stokes equations for a single continuum are then solved using the calculated mixture properties with the following source term added to the right-hand side of the momentum conservation equation. [130]

$$S_\alpha = - \sum_i (\alpha_i \rho_i u_{d,i}) (u_{d,i})^T \quad (5-4)$$

The interactions between the VOF phases account for the surface tension force F_σ through the Continuum Surface Force (CSF) approach [194]. The surface tension force depends on the calculated mean curvature of the interface κ and the imposed surface tension σ . Its tangential $F_{\sigma,T}$ and normal $F_{\sigma,n}$ components are given by equation (5-5) and equation (5-6). A semi-implicit stabilization scheme is then used to treat $F_{\sigma,n}$ as a body force in the momentum conservation equation.

$$F_{\sigma,n} = \sigma(\nabla \alpha_i) \kappa = \sigma(\nabla \alpha_i) [-\nabla \cdot (\nabla \alpha_i / |\nabla \alpha_i|)] \quad (5-5)$$

$$F_{\sigma,T} = |\nabla \alpha_i| (\nabla \sigma)_T \quad (5-6)$$

For jets in crossflow, maintaining a sharp interface is important to capture column stripping and breakup. The VOF approach's ability to capture and resolve a sharp interface depends on the mesh resolution and convective discretization scheme used for the volume fraction transport equation. For the latter, the High-Resolution Interface Capturing (HRIC) convection scheme is used with a 1st order face density reconstruction [195]. The convective term of the VOF transport equation is discretized according to the Normalized Variable Diagram (NVD) [196] by introducing a blended formulation for the normalized face value that depends on the interface orientation and local courant number. The value of the latter at the interface must be lower than 0.5 for the HRIC scheme to maintain a sharp interface. At most, it must be between 0.5 and 1 to blend the HRIC scheme with the 1st Order Upwind scheme.

To ensure a sufficiently small mesh resolution, AMR [130] is used to dynamically refine the cells marked as containing the interface. To maintain the sharpness of the interface

between adaptation events, the surrounding cells and those predicted to be near its next location are refined. The solution is interpolated on the adapted cells with a sharp interface reconstruction scheme that preserves the phase volume. To obtain the latter, the induced cut cell volume is considered proportional to α_i .

5.3.2 VOF-Lagrangian Approach

The VOF liquid phase can be considered either continuous or dispersed in the VOF gas phase based on its volume fraction. For jets in crossflow applications, the dispersed VOF liquid phase is formed by the ligaments and droplets resulting from the jet column breakup and shedding process. The hybrid approach first uses a VOF blob detection model to identify the dispersed VOF liquid phase and form spherical VOF droplets (blobs) in cells where the liquid phase volume fraction α_L is greater than an imposed value α_{blob} , which was set to 0.5. The impingement of Lagrangian particles on the dispersed VOF liquid phase is also accounted for by transforming them back into VOF blobs when they interact with these cells [130].

Different approaches can then be used to transform the VOF blobs into Lagrangian droplets. The Resolved hybrid transition model [40, 130, 136, 157] determines which VOF blobs are suitable to be completely transformed into Lagrangian droplets based on their characteristics. To ensure that only spherical VOF droplets are being transitioned into Lagrangian droplets, which are spherical particles that do not directly account for the surface deformation, the blob diameter D_{blob} must be less than a specified size and its shape must be close to spherical. The blob sphericity ϕ in equation (5-7), which is the ratio between its ideal (spherical) and actual surface area A_{blob} , must be greater than a specified value. The former is obtained from the blob volume and the latter by summing up the volume of the cells marked as containing the blob. [40, 130, 136, 157]

$$\phi = (4\pi(0.5D_{blob})^2)/A_{blob} \quad (5-7)$$

Moreover, only blobs with a liquid volume fraction close to unity are transformed to optimally conserve their mass, momentum, and energy as shown in **Figure 5-1**. A minimum value of 0.95 is imposed to ensure that the diameter and velocity of the formed Lagrangian droplet are similar to its parent blob (i.e. D_{blob} and u_{blob} respectively).

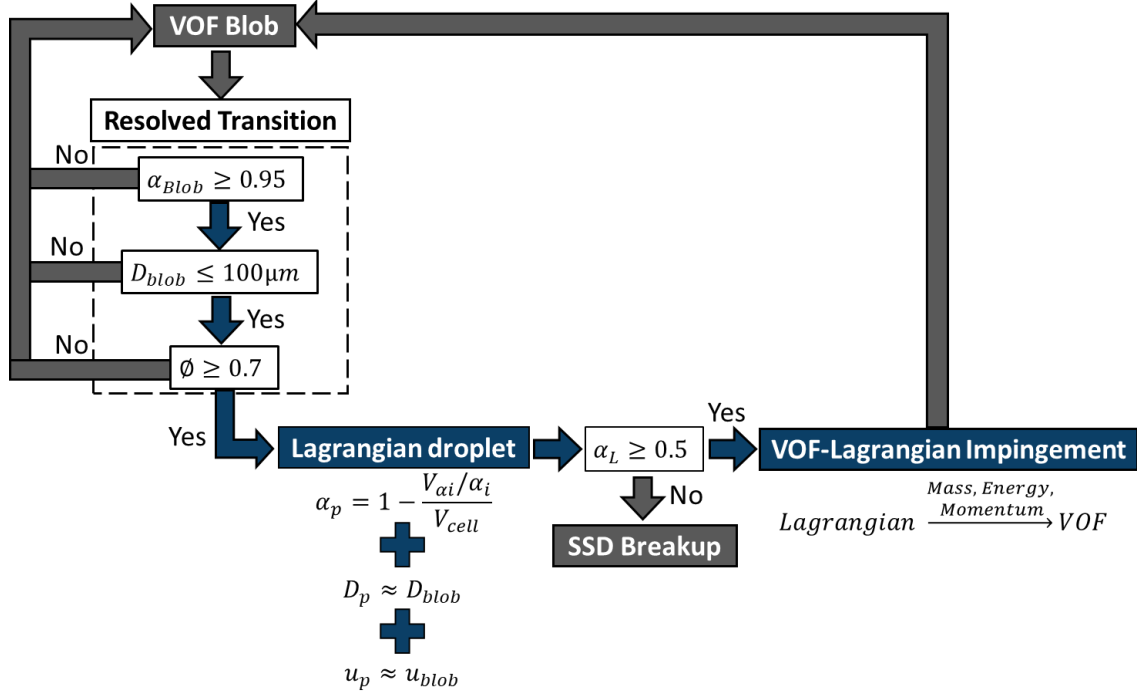


Figure 5-1: VOF-Lagrangian resolved transition model mechanism (Gray boxes: Solvers not represented).

The interactions between the Lagrangian particles and both VOF phases are modelled using the two-way coupling approach. Within the Lagrangian framework, the Lagrangian particles are considered dispersed in the continuous VOF phases. This is accounted for in the VOF framework by scaling the governing equations of the continuous VOF phases with the void fraction η , which is an indicator of the cell volume available for the VOF phases due to the presence of Lagrangian particles. It is calculated as the ratio of the cell volume available for both VOF phases to the cell volume V_{cell} [130]

$$\eta = \sum V_{\alpha_i} / V_{cell} = (V_{\alpha_i} / \alpha_i) / V_{cell} = 1 - \alpha_p \quad (5-8)$$

where V_{α_i} is the cell volume occupied by phase i and α_p the volume fraction occupied by Lagrangian particles in the cell. The two-way coupling approach also governs the VOF-Lagrangian impingement process so that the Lagrangian particles transfer their accumulated mass and momentum to the VOF Liquid phase. As for the governing equations of the continuous phases, additional source terms are included to account for the net transfer rate of momentum S_v and energy S_E from the Lagrangian particles, which are given by [130]

$$S_v = -\frac{1}{\Delta t} \sum_{\pi} \sum_{\delta t_p} n_{\pi}(F_s) \delta t_p \quad (5-9)$$

$$S_E = -\frac{1}{\Delta t} \sum_{\pi} \sum_{\delta t_p} n_{\pi}(F_s \cdot u_p) \delta t_p \quad (5-10)$$

where δt_p is an adaptive local parcel time step during which the Lagrangian solution is advanced at every global inner iteration and n_{π} is the number of particles within the Lagrangian parcel.

5.3.3 Lagrangian Approach

As seen in *section 5.3.2*, the interactions between the continuous VOF phase and the Lagrangian particles are governed by the aerodynamic and pressure gradient ∇P_{static} effects through the surface force F_s . The related drag force F_d and pressure gradient force F_p are calculated as [130, 132]

$$F_p = -(m_p/\rho_p) \nabla P_{static} \quad (5-11)$$

$$F_d = 0.5 C_D \rho A_p |u_s| u_s \quad (5-12)$$

where C_D is the drag coefficient and m_p , ρ_p and A_p are respectively the particle's mass, density and projected surface area. The particle slip velocity u_s is the difference between the continuous phase velocity u and particle velocity u_p , which is obtained by integrating over time equation (5-13) and used to calculate the particle's position vector. [130, 132]

$$m_p \frac{du_p}{dt} = F_s \quad (5-13)$$

The Lagrangian atomization process is accounted for using the SSD breakup model [33, 34], which predicts that breakup occurs when the particles contained within a parcel meet conditions based on the local flow characteristics. As indicated by the following equations, the particle's radius r_p and Weber number We must be respectively superior to a critical radius r_{crit} and critical Weber number We_{crit} , which is set equal to 12 [86]. The particle residence time $\tau_{R,p}$ in the domain must also be superior to the breakup time τ_{bu} , which depends on a breakup parameter B_1 as shown in equation (5-16) [33, 34].

$$\left[We = \frac{\rho |u_s|^2 (2r_p)}{\sigma} \right] > We_{crit} \quad (5-14)$$

$$r_p > \left[r_{crit} = \frac{We_{crit}\sigma}{2\rho|u_s|^2} \right] \quad (5-15)$$

$$\tau_{R,p} > \left[\tau_{bu} = B_1 \frac{r_p}{|u_s|} \sqrt{\frac{\rho_p}{\rho}} \right] \quad (5-16)$$

The parcels satisfying these conditions are replaced by several child parcels containing particles whose radius $r_{p,c}$ are sampled according to the following log-normal size-distribution function. Its mean value is given by the constant K_0 and its variance $\langle \xi^2 \rangle$ is given by K_1 and the local flow characteristics.

$$\Phi(r_{p,c}) = \frac{1}{2} \left(1 + erf \left[\left(\log \left(\frac{r_{p,c}}{r_p} \right) - K_0 \right) / \sqrt{2\langle \xi^2 \rangle} \right] \right) \quad (5-17)$$

$$\langle \xi^2 \rangle = K_1 \ln(We/We_{crit}) \quad (5-18)$$

The child particle velocity $u_{p,c}$ is then obtained by scaling the parent particle's velocity with the multiplication factor $|W_{bu}|$ to account for the momentum gained in the direction transverse to the slip velocity vector [33, 34]. This aspect is further controlled by the constant K_3 imposed to a value between 0 to 1.

$$u_{p,c} = |W_{bu}|u_p = (K_3 r_{p,c} / \tau_{bu})u_p \quad (5-19)$$

5.4 Numerical Methodology

To validate the predictive capabilities of the numerical methodology, the experimental conditions from datasets available in the literature for turbulent liquid fuel jets in high-speed crossflow presented in **Table 5-1** were reproduced. Only datasets at ambient temperatures were considered as further explained in *section 2.4.1*.

Table 5-1: Experimental datasets.

Datasets	Madabhushi et al. [30]	Freitag and Hassa [109]
Case #	1	2
u_g [m/s]	138	75
Re_g	6.1E+05	1.5E+06
$Re_{g,d}$	7.8E+03	1.8E+04
J	33.6	6
u_{jet} [m/s]	31	19.7
Re_{jet}	1.2E+04	5.2E+03

The kerosene fuel dataset from Freitag and Hassa [109] was selected due to its high-pressure condition ($P_g=8$ bar) and high atomization levels ($We_g=1172$, $We_{jet}=7032$). It includes data on the global SMD, spray trajectory and shadowgraph images.

The Jet A fuel dataset at ambient conditions from Madabhushi et al. [30] was selected due to its high momentum flux ratio J , high turbulent characteristics for both phases and also high atomization levels ($We_g=720$, $We_{jet}=24711$). It provides measurements for the transverse evolution of the droplets' characteristics at the centre of the spray, which will be used to validate the predictions in SMD and droplet axial velocity. The spray trajectory is validated by using correlations from Farvardin et al. [111] and Tambe et al. [81] obtained from experiments of turbulent liquid fuel jets in atmospheric crossflow. They were selected to ensure the conditions of case 1 were covered by their combined range of momentum flux ratios, Weber numbers and turbulence levels.

The numerical domains' dimensions presented in **Figure 5-2** correspond to the experimental test sections. This includes the length and diameter d of the plain orifice injector (0.762 mm for case 1 and 0.5 mm for case 2) located at their centre. The lengths of the numerical domains were elongated upstream of the injector by at least 1 time the measurement zone's length and elongated downstream of the latter by approximately 2 times its length. This improves the convergence by having an established gas flow field upstream of the phase interaction zone.

As previously mentioned, the VOF-Lagrangian approach is compared to the Lagrangian numerical methodology previously developed and validated using the same datasets [42, 43]. For the Lagrangian simulations, the injector geometry is removed and modelled using a point injector method, which injects droplets at the size of the nozzle diameter. The polyhedral volume mesh parameters were determined following a grid independence study previously conducted using the operating conditions of case 1. The cell size is refined to 0.4 mm in the near-field region and to 0.45 mm in the far-field region, which results in a mesh size of 3.37 million elements for case 1 and 2.79 million elements for case 2. For LES, more than 80% of the turbulent kinetic energy (TKE) spectrum was resolved on average.

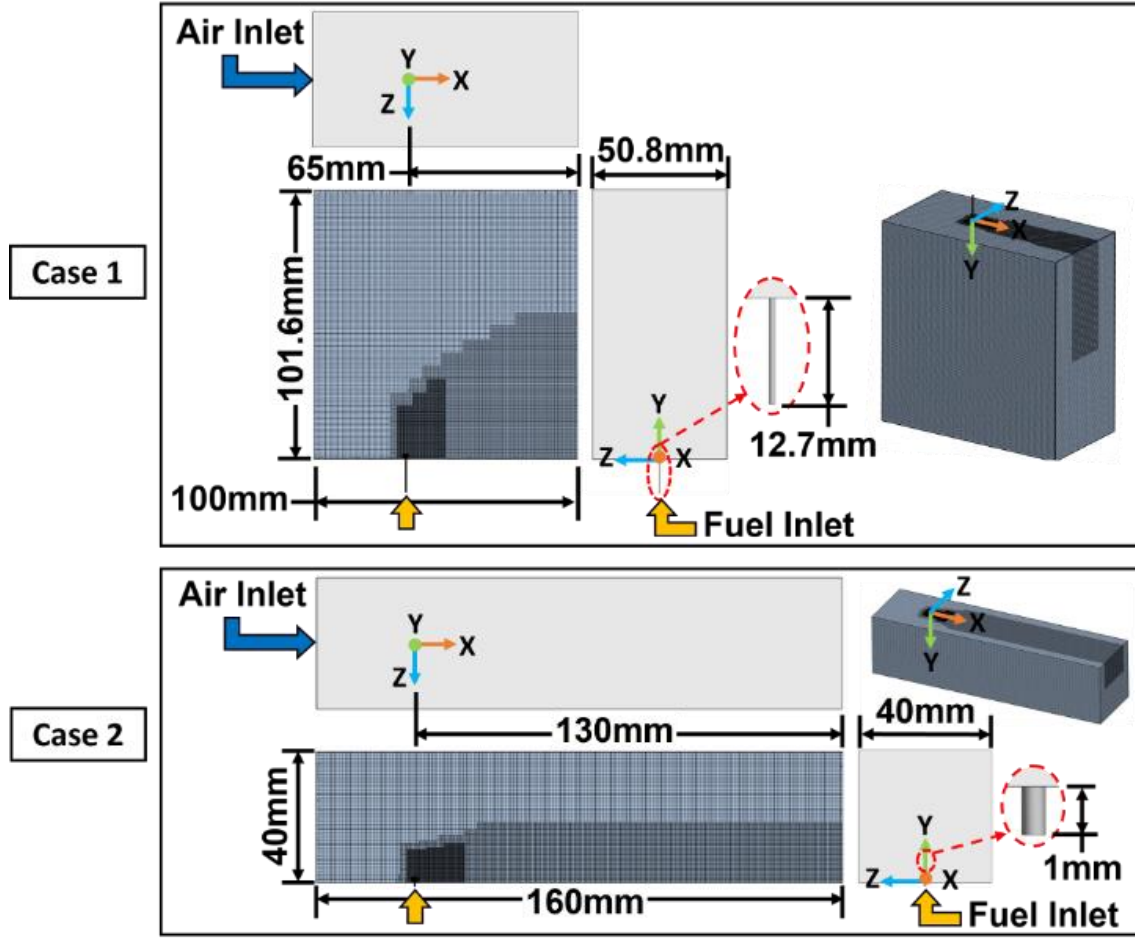


Figure 5-2: Numerical domain and baseline mesh on XY plane ($z/d=0$) for VOF-Lagrangian simulations.

For the VOF-Lagrangian simulations, the volume mesh is made of hexahedral elements to achieve a better adapted mesh quality with minimal monitoring required [130]. The baseline mesh includes refinement zones chosen based on the spray location predicted by the Lagrangian simulations. The initial cell size is refined to 0.4 mm in the far-field region, to 0.2 mm in the near-field region and to 0.1 mm near and within the injector where the VOF approach is expected to dominate. The resulting baseline mesh shown in **Figure 5-2** has 2.73 million elements for case 1 and 1.92 million elements for case 2.

The hybrid simulations use AMR every 10 time steps to ensure a sharp resolution of the interface and optimal mass conservation of the VOF phases. The cell sizes are progressively reduced to 0.01 mm by using 5 refinement levels. A transition width of 2 cells is used between each level to ensure a smooth volumetric size evolution. The resolution criterion used to detect and refine the interface is set to 5 cells. In addition, the

far-field cells within a volume delimited by the maximum droplet position are progressively reduced to 0.2 mm until the Lagrangian droplets reach the exit. To ensure they remain inside the refined volume between updates, its size is increased by 5 mm in the $+X$ and $+Y$ directions, and in both $\pm Z$ directions by 3 mm for case 2 and at least 6 mm for case 1. These AMR parameters allowed to resolve on average more than 90% of the TKE spectrum within the spray. The adapted mesh is shown at a random time step in **Figure 5-3**. Its size varied on averaged around 120 million elements for case 1 and 40 million elements for case 2.

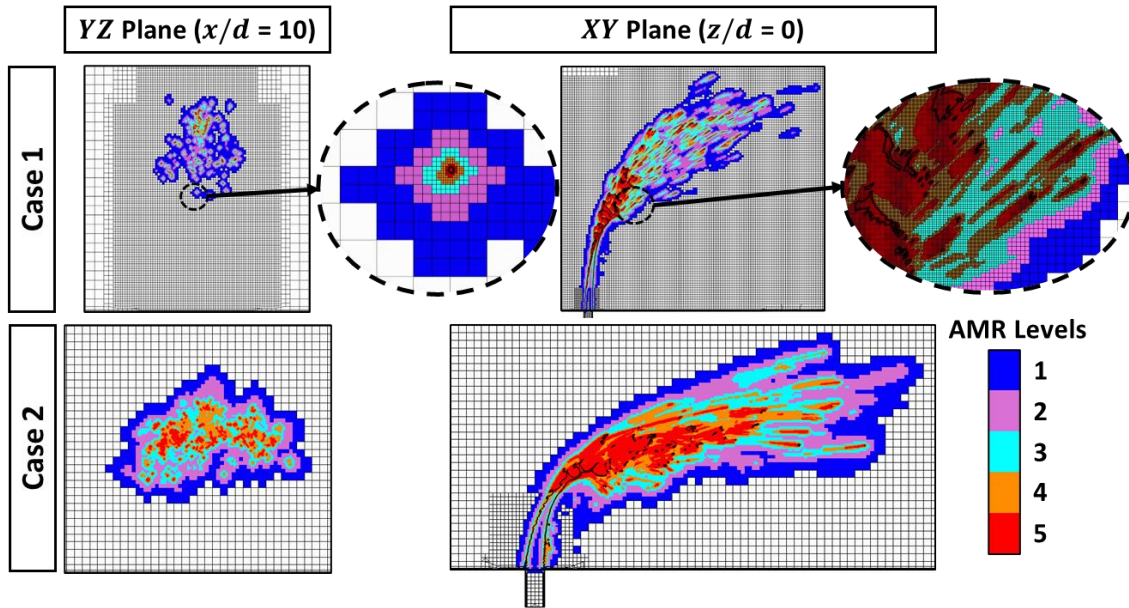


Figure 5-3: AMR levels on YZ plane ($x/d = 10$) and XY plane ($z/d = 0$) (zoomed) for case 1 and case 2 (black outline: instantaneous VOF interface).

All simulations are performed using Simcenter STAR-CCM+ and are turbulent, adiabatic and use an implicit unsteady solver. The latter uses a 2nd order temporal discretization scheme except for the hybrid approach due to limitations of the selected VOF-Lagrangian transition model [130]. For LES, the WALE subgrid-scale (SGS) model [134] is used with an all y^+ wall treatment and the segregated solver. For the URANS simulations, the coupled solver is used with a 2nd order discretization scheme to improve the phase coupling and turbulence is modelled by applying a two-layer approach [183] on the Realizable k-epsilon turbulence model [133] with a Two-Layer All y^+ wall treatment.

The Lagrangian droplets are modelled using two-way coupling, the SSD breakup model and the Liu drag coefficient [165]. The latter accounts for their distortion under

aerodynamic forces by scaling the drag coefficient [175] with the normalized droplet distortion parameter from the TAB breakup model [151]. The breakup parameter B_1 is set to $\sqrt{3}$ and the normal velocity coefficient K_3 to 1 as they were found to respectively enhance the accuracy of the SMD and the radial diffusion [42]. The constants K_0 and K_1 were set to their suggested values of -0.1 and 0.1. A turbulent dispersion model is used with URANS to model the droplet interactions with the turbulent eddies [180, 182].

The VOF solution is advanced once per time step and its transport equation is updated every inner iteration. The transition model is enabled after the VOF liquid phase reaches its column breakup point. Unless otherwise specified, the Resolved transition model is used with a transition blob diameter D_{blob} of 100 μm and minimum sphericity ϕ of 0.7.

With the Lagrangian approach, the time step is set to 1 μs to obtain a convective courant number below 1 in the spray region and the number of inner iterations is imposed to ensure the minimal convergence of the residuals to the 2nd or 3rd order of magnitude. With the hybrid approach, the global time step is set to 0.08 μs due to the significantly smaller cell sizes generated by AMR in regions of high velocity. Adaptive time-stepping is used to lower the computational cost of achieving a sharp interface. The time step is dynamically lowered from the global time step size and adapted to keep the convective courant number at the interface around 0.4. As a result, the time step was on average around 0.04 μs for case 1 and 0.07 μs for case 2. The number of inner iterations is also dynamically adapted to achieve good convergence and optimal mass conservation of the VOF phases.

5.5 Results

The results presented were time-averaged every 1 μs . The contours show time-averaged values on the centre XY plane ($z/d=0$), are zoomed near the injector and are overlaid with the projected time-averaged profile of the VOF interface. The 3D VOF interface and Lagrangian particles are represented in their instantaneous state and the latter are scaled by their sizes. The location of the VOF interface and Lagrangian particles were both considered to calculate the maximum spray trajectory and spray width. The transverse dispersion of the spray is defined as the difference between the maximum and minimum vertical trajectory. The time-averaged centreline profiles presented were evaluated at the

centre ($z/d=0$) of a YZ plane located at a normalized distance of $x/d \approx 33$ downstream the injector.

Error bands are used to better visualize the discrepancies between the data and numerical results. The experimental uncertainties for the datasets presented in **Table 5-1** were not provided. However, several studies have reported the error on the spray trajectories obtained from imaging techniques to be lower than $\pm 10\%$ [e.g. 106, 111, 197] when using 10 to 200 images and to decrease with an increasing sampling size. For the SMD, many studies have reported errors from laser instrumentation to decrease with an increasing droplet size and to be lower than $\pm 10\%$ for diameters larger than $10\mu\text{m}$ [e.g. 88, 89]. Droplet velocity measurements from laser instrumentation have been attributed to similar error ranges [e.g. 88, 89, 106]. This agrees with what has been reported by the research group that generated the dataset for case 1 [198, 199]. Considering the trajectory correlations used in the present study were obtained from 20 to 500 images [81, 109, 111] and that the SMD measured indicates the droplets are larger than $10\mu\text{m}$ [30, 109], it is deemed conservative to use $\pm 10\%$ error bands for all validation data.

5.5.1 Spray Trajectory

Regardless of the conditions, the hybrid approach tends to predict an overall smaller spray trajectory compared to the Lagrangian approach as seen in **Figure 5-4**. For case 1, the spray height predicted is on average 16% smaller compared to the Lagrangian approach. For case 2, it is lower on average by 26% and 17% compared to the Lagrangian approach using LES and URANS respectively. The overall higher discrepancies and more important differences in the near-field region with the higher-pressure conditions of case 2 indicate the hybrid approach is potentially sensitive to the operating conditions.

Within the regions shown in **Figure 5-4**, the spray trajectory predicted by LES tends to be overpredicted with the Lagrangian approach and underpredicted with the hybrid approach for both cases. Indeed, the latter predicts an overall spray trajectory on average 15% lower for case 2 compared to the data from Freitag and Hassa [109] and on average 11% lower for case 1 compared to both empirical correlations previously selected [81, 111].

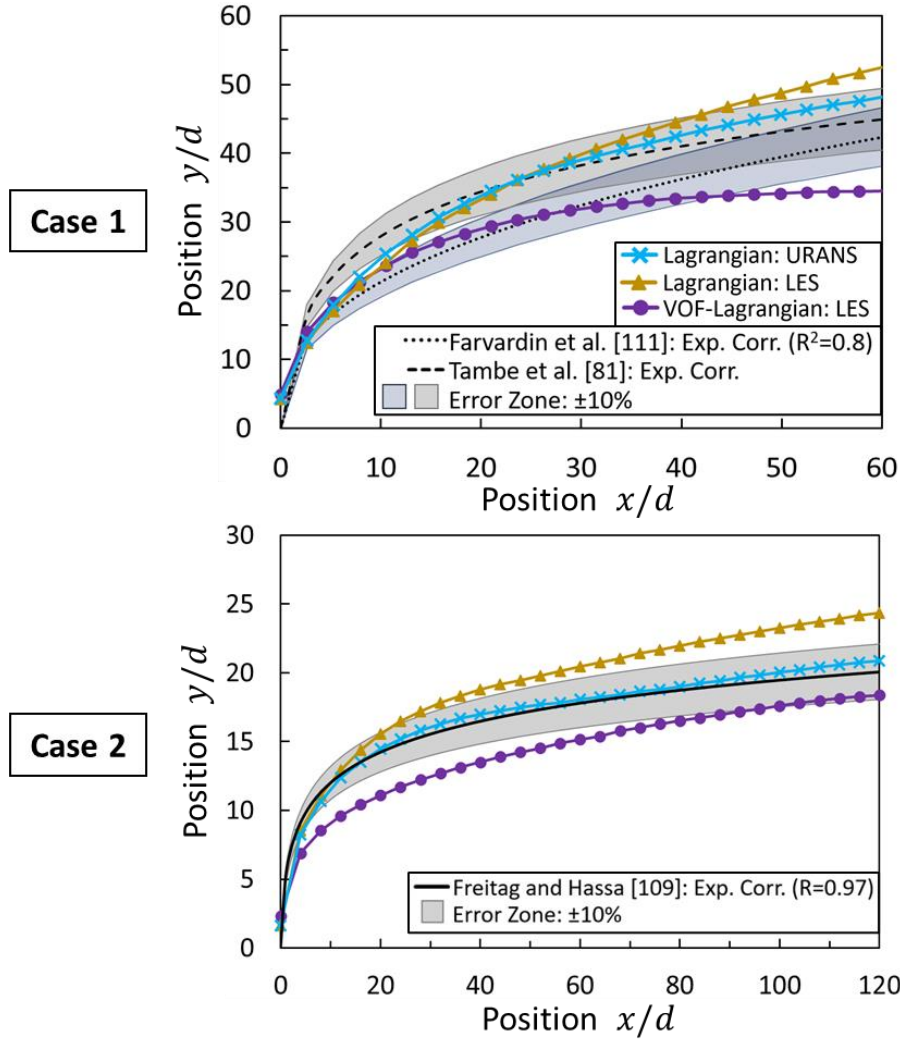


Figure 5-4: Time-averaged maximum spray trajectory for case 1 and case 2.

Although the effects of the hybrid approach on the accuracy of LES for case 1 vary with the empirical correlations, accounting for both yield similar overall absolute relative errors of 14% and 15% with and without the hybrid approach respectively. For case 2, the hybrid approach increases the discrepancies in the near-field region ($x/d \leq 60$) from 11% to 20%, but reduces them in the far-field region from 18% to 11%. This results in an overall absolute relative error predicted by LES for case 2 of 15% with and without the hybrid approach, which is similar to the values predicted for case 1. Moreover, the URANS methodology tends to agree better with the data as it predicts on average overall discrepancies of 3% for case 2 and 12% for case 1, which decreases to 6% compared only to the dataset from Tambe et al. [81]. Thus, the hybrid approach does not significantly

improve the overall predictive capabilities of LES for the spray height regardless of the operating conditions.

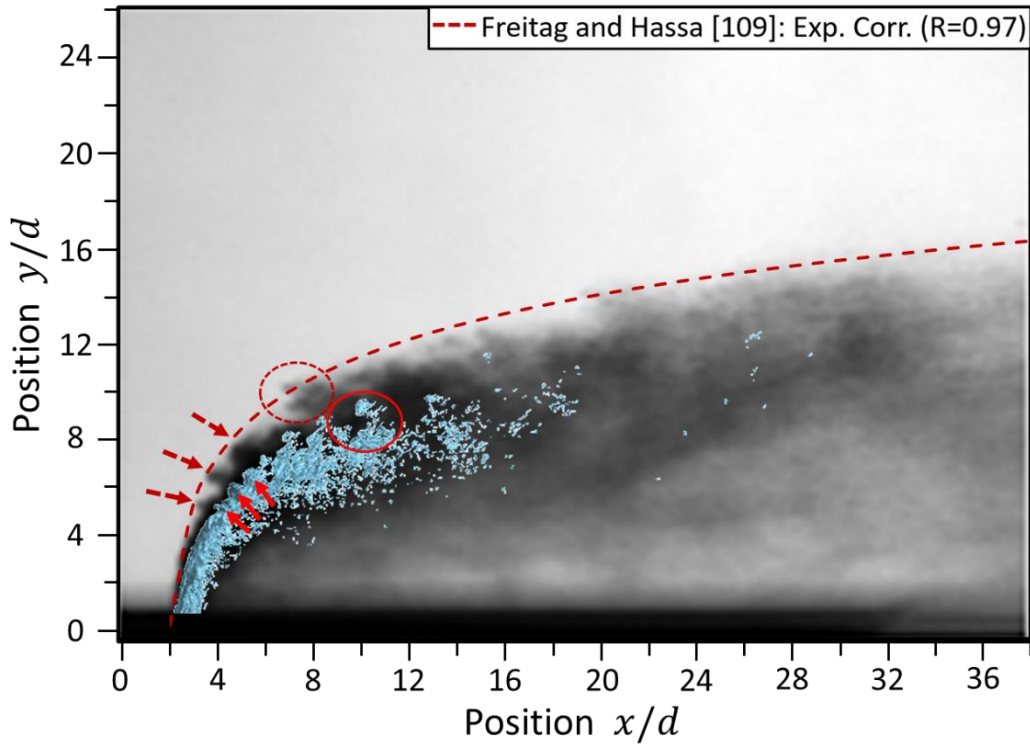


Figure 5-5: Experimental correlation, spray shadowgraph image and 3D VOF interface (blue) for case 2 (adapted from [109] with authorization from ILASS).

To assess the ability of the numerical methodology to capture the key primary breakup characteristics, the instantaneous VOF interface predicted for case 2 is compared to the spray's shadowgraph image in **Figure 5-5**. It is possible to observe that the aerodynamic effects on the jet surface are well captured by comparing the latter with the surface waves and stripped droplets formed by the dispersed VOF liquid phase. This demonstrates the ability of the proposed VOF numerical set-up to capture a sharp resolution at the interface, which is due to the combined use of AMR and the HRIC convection scheme.

5.5.2 Spray Dispersion

The VOF-Lagrangian approach significantly enhances the radial dispersion as it predicts a spray width on average 24 times larger for case 1 ($x/d \leq 60$) and 21 times larger for case 2 ($x/d \leq 120$) compared to both Lagrangian simulations. It also predicts a larger transverse dispersion as seen in **Figure 5-6**.

Without the VOF approach, the spray width predicted by LES is even smaller than the one predicted by URANS as it reduces the spray radial dispersion on average by 26% for case 1 and 23% for case 2. Moreover, the droplets' radial diffusion begins near the injector with the hybrid approach compared to further away from it ($x/d > 20$) with the Lagrangian approach.

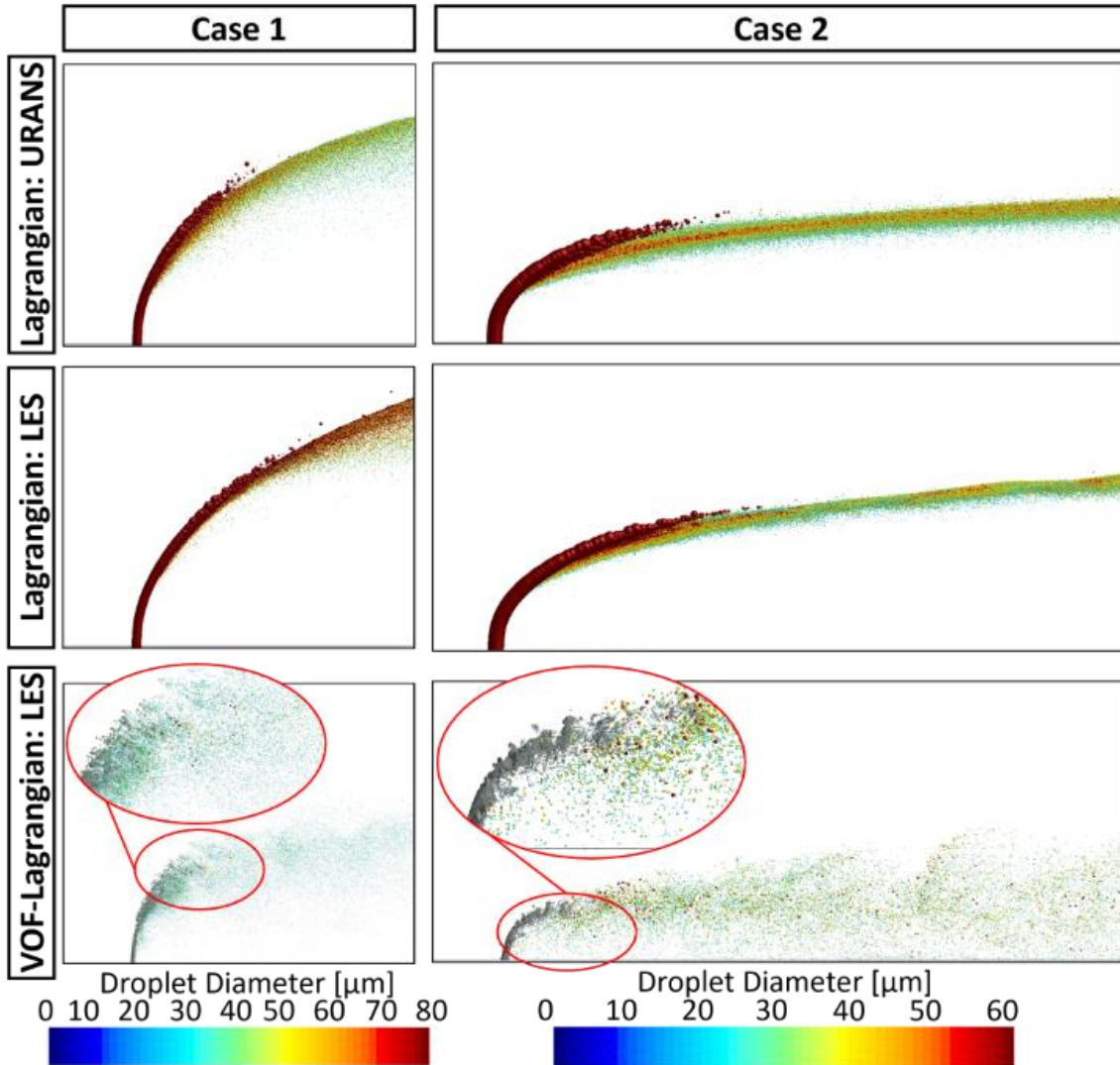


Figure 5-6: Instantaneous droplet diameter for case 1 and case 2 (3D VOF interface in grey).

These results indicate that the numerical methodology used for the Lagrangian approach struggles to capture on its own the important primary breakup processes of jets in crossflows, such as column breakup and shedding. This is most likely due to the Lagrangian approach applying a secondary breakup model on the entire spray, which was imposed considering its stochastic nature. The point injection method used might also

contribute to this issue as the resulting jet column is formed by large Lagrangian particles, which are less likely to fulfil the breakup time condition in equation (5-16). Considering the deterministic nature of the primary breakup models used in state-of-the-art CFD, it is recommended for future work to assess an injection method with a size distribution function to improve the radial and transverse dispersions of the Lagrangian approach.

5.5.3 Droplet Velocity

The VOF-Lagrangian approach tends to predict a higher droplet axial velocity in the windward spray region and lower in the leeward and core spray regions as seen in **Figure 5-7**. These discrepancies significantly improve the overall accuracy of the predictions compared to the data from Madabhushi et al. [30].

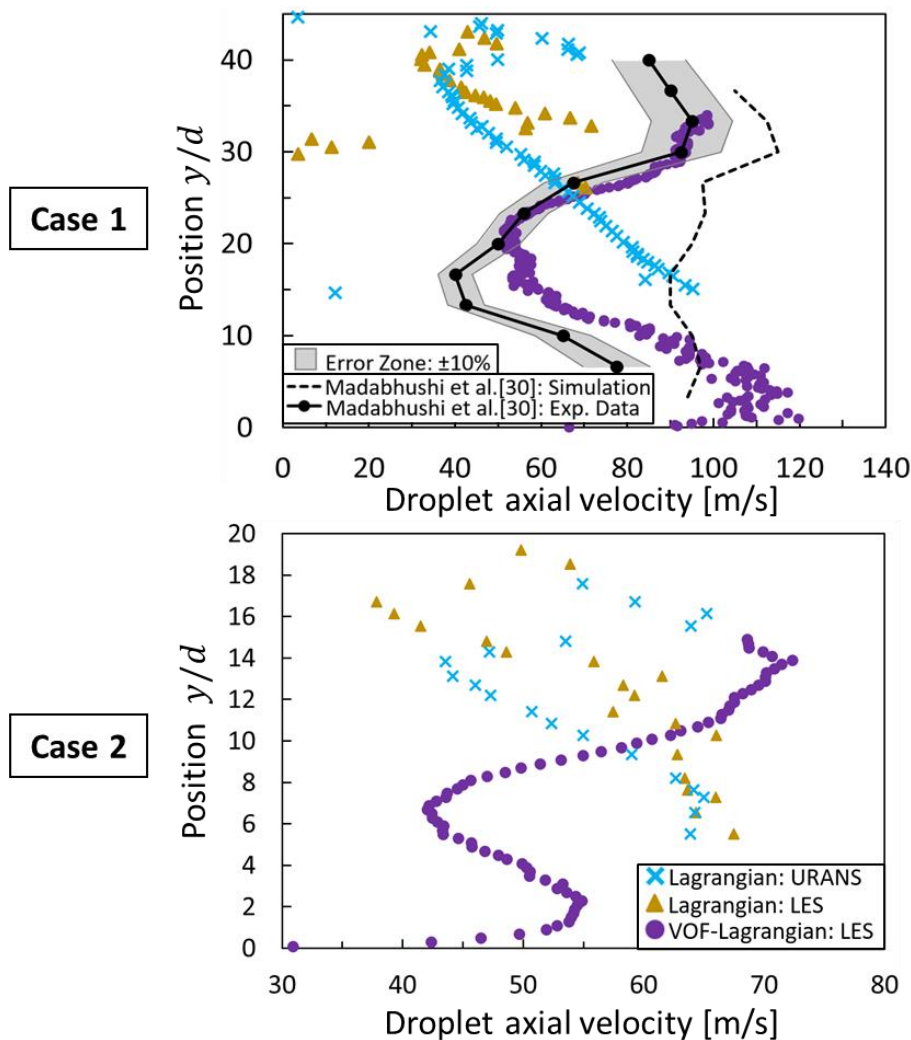


Figure 5-7: Time-averaged centreline droplet axial velocity for case 1 and case 2 ($x/d \approx 33$).

Indeed, although the hybrid approach tends to overpredict the droplet axial velocity in the leeward spray region ($y/d < 20$), its predictions are otherwise within $\pm 10\%$ accuracy on average. Moreover, its profile's shape agrees better with the experimental one. This is also true for case 2 when compared to profiles measured by other studies in the far-field region of turbulent liquid fuel sprays in crossflow at similar turbulence and atomization levels [30, 81], which are characterized by a lower droplet velocity zone in the wake region of the jet and higher zone in the windward spray region.

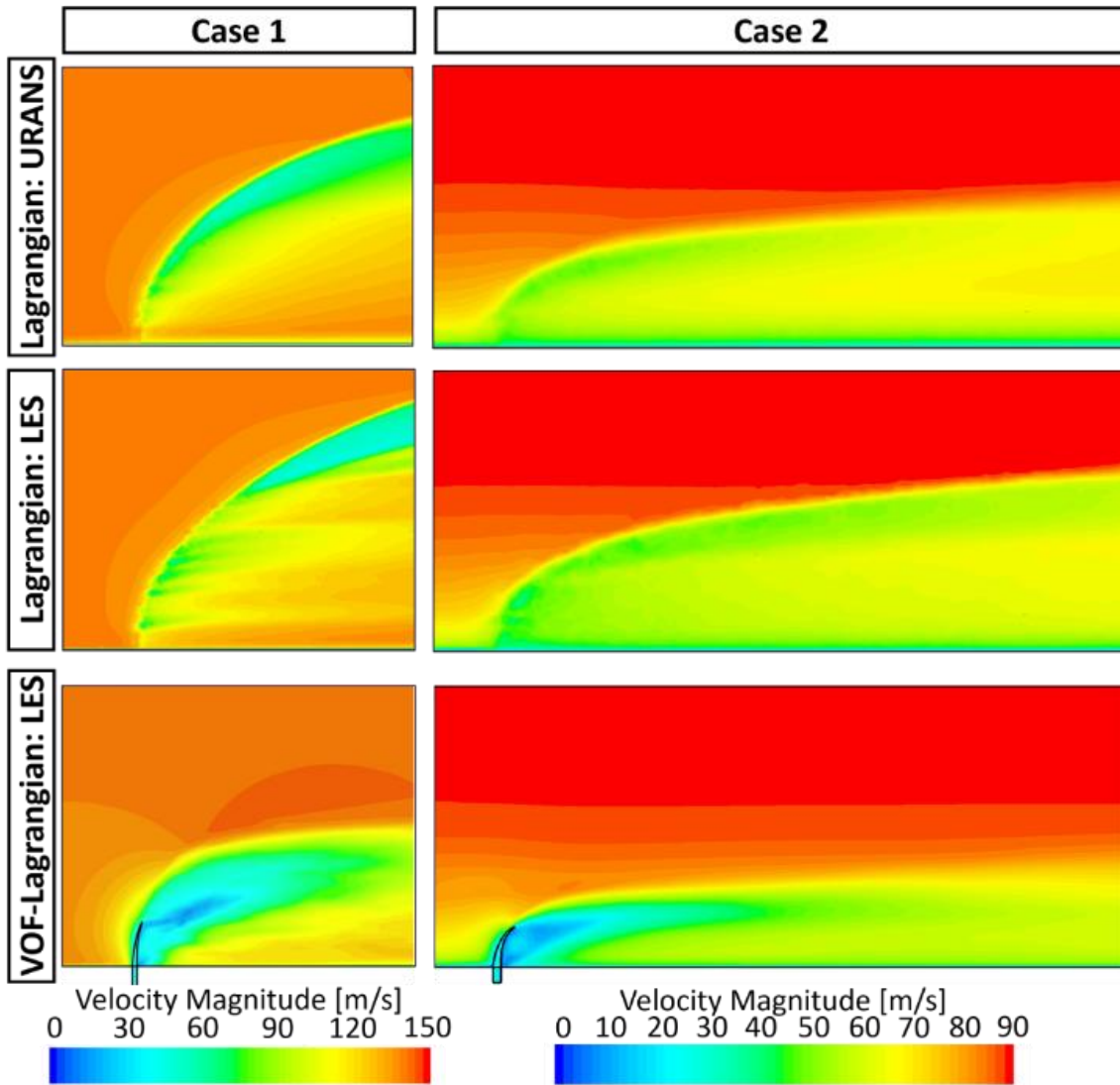


Figure 5-8: Time-averaged velocity magnitude for case 1 and case 2 (black outline: VOF interface).

These improvements are most likely due to the lower continuous phase velocity predicted by the VOF-Lagrangian approach in the wake region behind the liquid jet column as seen in **Figure 5-8**. According to the two-way coupling approach, it means that less axial

momentum is available to be transferred from the continuous phase to the droplets, hence the locally lower droplet axial velocities. It is also possible to observe a higher velocity zone above the interface due to the continuous flow field deviating from its straightforward trajectory when it first interacts with the liquid jet column. As a result, the axial momentum that can be transferred from the continuous phase locally increases, hence the higher droplet axial velocities predicted in the windward spray region.

These results indicate that the interactions between the continuous phase and liquid jet column are better captured when modelled by the VOF approach. Moreover, the increase in axial velocity over the windward interface could make it more difficult for the VOF liquid phase and droplets to penetrate vertically the continuous gas flow field. This would explain the smaller maximum spray trajectory predicted by the hybrid approach as presented in *section 5.5.1*.

5.5.4 Sauter Mean Diameter

The centreline SMD profile predicted by the VOF-Lagrangian approach tends to be more uniform as shown in **Figure 5-9**. As previously mentioned, it enhances the transverse dispersion of the spray due to its ability to capture the jet column stripping and breakup processes. As a result, larger Lagrangian droplets are transported in the wake region of the jet, which creates a more uniform local droplet size distribution compared to the Lagrangian approach, as seen in **Figure 5-6**. The enhanced transverse dispersion also explains why its centreline profiles reach lower transverse distances. The maximum transverse distance is lower due to its underpredicted trajectory.

For case 1, the URANS methodology tends to agree better with the data above the leeward region ($y/d > 20$) compared to the hybrid approach, which underpredicts the SMD. The breakup process could be overpredicted by its locally higher droplet velocity even if it agrees better with the data. Moreover, the maximum transverse position predicted by the hybrid approach is lower than the experimental one from Madabhushi et al. [30], which further supports its tendency to underpredict the trajectory. This also explains why the SMD predicted by URANS agrees better with the data near the windward interface ($y/d > 35$). However, the VOF-Lagrangian approach improves the predictions for the spray transverse dispersion as its centreline profiles reach low transverse distances similar to the data. As a result, it improves the SMD predictions in the leeward spray region (y/d

< 20) compared to the Lagrangian approach. The tendency of the hybrid approach to overpredict the droplet velocity in the leeward region could also explain why the SMD is locally underpredicted.

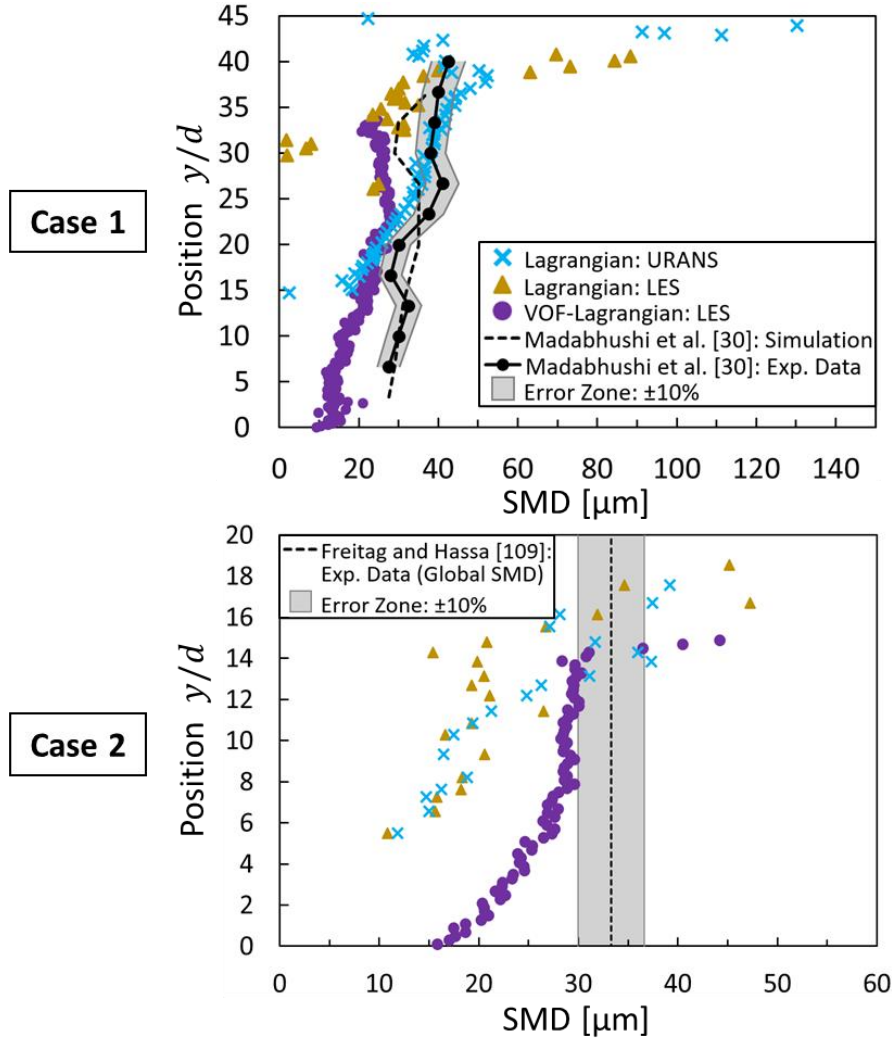


Figure 5-9: Time-averaged centreline SMD for case 1 and case 2 ($x/d \approx 33$).

Regardless of the operating conditions, the Lagrangian approach tends to overpredict the SMD at the windward interface. This is most likely due to the locally lower droplet velocity predicted as seen in **Figure 5-7**, which might be slowing down the breakup process. The VOF-Lagrangian approach tends to underpredict the SMD across the entire spray height, which indicates it might be overpredicting the overall breakup process. For case 2, the SMD predicted by the hybrid approach tends to agree more with the global SMD from Freitag and Hassa [109]. However, this is due to the Lagrangian approach underpredicting even more the overall SMD. Therefore, the predictive capabilities of the hybrid approach for the SMD might be sensitive to the operating conditions.

5.6 Discussion

The results previously presented show that using LES with the Lagrangian approach results in the highest spray trajectory and smallest spray width regardless of the operating conditions. It also yields the smallest vertical spray dispersion and overpredicts the SMD in the windward spray region. Moreover, using the VOF approach improves the overall predictive capabilities of LES, especially for the SMD due to its more uniform droplet size distribution.

The discrepancies between the LES and URANS simulations performed with the Lagrangian approach are mostly due to the effect of turbulence modelling. A related previous study on the effect of turbulence modelling on the predictive capabilities of the Lagrangian approach showed that coupling a turbulent dispersion model with URANS allows to better capture the important physical processes involved in turbulent liquid fuel jets in crossflows [43]. Indeed, the SGS models used in state-of-the-art CFD have been reported to struggle at capturing the impact on the Lagrangian particles of strong velocity gradients and large Reynolds numbers due to their filtering of the unresolved smaller-scale motions, which should not be considered negligible in such application [177, 179, 190, 191]. As a result, LES tends to underpredict the turbulent interactions and exchange of momentum and energy between the Lagrangian particles and continuous phase, which leads to an overpredicted spray trajectory and higher discrepancies with the experimental data [43, 177, 192, 193]. Thus, the results obtained using LES with the Lagrangian approach described in the previous paragraph agree with what has been reported in the literature.

The improved predictive capabilities of LES obtained by coupling the Lagrangian approach with the VOF approach might be due to the latter governing the spray modelling in the primary breakup region. Regardless of the conditions, the dispersed and continuous phases mostly interact in that zone of high-velocity fluctuations, as it is where most of the momentum and energy are exchanged. With the hybrid approach, the Lagrangian particles are formed further away from the nozzle and receive most of the momentum and mass from their parent VOF blobs. Thus, their properties in the near-field region depend less on their local interactions with the continuous phase and more on the upstream interactions between the VOF phases. As a result, the spray characteristics from the

hybrid approach might not be as sensitive to the ability of LES to model the turbulent interactions with the Lagrangian particles in the primary breakup region.

The tendency of the VOF-Lagrangian approach to underpredict the maximum spray trajectory compared to experimental data has also been reported by other studies on the hybrid approach [35, 36, 39, 40] and on different interface capturing methods including the VOF approach [135, 137]. Its underprediction of the SMD compared to the experimental data also agrees with what has been reported in the literature on the SSD breakup model [33, 34, 37, 172]. However, this is not strictly due to the breakup model used considering that this has also been reported by other studies on the hybrid approach conducted using different deterministic breakup models [40, 41] or without using the Lagrangian approach [137]. Moreover, a study conducted using the TAB breakup model also found that the SMD tends to be underpredicted in areas where the droplet velocity is locally overpredicted [41]. Thus, the better predictive capabilities achieved by the URANS numerical methodology for the spray trajectory and SMD further support the importance of capturing the turbulent interactions for turbulent jets in crossflow regardless of the multiphase modelling approach used. This could be achieved by incorporating a stochastic turbulent dispersion model into the Lagrangian framework. However, the latter is not compatible with the LES. Thus, future work should assess the predictive capabilities of the hybrid approach coupled with URANS and the turbulent dispersion model.

Using Direct Numerical Simulations (DNS) instead of LES has been shown to increase the spray trajectory and droplet size distribution when only using interface-capturing methods although improvements are still needed [137]. These results are not surprising considering that DNS resolves the important small-scale motions that are filtered by LES. However, the computational cost of DNS is not currently realistic for industrial applications and improvements are still needed for liquid jets in crossflow subjected to high Reynolds and Weber numbers [137]. Although the filtering done by LES could be attenuated by further refining the mesh, it would require achieving a TKE spectrum resolution significantly beyond the standard target value of 80% and would further increase the computational cost, which is already significant as discussed in *section 5.7*. Thus, to improve the hybrid approach within the LES framework, it is recommended

instead to focus on assessing the impact of using a SGS model recently developed to recover the sub-filtered acceleration of the Lagrangian particles [179]. In addition, as mentioned in *section 5.4*, the numerical coupling used for the Resolved VOF-Lagrangian transition is currently limited to 1st order unsteady accuracy for the LES solver. Therefore, future numerical development work could also be done to enable the capabilities for 2nd or higher-order temporal discretization, which could also potentially improve its predictive capabilities.

5.7 Computational Cost

The average solver CPU time per time step normalized by the total number of CPUs (256) Δt_{CPU} is presented in **Figure 5-10**. For the Lagrangian approach, Δt_{CPU} is 43% higher with URANS compared to LES, which is likely due to its use of a turbulent dispersion model. It is also on average 17 times higher with the hybrid approach compared to the URANS numerical methodology. The higher Δt_{CPU} of case 1 with the hybrid approach comes from its larger adapted total mesh size, which is caused by its lower pressure conditions enhancing the spray width and transverse dispersion. Indeed, normalizing Δt_{CPU} by the average mesh size reduces the cost difference between both cases. Moreover, the cost of the hybrid approach independently of AMR is 21% higher for case 2, which could be due to the effect of its higher pressure conditions on the solver.

As seen in **Figure 5-3**, the AMR settings used tend to over-refine the cells around the VOF interface, especially upstream/behind the latter. As a result, the total mesh size continues to increase over time despite a stable number of VOF blobs or Lagrangian droplets in the domain. To limit the maximum total mesh size, the adapted cells were coarsened by 1 AMR level (from 5 to 4) every 200-300 time steps. This prevented Δt_{CPU} from continuously increasing without affecting the interface resolution. Thus, the computational cost could be optimized for future work by reducing the AMR upstream swept distance or resolution criterion to avoid detecting an over-smeared interface. Moreover, it was found that continuously using 4 AMR levels for case 1 reduces Δt_{CPU} normalized by the mesh size by 26% and allows to double the time step size. Thus, conducting a preliminary assessment of the AMR settings is recommended for industrial applications as it can significantly improve the affordability of the hybrid approach.

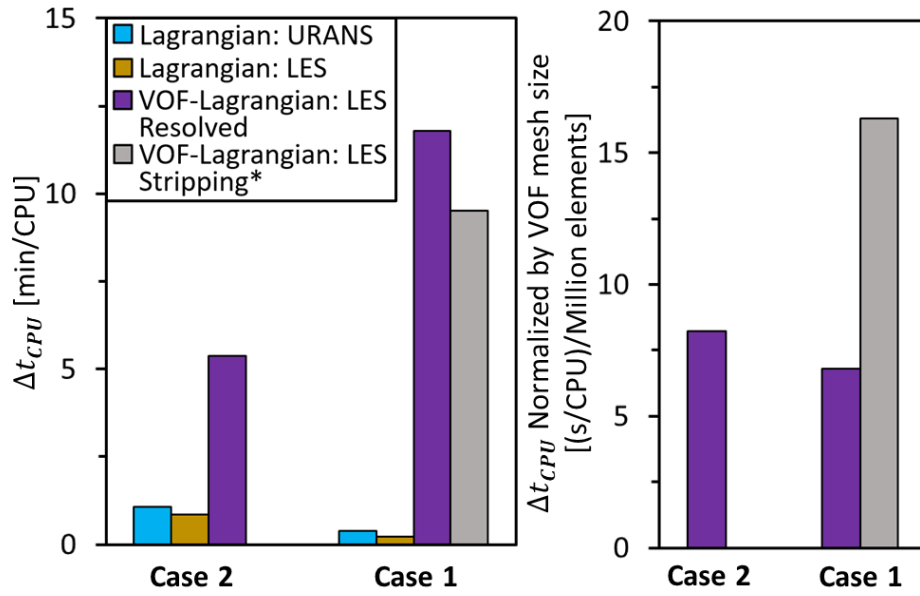


Figure 5-10: Time-averaged solver CPU time per time step Δt_{CPU} for case 1 and case 2
 (*averaged over 65 μ s after activating the stripping transition model).

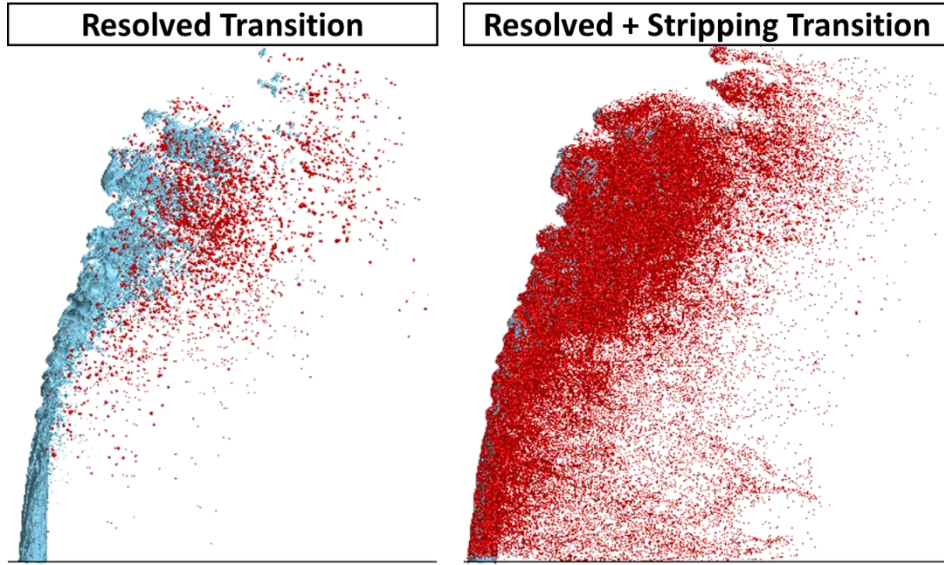


Figure 5-11: 3D VOF interface (blue) and Lagrangian particles (red) 65 μ s after activating the transition with and without the stripping model for case 1.

As mentioned in *section 5.3.2*, different models can be used to perform the VOF-Lagrangian transition, such as by stripping the Lagrangian droplets from the VOF liquid phase. This transition is controlled by imposing the size and mass flux of the stripped particles [130]. To ensure physical predictions, the transition is prevented if the droplet size exceeds 25% of the cell size and/or if the mass flux is not large enough to generate a full particle [130]. Thus, a variable diameter limited to 20% of the cell size was imposed

with a mass flux of $100 \text{ kg/m}^2\text{s}$. As shown in **Figure 5-11**, it generates significantly more particles and parcels within the same timeframe. This explains why its initial cost Δt_{CPU} normalized by the mesh size (averaged over $65\mu\text{s}$ after enabling the transition) is already 140% higher than the final cost of the resolved approach (averaged after the spray had reached the outlet). Thus, its final cost Δt_{CPU} with a fully developed spray region is expected to be significantly higher than the resolved approach. Therefore, the stripping approach was not further analyzed. It was also found that reducing the stripped diameter produces even more droplets, which further increases Δt_{CPU} .

To use the stripping transition model for industrial applications, the current numerical set-up needs to be optimized to reduce its computational cost. It might not be necessary with this transition model to maintain a sharp interface and capture the dispersed VOF liquid phase considering the droplets are shed from the jet column. Thus, future studies on the stripping VOF-Lagrangian transition model should be done to assess its predictive capabilities without the HRIC convection scheme and/or with coarser AMR settings. This modification could potentially reduce the overall cost of the hybrid approach and achieve better predictive capabilities considering the stripping transition model is compatible with 2nd order LES.

5.8 Conclusion

In summary, the predictive capabilities and computational cost of using the VOF-Lagrangian approach with a stochastic breakup model were assessed for turbulent liquid fuel jets in high-speed crossflow. The overall predictive capabilities of LES were significantly improved by coupling the Lagrangian and VOF approaches for a wide range of pressures and atomization conditions, except for the spray trajectory as the absolute error remained similar. Compared to the URANS numerical methodology previously developed and validated, better agreement with the experimental data for the SMD in the leeward spray region and for the overall droplet axial velocity were achieved with the hybrid approach. However, it is the opposite for the spray trajectory as it tends to be underpredicted.

Therefore, it is recommended to prioritize the hybrid approach for applications that would benefit from using higher-fidelity models compatible with LES, such as in combustion

modelling. To improve its predictive capabilities, future work should assess using SGS models developed to capture the Lagrangian subgrid acceleration and using the turbulent dispersion model with the URANS approach. Although further increasing the mesh resolution to enhance the portion of resolved TKE could potentially improve the predictions, it would be at the expense of the computational cost. To improve its affordability for industrial research and development purposes, the numerical methodology presented could be optimized by modifying the AMR settings or the VOF-Lagrangian transition model.

Moreover, the VOF-Lagrangian approach was found to significantly enhance the spray radial dispersion. Therefore, it should be used when designing test sections for jets in crossflow experiments to conservatively assess the wall-impingement risks, which could affect data collection. Considering the ability of the hybrid methodology developed to capture the jet column stripping and breakup, it will be used to select the measurement locations for experiments on diesel jets in crossflow at similar conditions. Future work will validate its predictive capabilities with the added complexity of evaporation modelling.

5.9 Acknowledgment

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6 An Optimized VOF-Lagrangian Numerical Methodology for Turbulent Liquid Fuel Jets in High-Speed Crossflow

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6.1 Abstract

This study aims to improve the affordability of the VOF-Lagrangian approach without relying on empirical correlations to predict the complex spray characteristics of turbulent liquid fuel jets in high-speed crossflow for low-emission gas turbine applications. An optimized transition model is proposed to remove the need to have a fine mesh resolution in the near-field region by stripping the Lagrangian droplets from a coarse VOF liquid jet column. To provide a numerical methodology suitable for a wide range of conditions, the properties and size of the transitioned Lagrangian droplets are inherited directly from the donor VOF liquid cell. A stochastic breakup model is then used to predict the primary and secondary atomization of the stripped droplets. The predictive capabilities of the optimized hybrid stripping method are assessed using experimental data for a turbulent Jet A jet at a high momentum flux ratio ($J=33.6$) and Weber numbers ($We_g = 720$, $We_{jet} = 24711$).

The discrepancies with the experimental data were found to be similar to those predicted by the numerical methodology previously developed and validated using the higher fidelity resolved transition model. Although the optimized methodology proposed tends to predict a slightly smaller centreline SMD and higher centreline droplet axial velocity, the average relative difference between the two methods is less than 15% and their average droplet properties in the far-field region are not significantly different. Considering the proposed numerical methodology speeds up the solver CPU time per time step by 78%, the trade-off between accuracy and computational cost is deemed reasonable. It was also found that using a higher-order temporal discretization scheme does not improve the predictive capabilities of the proposed numerical methodology, which is likely due to using a lower-order convection scheme with a coarser interface

resolution. Nonetheless, several recommendations were made to improve the accuracy of the optimized methodology without compromising its lower computational cost.

Keywords: CFD; Volume of Fluid; VOF-Lagrangian; Turbulent; Liquid fuel; Crossflow; Atomization; Gas Turbine.

6.2 Introduction

Emissions from aero and industrial gas turbines can be reduced by enhancing the mixing quality of the fuel and air, which can be achieved by injecting the fuel transversely into the hot air and further enhanced by the turbulent characteristics [5, 6, 10]. For combustion systems using liquid injectors, the crossflow configuration represents an additional challenge to combustion modelling as it changes the atomization process and the resulting spray characteristics. The breakup mechanism of turbulent liquid jets in crossflow first involves stripping ligaments and large droplets from the liquid jet column, which then further breaks up to form a large droplet cloud downstream of the injector [9, 82, 88]. The primary and secondary atomization process can be modelled using the high-fidelity interface-capturing method Volume-of-Fluid (VOF), but its high computational cost makes it unpractical for industrial applications and also for academic research projects that only need to incorporate atomization modelling in the Computational Fluid Dynamics (CFD) framework to study other complex phenomenon (e.g. combustor design, flame characteristics, etc.). This is due to the fine mesh required to capture both breakup processes and the higher-order convection schemes needed to achieve a sharp interface resolution.

The Lagrangian approach is often used as a lower-cost alternative, which is attributed to its use of breakup models to predict the primary and secondary breakup process. However, the breakup models used in state-of-the-art CFD often rely on empirical constants that require exhaustive calibration to accurately predict the spray characteristics [5, 14] as discussed in further detail in previous chapters. To the best knowledge of the author, this is also true for the breakup models that have been developed to address the challenges of capturing the primary breakup process of liquid jets in crossflow. Indeed, they all rely on empirical or single-droplet correlations to predict the properties of the droplets being shed from the jet column [29, 30, 31, 32] and use deterministic breakup models to predict the secondary droplets as summarized by Mashayek et al. [29].

The deterministic nature of the Lagrangian breakup models motivated the development of an unsteady numerical methodology using a Stochastic Secondary Droplet (SSD) breakup model [33, 34], which is covered in Chapter 3 and Chapter 4 [42, 43]. The unsteady Reynolds-Averaged Navier-Stokes (URANS) methodology proposed was found to have good predictive capabilities for the Sauter Mean Diameter (SMD) and spray trajectory over a wide range of pressures and atomization characteristics for turbulent liquid fuel jets in high-speed crossflow. Despite additional attempts to improve its accuracy in the leeward spray region, the local discrepancies with the experimental data remain significant due to not explicitly modelling the liquid jet column shedding and breakup process.

Coupling the VOF and Lagrangian approach alleviates the computational cost of modelling the breakup process in the far-field region while simultaneously removing the need to rely on empirical models to capture the jet column atomization process. This is done by tracking the small spherical droplets constituted of the dispersed liquid phase and transforming them into Lagrangian particles once they meet specific transition criteria, which are often based on their sphericity and diameter [40, 136, 157]. Although this resolved transition model limits the modelling of the VOF liquid phase to the near-field region, a fine mesh is still required to capture and track these small VOF blobs. Thus, it is not surprising that concerns are still being raised about the computational cost of the VOF-Lagrangian approach even when coupled with Adaptive Mesh Refinements (AMR) [27, 38, 41]. While Heinrich and Schwarze [40] reported that using the VOF-Lagrangian approach with a resolved transition model reduced the CPU time per time step by a factor of 3 compared to the VOF approach, the previous study presented in Chapter 5 [44] found that the VOF-Lagrangian approach can be up to 30 times more computationally expensive than the Lagrangian approach. In spite of that, the hybrid approach was found to significantly improve the predictions in overall droplet velocity and SMD in the leeward region compared to the unsteady Lagrangian numerical methodology as well as the overall predictive capabilities of Large Eddy Simulations (LES) for turbulent liquid jets in crossflow. Therefore, there is a strong incentive to improve the affordability of the previous methodology proposed for the VOF-Lagrangian approach.

Recent efforts have been made to reduce the computational cost of the VOF-Lagrangian approach for liquid jets in crossflow applications. Feiz et al. [27] suggested reverting to the purely Lagrangian approach by using an enhanced version of the deterministic Madabhushi breakup model developed for jets in crossflow [26, 200], which aims to better account for the jet column breakup process by scaling the droplet diameter with a ligament factor. Although they were able to achieve similar predictive capabilities as the VOF-Lagrangian approach, they emphasize that it required rigorous calibration of the model constants due to their strong influence on the spray characteristics [27] especially for non-uniform crossflow conditions [26]. Wang et al. [38] proposed to decouple the VOF and Lagrangian approaches by solving the VOF liquid jet column solution separately and using the time-averaged results to determine the properties and position of the Lagrangian droplets that are injected in a separate simulation. Despite significantly reducing the cost of coupling atomization and combustion modelling due to the coarser mesh resolution required by the Lagrangian approach, this method still implies running an expensive VOF simulation to track when the VOF-Lagrangian criteria are satisfied for both stripping and resolved transition models. Moreover, new modelling challenges arise from decoupling the VOF and Lagrangian approaches to account for the VOF-Lagrangian interactions, such as blockage modelling [38]. The decoupled VOF-Lagrangian methodology was also assessed by Feiz et al. [27] and compared to using the Lagrangian approach with the enhanced Madabhushi breakup model. Fontes et al. [41] explored the idea of relaxing the mesh resolution requirements in the near-field region by only stripping Lagrangian droplets from the jet column breakup point. However, the proposed methodology uses a deterministic breakup model in the far-field region (AB-TAB [201]) and relies heavily on empirical correlations to predict the position, diameter, and velocity of the stripped droplets [41].

The strategy proposed by Fontes et al. [41] of implementing a transition model that does not require a fine resolution of the jet column aligns with the recommendations made in Chapter 5 to reduce the computational cost of the VOF-Lagrangian approach. Therefore, the present study further expands on this idea by proposing an optimized transition model based solely on the surface stripping of the jet column, which should remove the need to capture the dispersed VOF liquid phase. To the best knowledge of the author, no other studies available in the literature on the VOF-Lagrangian approach have been conducted

using only such a transition model. In fact, the vast majority have been conducted with the resolved transition model previously described [25, 35, 36, 39, 40, 41]. The proposed methodology employs a stripping mechanism similar to the Multiple Injector Model (MIM) [29] and the Boundary Layer stripping (BLS) model [156] used by many breakup models developed for jets in crossflow [29, 31, 32], which strip the Lagrangian droplets according to the specified formulation for the shedding mass. However, the VOF-Lagrangian transition criteria proposed do not rely on empirical correlations to predict the stripped droplet properties unlike with these primary breakup models for jets in crossflow. Moreover, the liquid jet column is directly resolved using the higher-fidelity VOF approach instead of using experimental trajectory correlations to predict the bending of a Lagrangian droplet column [29]. To reduce the computational cost of modelling the VOF liquid jet column, the numerical methodology previously developed and validated in Chapter 5 is optimized by using a lower-order VOF convection scheme and coarser AMR settings. In addition, the effect of using a higher-order temporal discretization on the predictive capabilities of the VOF-Lagrangian approach is assessed using the optimized VOF stripping method following the recommendations from Chapter 5. The predictive capabilities and computational cost of the optimized stripping mechanism and resolved stripping mechanism are compared using an experimental dataset for turbulent liquid fuel jets in high-speed crossflow.

6.3 Governing Equations

The description of the governing equations is limited to highlighting the differences between the previous (“hybrid resolved method”) and the newly proposed (“optimized hybrid stripping method”) numerical methodologies. The implementation of the Lagrangian approach [132] follows the stochastic methodology previously developed and validated, which is described in detail in *section 4.3.1* to *section 4.3.3* of Chapter 4 as well as *section 5.3.3* of Chapter 5 [43, 44].

6.3.1 VOF Approach

The fundamental equations of the VOF approach [11] do not change with the numerical methodologies compared in the present study. The position and distribution of the VOF interface are captured by solving equation (6-1), which is the transport equation for the volume fraction α of phase i . A cell is marked as containing the VOF interface if the latter

is more than 0 but less than 1. The volume fractions of the remaining N phases contained within the interface cell are then obtained using equation (6-2). [11, 130]

$$\frac{\partial \alpha_i}{\partial t} + \nabla(\alpha_i u) = -\alpha_i \frac{D\rho_i}{Dt} - \frac{1}{\rho_i} \nabla(\alpha_i \rho_i u_{d,i}) \quad (6-1)$$

$$\sum_{i=1}^N \alpha_i = 1 \quad (6-2)$$

Where $u_{d,i}$ is the slip velocity between the mixture and phase i and ρ_i the density of the latter. The mixture contained within the interface cell inherits the properties of each phase scaled by their respective volume fraction and its velocity u is averaged based on their respective mass [130].

In addition, both numerical methodologies model the effect of the surface tension σ between the VOF phases by using the Continuum Surface Force (CSF) [194] approach with a semi-implicit stabilization scheme. The latter incorporates the normal component of the surface tension force as a body force in the conservation equation for the momentum [194]. Moreover, they both use a 1st order face density reconstruction. However, their respective implementation of the VOF approach differs beyond this point.

The hybrid resolved method uses a High-Resolution Interface Capturing (HRIC) convection scheme [195] to capture the stripping and breakup of VOF blobs from the liquid jet column because it allows to maintain a sharp interface. However, this is not needed for the optimized methodology as explained in *section 6.2* considering the Lagrangian droplets can be stripped from any interface cells where the stripping criteria are respected. Thus, it is deemed likely acceptable to replace the high-order scheme with a 1st Order Upwind scheme [202] to discretize the convective term of the VOF transport equation.

Although AMR is utilized in both methodologies to dynamically refine the interface cells, it is not deemed necessary to use a sharp interface reconstruction scheme with the optimized hybrid stripping method for the same reasons mentioned above. Thus, the interface resolution of the latter is only captured by refining the cells surrounding the current and estimated future position of the interface [130].

6.3.2 VOF-Lagrangian Approach

The main difference between both methodologies is the VOF-Lagrangian transition model used. The methodology previously developed and validated utilizes the resolved VOF-Lagrangian transition model [40, 136, 157] to completely transform the VOF blobs into Lagrangian particles. To ensure an optimal conservation of the mass, momentum, and energy, the VOF blobs are only transitioned if their diameter D_{blob} , sphericity ϕ and liquid phase volume fraction α_{blob} respect the imposed conditions specified in equation (6-3) to equation (6-5) [130].

$$\phi = \frac{(4\pi(0.5D_{blob})^2)}{A_{blob}} \geq 0.7 \quad (6-3)$$

$$D_{blob} \leq 100 \mu m \quad (6-4)$$

$$\alpha_{blob} \geq 0.95 \quad (6-5)$$

Where A_{blob} is the actual surface area of the interface cells containing the VOF blob. As explained in *section 5.3.2* from Chapter 5, this transition model requires using a VOF blob detection model to identify the spherical droplets formed by the VOF liquid phase. The dispersed VOF liquid phase is contained in the cells where $\alpha_L \geq 0.5$. This implies that the VOF liquid jet column is also marked as a VOF blob, hence the importance of using additional criteria to control the resolved transition mechanism.

Unlike the resolved transition model, the stripping transition model does not completely transform the VOF liquid phase into a single Lagrangian droplet of similar size and velocity that follows the path of the parent VOF blob. It also does not limit the transition to occur only in cells forming a spherical VOF liquid droplet. Instead, the mass of the latter contained in an interface cell is progressively reduced to form smaller Lagrangian droplets dispersed in different directions. The stripping transition model aims to generate Lagrangian droplets with a diameter $(D_{p,s})_{Target}$ and mass flux $(\dot{m}_{L,s})_{Target}$ corresponding to imposed values. However, the VOF mass that can be stripped $m_{L,s}$ is ultimately limited by the VOF liquid mass available in the interface cell m_L regardless of the target stripping mass $(m_{L,s})_{Target}$ imposed indirectly through the mass flux criterion as described in equation (6-6). The former is proportional to the cell volume V_{cell} scaled by the liquid volume fraction as expressed in equation (6-7) while equation (6-8) shows

the latter uses the interaction area density A_{cd} as a scaling factor instead. The interfacial interaction area between the VOF liquid phase and the Lagrangian particles depends on the liquid volume fraction in the cell and a characteristic interaction length scale l_{cd} . [130]

$$m_{L,s} = \min \left(m_L, (m_{L,s})_{Target} \right) \quad (6-6)$$

$$m_L = \alpha_L \rho_L V_{cell} \quad (6-7)$$

$$(m_{L,s})_{Target} = A_{cd} V_{cell} \Delta t (\dot{m}_{L,s}'')_{Target} = \left(\frac{6\alpha_L}{l_{cd}} \right) V_{cell} \Delta t (\dot{m}_{L,s}'')_{Target} \quad (6-8)$$

The stripped droplet diameter $D_{p,s}$ is also limited to 50% of the cell size L_{cell} as shown in equation (6-9), which ensures the volume fraction of the Lagrangian droplets stripped is inferior to 75% of the cell volume [130]. In addition, the stripping process only occurs if the VOF liquid mass is sufficient to produce one parcel with at least one particle. In other words, the stripped VOF liquid mass $m_{L,s}$ must be larger than the particle mass that will be stripped $m_{p,s}$, which is calculated using equation (6-10). [130]

$$D_{p,s} = \min \left((D_{p,s})_{Target}, 0.5 L_{cell} \right) = \min \left((D_{p,s})_{Target}, 0.5 (V_{cell})^{1/3} \right) \quad (6-9)$$

$$m_{p,s} = \rho_L \left(\frac{\pi}{6} D_{p,s}^3 \right) \quad (6-10)$$

If the stripping conditions are not respected or if the stripped mass flux imposed is too large, the VOF liquid mass is accumulated in the interface cell until it can be stripped. When stripping occurs, the number of particles stripped $n_{\pi,s}$ is calculated using equation (6-11) and the stripped droplets inherit their properties from the VOF liquid phase, such as density and volume fraction. Their velocity is also inherited from the continuous phase, but a perturbation vector is applied to transport them away from the stripping cell centre. [130]

$$n_{\pi,s} = \frac{m_{L,s}}{m_{p,s}} \quad (6-11)$$

The optimized numerical methodology introduces an additional stripping criterion to mitigate the risk of underpredicting the SMD due to the limitations imposed by the interface cell size on the maximum stripped diameter. Indeed, there seems to be an incongruity between the inner workings of the stripping transition model and the mesh resolution required by the VOF approach to capture the liquid jet column, which needs to be refined to small sizes even when aiming for a coarser interface resolution. Therefore,

the VOF-Lagrangian transition is prevented from taking place in interface cells that have a size smaller than a specified value. Although the latter could be imposed based on the expected SMD or by an empirical correlation, the alternative approach suggested is to avoid stripping from interface cells that have an adapted size indicating they have been refined up to the maximum AMR level. This implementation strategy aligns better with the overall objective of the work, which is to develop and validate a numerical methodology that does not rely on having prior knowledge of the spray characteristics. The target droplet diameter $(D_{p,s})_{Target}$ and mass flux $(\dot{m}_{L,s})_{Target}$ are set to zero if the adapted cell size L_{AMR} is smaller than the specified value $L_{AMR\ Max-1}$, which should enforce that no VOF mass nor particle mass can be stripped according to equation (6-6) and equation (6-9). To further prevent the stripping of small Lagrangian droplets, the stripped droplet diameter is maximized by imposing the target value $(D_{p,s})_{Target}$ equal to 50% of the adapted cell size. Taking into account that the latter represents the diameter of a sphere encapsulating the cell [130], this formulation ensures that $D_{p,s}$ will never be smaller than 50% of the cell size. The proposed VOF-Lagrangian transition mechanism is illustrated in **Figure 6-1**. The gray boxes refer to solvers that are not represented to improve clarity.

Considering the optimized hybrid stripping method is not expected to capture the stripping and breakup process of VOF liquid droplets (blobs) from the VOF liquid jet column, it is not necessary to use a VOF blob detection model to track their presence in the domain. However, it is still relevant to use for this study as it allows the comparison of how both methodologies are modelling the VOF phase interactions in the near-field region.

In addition, both methodologies use a VOF-Lagrangian impingement model to transform the Lagrangian particles into VOF blobs when they interact with interface cells marked as containing the VOF liquid phase [130]. Although the Lagrangian droplets are not expected to interact with any dispersed VOF liquid phase when using the optimized hybrid stripping method, the impingement model is expected to restrict the stripping process to the interface cells located in the leeward region of the VOF liquid jet column. Indeed, coupling both transition models has been reported in *section 5.7* of Chapter 5 to be more computationally expensive due to the significantly higher number of Lagrangian

droplets stripped from the entire surface area of the liquid jet column. Thus, the numerical methodology proposed might benefit from using the impingement model due to the additional limitations on the VOF-Lagrangian transition that could reduce its computational cost.

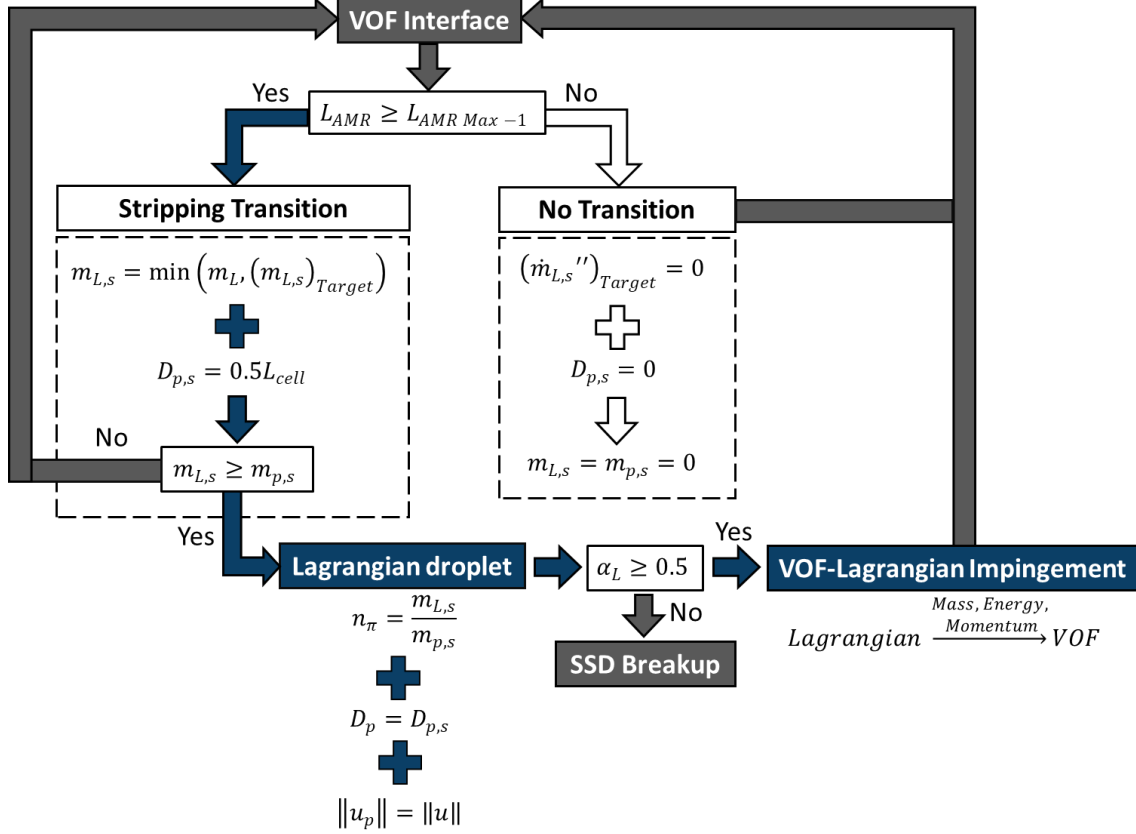


Figure 6-1: Optimized VOF-Lagrangian stripping transition model mechanism (Gray boxes: solvers not represented).

6.3.3 Time Discretization

The governing equations are discretized in space and time using the Finite-Volume method, which involves using an Algebraic Multigrid (AMG) method to solve a set of linear equations [130]. To do so, a transport equation that incorporates the transient, convective, diffusive and source terms of a given fluid property is integrated over a control volume [130].

Time integration methods are then used to solve the transient term, such as the implicit linear backward difference multi-step (BDF) method [203]. The latter can be formulated to achieve a higher-order k_{BDF} of time accuracy by considering the numerical solution

(S_t) at the current time $(n_t + 1)$ and during the previous k_{BDF} time levels $(n_t, n_t - 1, \dots, n_t + 1 - k_{BDF})$ [130, 204]. However, the BDF method is only unconditionally stable with the 1st (BDF1) and 2nd (BDF2) orders [205, 206, 207]. Thus, the present study will be limited to those two first orders. The BDF1 scheme solves the transient term by storing the current and previous solution as expressed by equation (6-12) while the BDF2 scheme considers the previous solution at an additional time as expressed by equation (6-13) [130, 203, 207].

$$\frac{d}{dt}(S_t)^{n_t+1} = [(S_t)^{n_t+1} - (S_t)^{n_t}] \frac{1}{\Delta t} \quad (6-12)$$

$$\frac{d}{dt}(S_t)^{n_t+1} = \left[\frac{3}{2}(S_t)^{n_t+1} - 2(S_t)^{n_t} + \frac{1}{2}(S_t)^{n_t-1} \right] \frac{1}{\Delta t} \quad (6-13)$$

6.4 Numerical Methodology

The computational cost assessment of the hybrid resolved method presented in *section 5.7* of Chapter 5 [44] revealed the VOF-Lagrangian approach is significantly more expensive under lower pressure conditions and higher momentum flux ratios because of the resulting larger spray width and height, which requires additional modelling efforts from both VOF and Lagrangian phases. Indeed, the average solver CPU time per time step normalized by the total number of CPUs Δt_{CPU} is 119% higher with the experimental conditions from Madabhushi et al. [30] compared to the higher-pressure conditions from Freitag and Hassa [109] despite their relatively similar initial mesh size. In addition to having a higher momentum flux ratio ($J=33.6$), the dataset from Madabhushi et al. [30] consists of a turbulent liquid fuel jet (Jet A) injected at higher velocity ($u_{jet} = 31$ m/s, $Re_{jet} = 1.2E+04$) into a higher-speed turbulent crossflowing air stream ($u_g = 138$ m/s, $Re_g = 6.1E+05$). This implies that the numerical models have to deal with strong velocity gradients, which could put more strain on the computational cost and predictive capabilities of the VOF-Lagrangian approach. Its significantly higher jet Weber Number and relatively high gas Weber number ($We_g = 720$, $We_{jet} = 24711$) could also be further contributing to increasing the computational cost as it suggests an enhanced breakup process from the liquid jet column. Thus, the ability of the proposed optimized hybrid stripping method to improve the affordability of the VOF-Lagrangian approach while maintaining an acceptable accuracy will be assessed under the most computationally

demanding conditions from the dataset of Madabhushi et al. [30]. The results will be compared to those previously obtained using the hybrid resolved method under the same conditions.

The numerical domain previously used to assess the hybrid resolved method that is presented in **Figure 5-2** of *section 5.4* from Chapter 5 is re-used in the present study. It includes the outlet geometric features of the plain orifice injector ($d = 0.762$ mm, $L/d = 16.7$) used during the experiments conducted by Madabhushi et al. [30] as well as the cross-section area of the rectangular test section ($H = 101.6$ mm, $W = 50.8$ mm). To improve convergence, an additional length was added upstream and downstream of the measurement plane ($\Delta x_m = 25.4$ mm) and the zone numerically studied ($-2.7 \leq x/d \leq 60$).

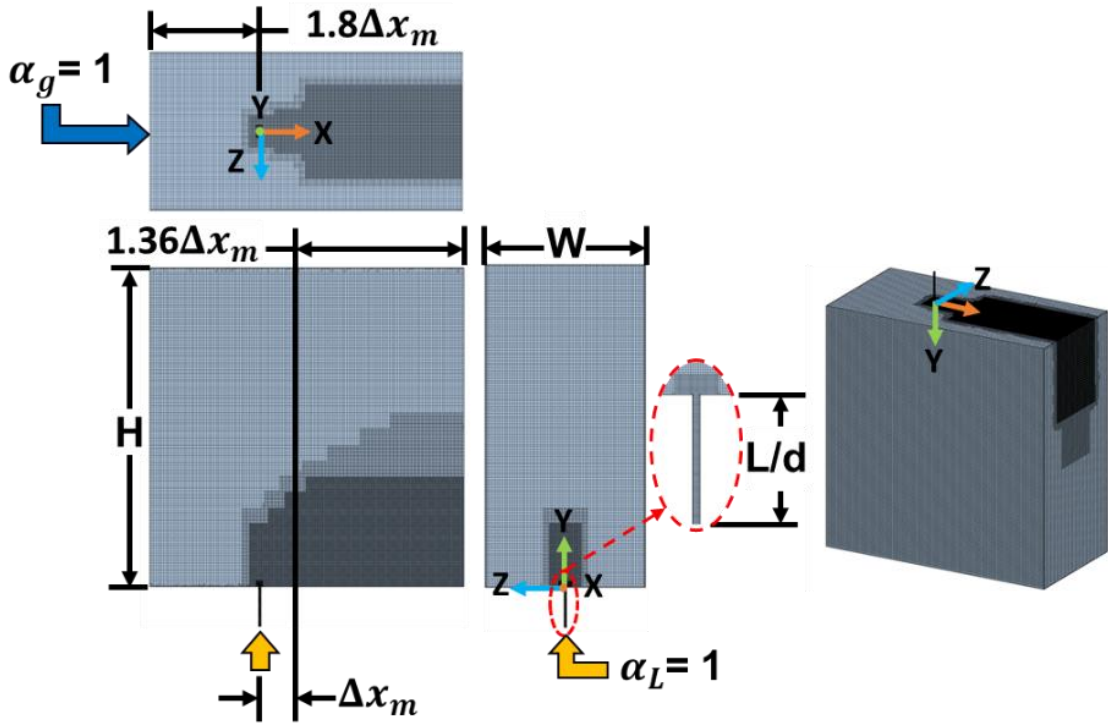


Figure 6-2: Numerical domain and cross-section planes (XY at $z/d=0$, XZ at $y/d=2$ and YZ at $x/d=0$) of the baseline mesh for the optimized hybrid stripping method.

Both methodologies have the same baseline hexahedral volume mesh, except in the far-field region. With the hybrid resolved method, the mesh in the far-field region was dynamically refined from 0.4 mm to 0.2 mm as the Lagrangian droplets were progressing in the domain to reduce the computational cost while the near-field spray was being formed. However, this is not deemed necessary for the optimized hybrid stripping method considering the significantly smaller adapted mesh size expected. Although the extra

computational cost associated with this additional AMR setting is estimated to be small, it could end up being counterproductive in this instance. Thus, the mesh is uniformly refined to 0.2 mm in the spray region and to 0.1 mm inside the injector and near its exit. The numerical domain and the cross-section pictures of the baseline mesh used for the optimized hybrid stripping method are presented in **Figure 6-2**. The resulting baseline mesh is constituted of 9.24 million elements, which is 3.4 times the baseline mesh size previously used with the hybrid resolved method.

All simulations were conducted using Simcenter STAR-CCM+. As detailed in *section 6.3*, there are some similarities and differences between both numerical methodologies, which are highlighted in **Table 6-1**. They both consider the properties of the VOF phases and Lagrangian droplets to be constant as evaporation is not modelled due to the ambient conditions used for validation. Moreover, the values imposed for the SSD breakup model constants follow the recommendations from the parametric study conducted in Chapter 3 to improve the accuracy of the SMD predictions and enhance the spray width.

To assess the effect of using a higher-order temporal discretization scheme with the optimized hybrid stripping method, only the flow solvers are modified by replacing the BDF1 scheme with the BDF2 scheme. The entire unsteady simulation procedure was repeated with the BDF2 scheme, which first involves establishing the unsteady continuous gas flow field before injecting the VOF liquid phase. The VOF-Lagrangian transition model is enabled once the VOF liquid jet column has stopped progressing in the domain, which indicates the VOF liquid mass is stabilized.

The AMR settings are first optimized for the hybrid stripping method based on the recommendations made in the previous VOF-Lagrangian approach study presented in Chapter 5 [44]. Thus, the upstream swept distance is reduced to prevent the detection of an over-smearred interface. To further reduce the computational cost, the number of AMR levels is also reduced, and the minimum element size is increased. To avoid any potential mass imbalance problems due to the coarser interface resolution expected, the criterion used to detect the interface is doubled and the mesh is adapted more frequently. The differences in the AMR settings used by both methodologies are highlighted in **Table 6-2**.

Table 6-1: Numerical models comparison between the hybrid resolved method and the proposed optimized hybrid stripping method.

Models	Hybrid resolved method	Optimized hybrid stripping method
Turbulence	• LES • WALE Subgrid Scale model [134] • All y^+ Wall Treatment	
Flow	• Segregated flow solver with 2nd order convection scheme • Implicit Unsteady with BDF1 temporal discretization scheme • Adaptive Time-Step	
Lagrangian	• Two-way coupling • SSD breakup model [33, 34] ($B_1 = \sqrt{3}$, $K_3 = 1$, $K_0 = -0.1$ and $K_1 = 0.1$ [42]) • Drag Force with TAB Distortion model [151, 165, 175] (Distorted droplet) • Pressure Gradient Force	
VOF	• HRIC convection scheme	• 1 st order convection scheme
	• 1st Order density reconstruction • Surface tension force (CSF model)	
VOF-Lagrangian	• Resolved Transition model	• Stripping Transition model
	• Blob Detection Model • VOF-Lagrangian Impingement • Free Surface AMR	

Table 6-2: AMR settings comparison between the hybrid resolved method and the proposed optimized hybrid stripping method.

AMR settings	Hybrid resolved method	Optimized hybrid stripping method
AMR levels	5	4
Minimum adaptation cell size [μm]	10	15
Interface detection [cells]	5	10
Upstream Swept distance factor	1.5	1.0
Downstream Swept distance factor	1.5	
Transition width between levels [cells]	2	
Adaptation frequency [time steps]	10	5
Adaptive Mesh Interpolation	Sharp reconstruction	N/A

As detailed in *section 6.3.2*, an additional stripping criterion was introduced to limit the VOF-Lagrangian transition based on the maximum AMR level. Thus, the AMR settings imposed restrict the VOF-Lagrangian transition to only occur from interface cells where $L_{AMR\ Max-1} \geq 50\ \mu\text{m}$, which should cover up to 3 AMR levels. Moreover, the baseline mesh size used within the spray region suggests that the droplets stripped in the present

study should have a diameter between 25 μm to 100 μm according to the minimum adapted cell size condition imposed.

Regarding the target stripping mass flux, its value could be set to an astronomically large number (e.g. $10^{1000} \text{ kg/m}^2\text{s}$) to force the stripping mechanism into using the local VOF mass available in the cell. Although this strategy has the advantage of removing the need to estimate inputs, it might compromise the affordability of the optimized hybrid stripping method as it could generate a significantly large number of stripped particles according to equation (6-11). Indeed, a preliminary study conducted on the effect of the target mass flux by varying its value from $1000 \text{ kg/m}^2\text{s}$ to $10000 \text{ kg/m}^2\text{s}$ found that the number of particles generated within the same time frame increased proportionally to $(\dot{m}_{L,s}'')_{Target}$. This also indicates that the VOF mass available in the cells tends to be much larger than the target mass specified for the conditions used in the present study. In addition, increasing the target mass flux tends to increase the frequency of the stripping transition process. Thus, it is likely more computationally efficient to impose a value that would yield a target stripping mass smaller than the VOF mass available in the interface cell. Replacing equation (6-7) and equation (6-8) into this condition $((m_{L,s})_{Target} < m_L)$ gives the following expression for the maximum stripping mass flux.

$$(\dot{m}_{L,s}'')_{Target} < \frac{\rho_L l_{cd}}{6\Delta t} \quad (6-14)$$

The maximum value to impose can be estimated by replacing the liquid density ρ_L with the initial jet density and by replacing the time-step Δt with the average adapted value before activating the VOF-Lagrangian transition model. Considering the interaction length scale between the Lagrangian particles and VOF liquid phase can be estimated using the SMD [130], it is suggested to use instead the target diameter $(D_{p,s})_{Target}$ value calculated using the minimum adapted cell size, which should be 50% of the latter. This gives a maximum $(\dot{m}_{L,s}'')_{Target}$ value of approximately $32500 \text{ kg/m}^2\text{s}$ for the conditions and mesh resolution used in the present study. Considering that targeting a stripping VOF mass too small might prevent the transition process from occurring altogether as mentioned in *section 6.3.2*, the stripping mass flux was set to $1000 \text{ kg/m}^2\text{s}$ as it corresponds to the smallest value used during the preliminary assessment that successfully transitioned the VOF liquid phase.

As indicated in **Table 6-1**, both methodologies use adaptive time-stepping to efficiently maintain the courant number at the interface inferior to 0.5 when using the HRIC convection scheme or lower than 0.5-0.7 depending on the implicit temporal discretization (BDF2-BDF1) when using the 1st order Upwind convection scheme [130, 195]. To further improve the computational efficiency, the number of inner iterations is also dynamically adapted based on the asymptotic values of the residuals. The larger minimum cell size and lower order VOF convection scheme used by the optimized hybrid stripping method allowed the adapted time-step size to be on average twice as large as with the hybrid resolved method. Indeed, the time-step was adapted on average to 0.08 μ s when using the hybrid optimized stripping method with the BDF1 scheme, which even increased by 5% on average with the BDF2 scheme.

6.5 Results

The adapted mesh from both numerical methodologies is compared in **Figure 6-3**. It can be seen that the coarser AMR settings of the optimized hybrid stripping method operate as intended. Indeed, they are not over-refining the cells surrounding the liquid jet column and do not tend to refine cells located outside the latter. In fact, its adapted mesh had 10 million elements on average, which is only an 8.4% increase from its baseline mesh size. In comparison, the AMR settings used with the hybrid resolved method resulted in an adapted mesh size on average 37 times larger than its baseline mesh size. Therefore, the optimized AMR settings proposed were successful in reducing the adapted mesh size with an average decrease of 90% compared to the hybrid resolved method despite its smaller baseline mesh size.

Figure 6-4 compares the instantaneous image of the VOF interface and Lagrangian droplets scaled by their diameter 65 μ s after activating the VOF-Lagrangian transition with the optimized hybrid stripping method to the snapshots taken within the same time frame presented in **Figure 5-11** of *section 5.7* from Chapter 5 [44]. Compared to the hybrid resolved method, the proposed methodology does not capture the dispersed VOF liquid droplets resulting from the column shedding process and results in a smooth interface. This indicates that the aerodynamic effects on the jet surface are not as well captured, which was expected considering the coarser mesh resolution and lower-order VOF convection scheme used. However, the presence of Lagrangian droplets in the

domain confirms the hypothesis that the stripping transition model does not require capturing a sharp interface to transition the VOF liquid phase within the interface cells.

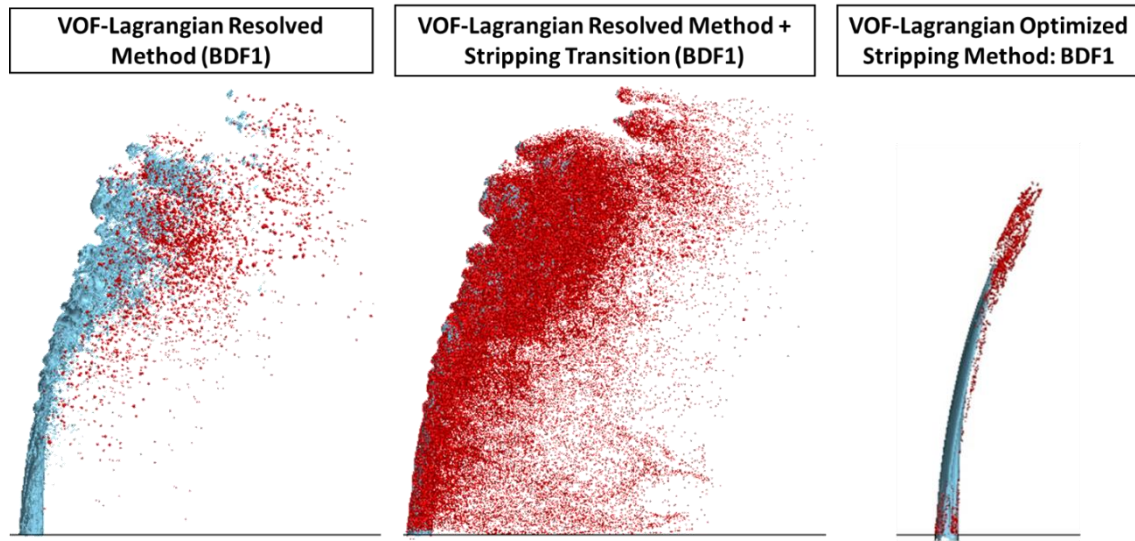


Figure 6-3: Instantaneous VOF liquid phase (blue) and Lagrangian particles (red) 65μs after enabling the VOF-Lagrangian transition for different numerical methodologies.

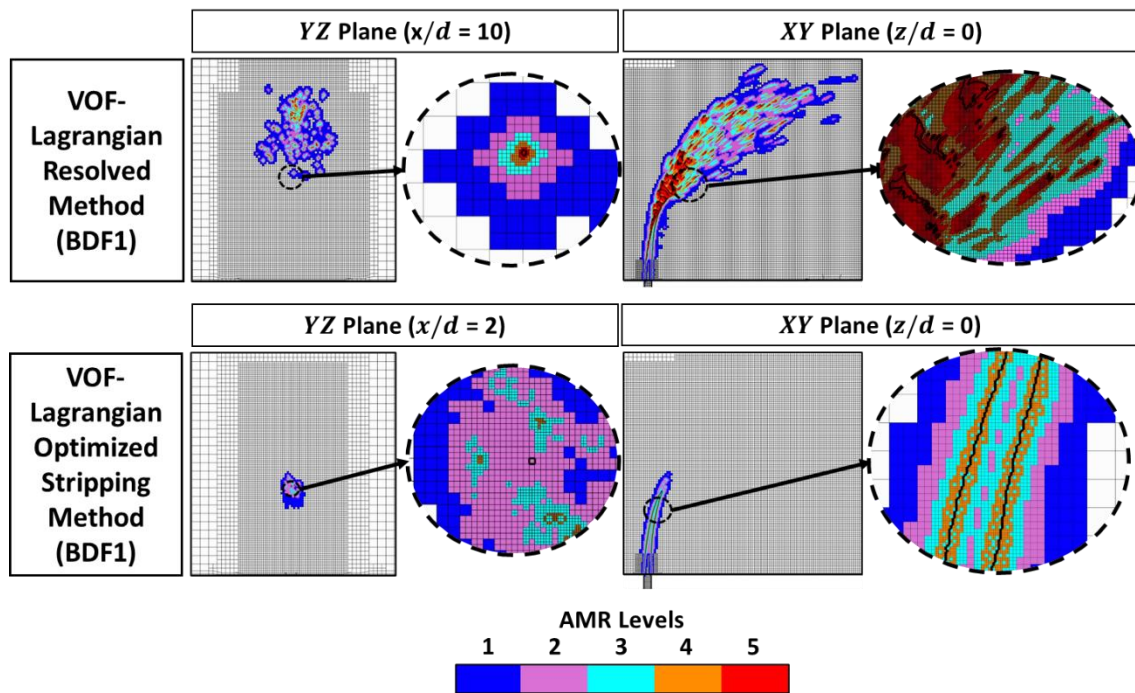


Figure 6-4: Instantaneous adapted mesh on the YZ and XY ($z/d = 0$) cross-section planes coloured by the AMR levels (black outline: instantaneous VOF interface).

It is also possible to observe in **Figure 6-4** that unlike the hybrid resolved method coupled with both transition models, the optimized hybrid stripping method introduces far fewer Lagrangian droplets in the domain within the same timeframe and only from cells located

within the leeward region of the liquid jet column. This confirms that the VOF-Lagrangian impingement model and the stripping criterion selected are restricting the VOF-Lagrangian transition mechanism. Therefore, it can be concluded that the proposed numerical set-up has the expected behaviour regarding the atomization modelling.

The predictive capabilities can now be assessed for the Sauter Mean Diameter (SMD) and droplet axial velocity by comparing the numerical predictions with the experimental measurements from Madabhushi et al. [30] taken at the centreline ($z/d=0$) of a YZ cross-section plane located $x/d \approx 33$ downstream the injector. The predictive capabilities in spray trajectory are assessed by comparing the numerical predictions to the correlations derived by Farvardin et al. [111] and Tambe et al. [81] by conducting turbulent liquid fuel jets in crossflow experiments under ambient conditions with similar turbulence and atomization characteristics.

Error zones representing a conservative deviation of $\pm 10\%$ from the experimental data and correlations are added to the graphics to help visualize the discrepancies with the numerical predictions. The error band was selected following an exhaustive literature review on the experimental uncertainties reported with similar data collection procedures for the imaging techniques used by Farvardin et al. [111] and Tambe et al. [81] to extract the spray trajectory correlations and for the laser instrumentation used by Madabhushi et al. [30] to obtain the droplet properties. Further details can be found in *section 5.5* of Chapter 5 [44].

The predictions obtained with the URANS numerical methodology previously developed and validated in Chapter 3 and Chapter 4 [42, 43] are included in the graphics to provide a visual reference with the most affordable numerical methodology developed throughout this work. However, the analysis and discussion are limited to comparing the different VOF-Lagrangian methodologies. A detailed comparison of the hybrid resolved method and URANS stochastic Lagrangian method can be found in Chapter 5 [44].

The results shown in the graphics and contours are time-averaged at a constant interval of $1 \mu s$ while the images showcasing the Lagrangian droplets are instantaneous. The contours are presented on the XY cross-section plane ($z/d=0$) with the time-averaged outline of the VOF liquid interface. Unless otherwise specified, the Lagrangian droplets

represented are scaled by their diameter and all the images presented are cropped between $-15 \leq x/d \leq 60$ and $y/d \leq 60$ to better visualize the measurement zone.

6.5.1 Spray Trajectory

Figure 6-5 shows that for the same temporal discretization scheme, the optimized hybrid stripping method predicts an overall spray trajectory on average 6% smaller than the hybrid resolved method. The discrepancies in spray trajectory mainly occur in the first half of the spray region ($x/d \leq 30$) where the relative difference is on average 8%. Indeed, there are no significant differences in the far-field region ($30 < x/d \leq 60$) as the average relative difference decreases to 3%.

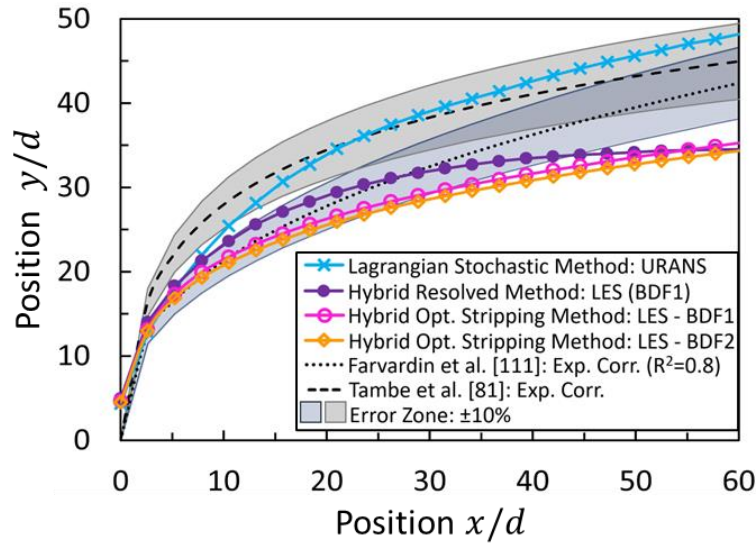


Figure 6-5: Time-averaged maximum spray trajectory for different VOF-Lagrangian transition methods and temporal discretization schemes.

Moreover, the optimized hybrid stripping method tends to predict a slightly lower overall spray trajectory compared to the hybrid resolved method regardless of the temporal discretization scheme used. This results from the non-significant impact of the temporal discretization scheme on the spray trajectory predicted by the former. Although it can be observed in **Figure 6-5** that the BDF2 scheme tends to predict a spray trajectory slightly lower than the BDF1 scheme, the relative difference is only 3% on average across the entire spray and within both breakup regions.

Compared to the empirical correlations previously selected [81, 111], the VOF-Lagrangian approach tends to underpredict the overall spray penetration regardless of the

transition method used with the same temporal discretization scheme. Indeed, the overall spray trajectory is on average 16% lower with the optimized hybrid stripping method and 11% lower with the hybrid resolved method. Although the latter tends to underpredict less the overall spray trajectory, its absolute relative error of 14% is not significantly different from the optimized hybrid stripping method's absolute relative error of 16%. Moreover, the latter tends to agree more with the empirical correlation from Farvardin et al. [111] within the primary breakup region as it locally underpredicts the trajectory on average by 3% lower while the hybrid resolved method locally overpredicts it by 5%. This opposite prediction trend in the primary breakup region balances their underprediction of the far-field region trajectory, which leads to both methods having an absolute relative error of 9% compared to the empirical correlation from Farvardin et al. [111]. Thus, the transition method does not significantly impact the average accuracy of the VOF-Lagrangian approach when it comes to predicting the overall spray trajectory. This conclusion is also applicable regardless of the temporal discretization scheme used by the optimized hybrid stripping method because of the similar spray trajectories predicted by the BDF1 and BDF2 schemes within both breakup regions.

6.5.2 Droplet Velocity

Figure 6-6 shows that for the same temporal discretization scheme, the optimized hybrid stripping method tends to predict a centreline droplet axial velocity on average 15% higher than the hybrid resolved method. Although the discrepancies in the leeward region ($y/d \leq 10$) are not significant as the average relative error is only 3%, they tend to increase with the transverse distance up to the windward interface. Indeed, the average relative difference increases to 17% within the spray core region ($10 < y/d \leq 20$) and to 25% within the windward region ($20 < y/d \leq 30$) before decreasing to 8% on average near the windward interface ($y/d > 30$).

Compared to the experimental data from Madabhushi et al. [30], the VOF-Lagrangian approach tends to overpredict the droplet axial velocity in the leeward spray region regardless of the transition method used with the same temporal discretization scheme. While the accuracy of the hybrid resolved method significantly improves above the leeward region, the opposite occurs with the optimized stripping method as its overprediction of the droplet axial velocity tends to increase with the transverse distance.

However, the accuracy of the latter improves near the windward interface as its prediction falls within $\pm 10\%$ of the experimental data. Moreover, the shape of its centreline profile in this region agrees better with the experimental one as they are both characterized by a decrease in axial droplet velocity near the windward interface.

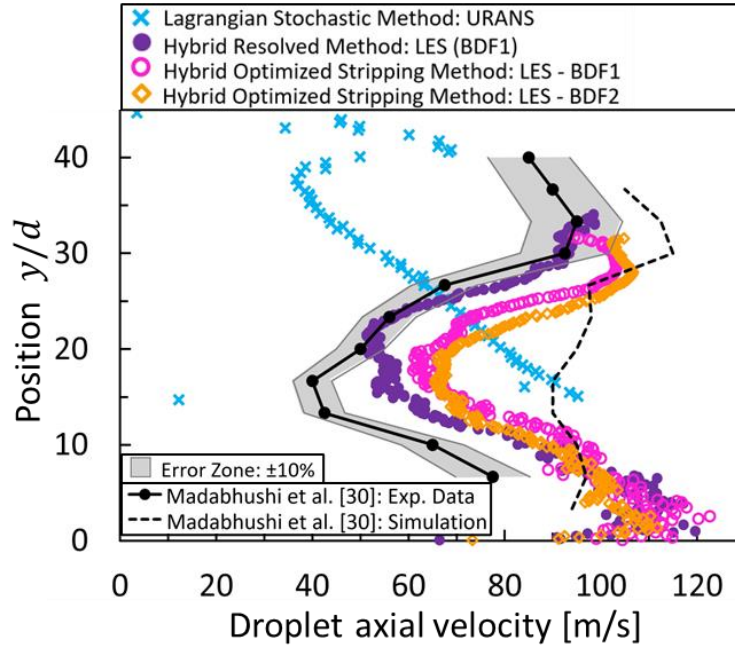


Figure 6-6: Time-averaged centreline droplet axial velocity for different VOF-Lagrangian transition methods and temporal discretization schemes.

In addition, the optimized hybrid stripping method tends to overpredict the droplet axial velocity regardless of the temporal discretization scheme used. Although using the BDF2 scheme tends to reduce the accuracy in the windward region ($20 < y/d \leq 30$) as it predicts a droplet axial velocity on average 9% higher than the BDF1 scheme, it does not have a significant impact below or above this region. In fact, using the BDF2 scheme tends to slightly decrease the droplet axial velocity on average by 3% below the windward region ($y/d \leq 20$) and to slightly increase it by 3% above it ($y/d > 30$). As a result, the average relative difference in centreline droplet axial velocity across the spray height is only 1%. Thus, it can be concluded that the temporal discretization scheme does not have a significant impact on the predictive capabilities of the optimized hybrid stripping method for the droplet velocities.

6.5.3 SMD

As shown in **Figure 6-7**, the VOF-Lagrangian approach tends to underpredict the centreline SMD compared to the experimental data from Madabhushi et al. [30] across the entire spray height regardless of the transition method when using the same temporal discretization scheme. Although the optimized hybrid stripping method tends to predict a centreline SMD on average 10% smaller than the hybrid resolved method, its lesser agreement with the experimental data is confined to the windward and spray core regions ($10 < y/d \leq 30$) where the centreline SMD predicted is on average 20% smaller. In fact, the optimized hybrid stripping tends to be more accurate within the leeward spray region ($y/d \leq 10$) and near the windward interface ($y/d > 30$) as it predicts a larger centreline SMD on average by 6% and 19% respectively. Moreover, similar to its predictions in the centreline droplet axial velocity profile near the windward interface, the shape of the centreline SMD profile agrees better with the experimental one as they are both characterized by a local increase in droplet sizes.

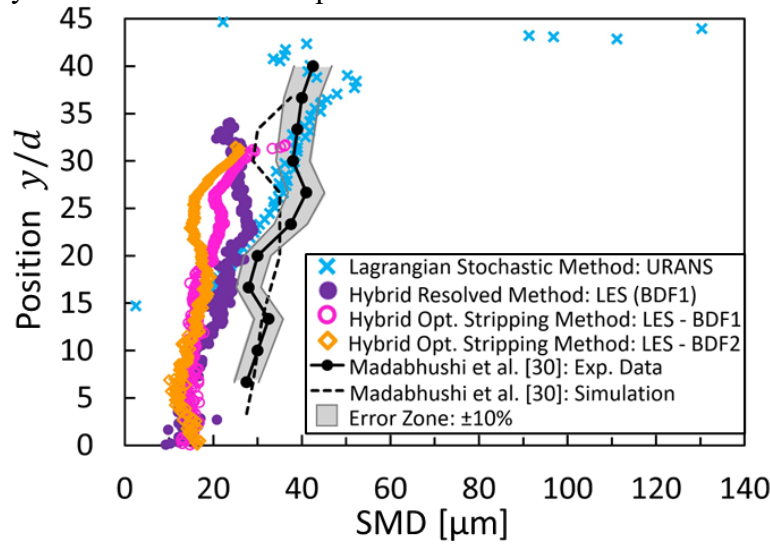


Figure 6-7: Time-averaged centreline SMD for different VOF-Lagrangian transition methods and temporal discretization schemes

The tendency of the optimized hybrid stripping method to enhance the underprediction of the overall centreline SMD is independent of the temporal discretization scheme. Indeed, the BDF2 scheme predicts an average centreline SMD 9% smaller than the BDF1 scheme. Although the temporal discretization scheme does not have a significant impact on the accuracy within the leeward and spray core regions ($y/d \leq 20$) considering the

relative difference is only 3% on average, it tends to significantly underpredict the SMD at higher transverse distances. Indeed, the main source of discrepancy is located above the spray core region ($y/d > 20$) as the average relative difference increases to 20%.

6.6 Discussion: VOF-Lagrangian Methodology

The results previously presented on the effect of the VOF-Lagrangian transition method show that the optimized hybrid stripping method tends to predict a lower spray trajectory, smaller centreline SMD and higher centreline droplet axial velocity. Although the discrepancies in spray trajectory and droplet velocity can be attributed to differences in the modelling of the VOF liquid phase and the VOF phase interactions in the near-field region, those in droplet diameter are more likely caused by the stripping mechanism and the related imposed stripping criterion.

Despite the tendency of the optimized hybrid stripping method to yield higher discrepancies with the experimental data, its predictive capabilities agree with those reported in the literature using other alternative VOF-Lagrangian transition/coupling methodologies to lower its cost. Indeed, decoupling the VOF-Lagrangian approach also tends to underpredict the average SMD [27, 38] and spray trajectory [27] when using the SSD [38] or Wave [27, 38] breakup models. It also tends to underpredict the SMD within the leeward and spray core regions [27, 38] as well as overpredict the local droplet axial velocity [38]. The deterministic stripping transition model proposed by Fontes et al. [41] also tends to predict lower droplet diameters in regions where the droplet velocity is overpredicted. In addition, the predictive capabilities of both methodologies proposed in this work tend to agree with those reported in the literature for coupling the Lagrangian approach with an interface-capturing method, such as the VOF approach. Indeed, regardless of the transition model (resolved/stripping), transition methodology (coupled/decoupled), secondary breakup model (stochastic/deterministic) or operating conditions used, the hybrid approach tends to underpredict the spray trajectory [27, 35, 36, 39, 156] and the average SMD/droplet size distribution [27, 38, 40, 41].

6.6.1 Hybrid Methodology: Effect on Spray Trajectory

The discrepancies in spray trajectories between both transition methods can be explained by their respective modelling of the VOF liquid phase and its resulting influence on the

properties of the Lagrangian droplets. For the hybrid resolved method, the near-field spray is mainly constituted of the VOF blobs shedding from the VOF liquid jet column. **Figure 6-8** shows that the VOF blob cloud, which is represented by the instantaneous position of the VOF interface at a given time-step, penetrates almost 1.9 times the height and 15.4 times the length of the liquid jet column, which is represented by the time-averaged position of the VOF interface. Thus, the spray trajectory in the primary breakup region is mostly governed by the penetration of the VOF blobs when using the hybrid resolved method.

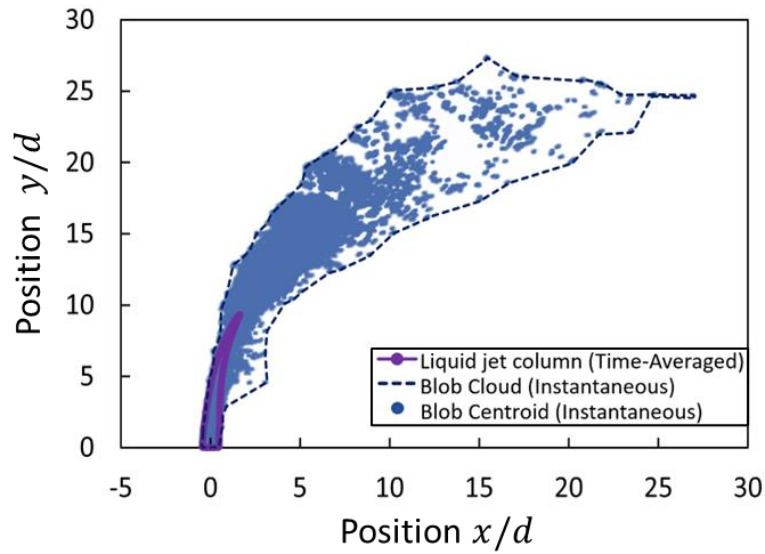


Figure 6-8: Instantaneous (blob cloud) and time-averaged (jet column) position of the VOF interface for the hybrid resolved method.

However, it is the opposite with the optimized hybrid stripping method which removes the need to generate a large number of VOF blobs by limiting the influence of the VOF liquid phase on the Lagrangian droplets to the modelling of the jet column. As a result, the average blob count generated during the transition process of the optimized hybrid stripping method was 1.03 blobs per time step compared to 8982.26 blobs per time step for the hybrid resolved method, with the minimum possible value of 1 representing the liquid jet column. This explains why the time-averaged and instantaneous positions of the VOF interface predicted with the optimized hybrid stripping method shown in **Figure 6-9** are more similar, which indicates that the VOF blob cloud is almost non-existent. Although the jet column penetration is on average 17% higher and 19% longer than the hybrid resolved method, the interface resolution is not sufficient to capture a vertical penetration similar to the resolved VOF blob cloud's maximum height. This could explain

the tendency of the optimized hybrid stripping method to underpredict the overall spray trajectory as described in *section 6.5.1*.

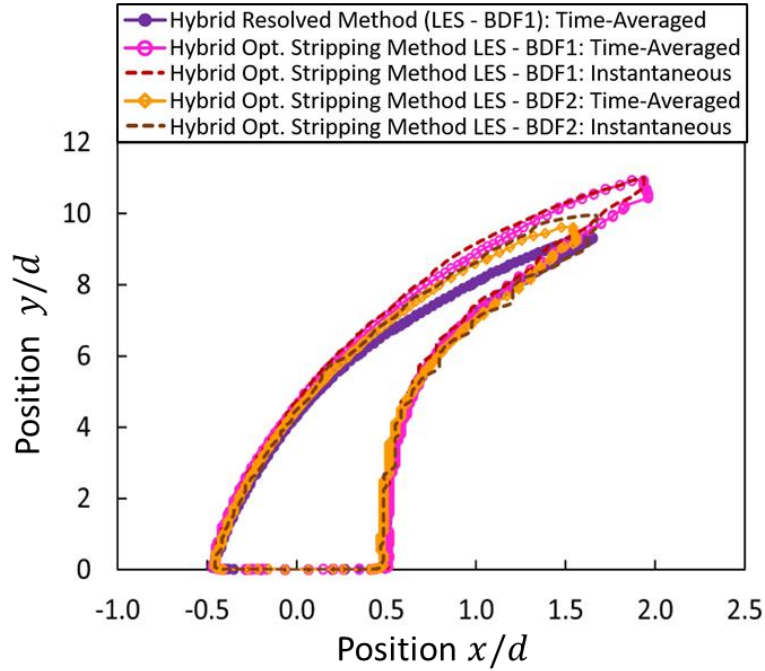


Figure 6-9: Instantaneous (blob cloud) and time-averaged (jet column) position of the VOF interface for the optimized hybrid stripping method with different temporal discretization schemes.

The lower discrepancies in spray trajectory within the far-field region, which is dominated by the presence of Lagrangian droplets for both methods, can be explained by their interactions with the continuous phase. As explained in *section 5.6* of Chapter 5 [44], the Lagrangian droplets transformed by the hybrid resolved transition method mostly inherit their properties from the VOF blobs located within the primary breakup region. As shown in **Figure 6-8**, the VOF-Lagrangian transition can occur quite far away from the jet column breakup point as the VOF blobs were found to travel up $x/d = 32.5$ during the transition process, which is over half the spray length analyzed. It is also coincidentally close to the region where the axial relative change in spray trajectory becomes non-significant (lower than 2%) as seen in **Figure 6-5**. This indicates that the spray trajectory in the far-field region is strongly limited by the penetration of the VOF blob cloud for the hybrid resolved method. Moreover, the maximum spray trajectory point is 26% higher than the VOF blob cloud's maximum penetration with the hybrid resolved method. This difference is significantly more important with the optimized hybrid stripping method as the maximum spray trajectory is on average 2.2 times higher than the maximum

penetration of the jet column. This indicates that the Lagrangian droplets interact more with the continuous phase when using the optimized hybrid stripping method, which results in a stronger influence of the continuous phase interactions on the overall spray properties.

Therefore, refining the AMR settings to better capture the maximum penetration of the liquid jet column could potentially result in the hybrid stripping method agreeing better with the experimental correlations from Farvardin et al. [111] and Tambe et al. [81]. To avoid impacting the computational cost, a user-defined function could be developed to restrict the use of an additional AMR level to the interface cells located above a specified transverse distance close to the expected maximum penetration of the liquid jet column. This approach would require a rough estimate of the jet column breakup point coordinates, which can be obtained using different empirical correlations available in the literature such as those summarized by Broumand and Birouk [9] and references therein. Alternatively, the application of an additional AMR level could be determined based on the local jet column bending by tracking the position of the interface cells. The cells only go through further refinement if they are located within and after the region where the initial variation in the horizontal position of the liquid VOF phase is significant, which indicates that the jet column is bending as it gets closer to reaching its maximum penetration. Although it is expected that more work will be required to successfully implement this approach, it has the advantage of not depending on any empirical estimation of the jet column penetration.

6.6.2 Hybrid Methodology: Effect on Droplet Velocity

As explained in *section 4.5.1* from Chapter 4 [43], the droplet velocity for jets in crossflows is expected to increase with the axial distance until it reaches a constant value close to the average gas phase velocity, which marks the completion of the momentum exchange between the droplets and continuous phases. **Figure 6-10** shows that the evolution of the droplet velocity with the hybrid resolved method follows the expected behaviour. Indeed, it predicts that the droplet velocity increases with the axial distance and that the rate of change is much higher in the primary breakup region, which is where most of the momentum exchange is expected to occur as detailed in *section 4.5.1*. However, this is not the case with the optimized hybrid stripping method as the droplet

velocity is almost constant over a short distance immediately after the jet column breakup point until it starts increasing again to much higher values and at a faster rate than the hybrid resolved method. Considering that both transition methods are predicting similar droplet velocities within the jet column region ($x/d \leq 2$) as the relative difference is only 2%, the discrepancies in the far-field region are likely caused by differences in the modelling of VOF phase interactions and the related impact on the Lagrangian droplets.

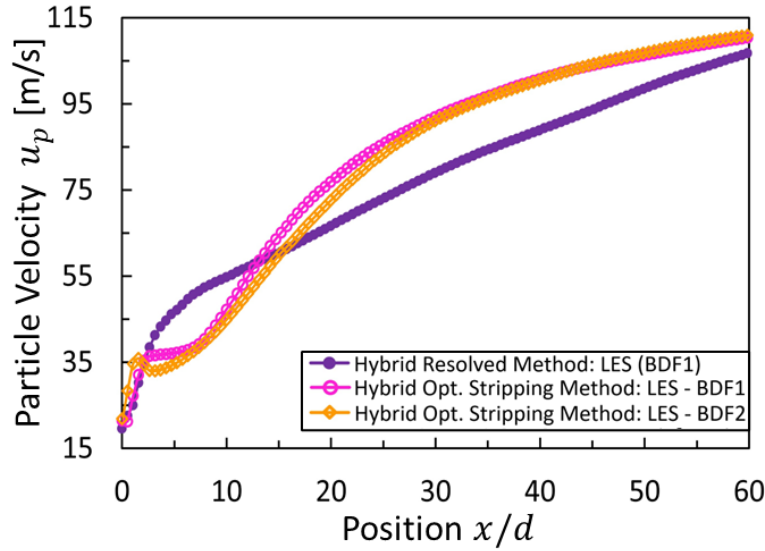


Figure 6-10: Time-averaged axial evolution of the droplet velocity magnitude u_p for different VOF-Lagrangian transition methods and temporal discretization schemes.

Using the two-way coupling model with the VOF-Lagrangian approach means that the effect of the VOF liquid jet column on the continuous gas phase velocity will indirectly impact the Lagrangian droplet properties. As shown in **Figure 6-11**, the VOF-Lagrangian approach captures the presence of a lower gas phase velocity zone in the wake of the liquid jet column regardless of the transition methods. Although the local velocity magnitude is much lower with the optimized hybrid stripping method, this low-velocity zone spreads further away downstream and penetrates to higher transverse distances with the hybrid resolved method. Therefore, while the Lagrangian droplets from the hybrid resolved method interact with a higher velocity flow near the jet column compared to the hybrid stripping method, they interact with an overall lower velocity flow on a longer axial distance. Hence why its average droplet velocity increases at a faster rate in the near-field region, but at a slower rate in the far-field region. Once the Lagrangian droplets from the hybrid stripping method have finished crossing their shorter and much lower velocity

zone, their velocity magnitude starts to increase again at a faster rate as seen in **Figure 6-10** because of their interaction with a higher gas velocity field. As a result, the droplet velocity predicted by the hybrid stripping method is on average 18% lower within the wake region of the jet ($2 < x/d \leq 10$) and on average 11% higher afterwards ($x/d > 10$).

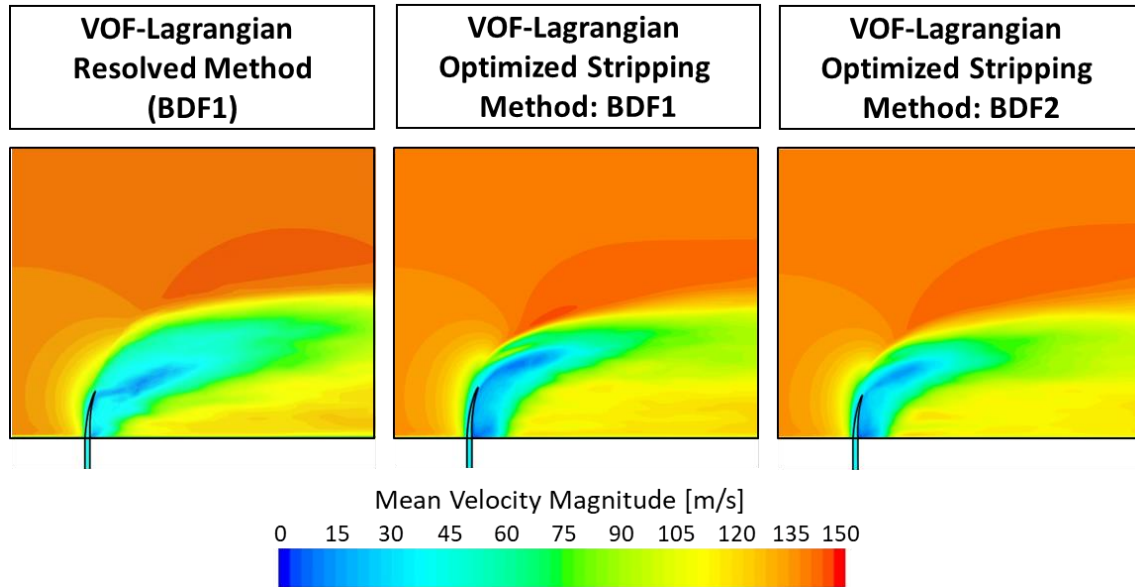


Figure 6-11: Time-averaged continuous phase velocity magnitude u for different VOF-Lagrangian transition methods and temporal discretization schemes (black outline: time-averaged VOF interface).

Considering the measurement plane used in **Figure 6-6** is located downstream of the recirculation zone, the discrepancies in VOF phase interactions observed in **Figure 6-11** are likely responsible for the hybrid stripping method overpredicting the centreline droplet axial velocity compared to the experimental data from Madabhushi et al. [30]. It should also be considered that the droplets are subjected to stronger velocity gradients when they exit the recirculation zone and disperse transversely, which could explain why the discrepancies within the leeward region are not as significant despite the local differences in velocity magnitude.

The differences in the modelling of the VOF phase interactions within the near-field region are likely caused by the hybrid resolved method shedding a significantly large number of VOF blobs from the liquid jet column's interface unlike the hybrid stripping method as explained in *section 6.6.1*. As a result, a large VOF blob cloud also interacts with the continuous flow behind the jet column region and even further downstream the injector, which is likely modifying the local flow properties that the Lagrangian droplets

are interacting with. Therefore, the predictions of the hybrid stripping method could probably be improved by having a similar resolution at the VOF liquid interface. However, this would go against the fundamental purpose of the proposed optimized hybrid stripping method because it would significantly increase the computational cost of the VOF-Lagrangian approach as previously demonstrated in *section 5.6* of Chapter 5. Therefore, the tendency of the optimized hybrid stripping method to overpredict the droplet axial velocity could be considered a limitation of the proposed lower-cost methodology.

6.6.3 Hybrid Methodology: Effect on SMD

The larger centreline SMD predicted near the windward interface by the hybrid stripping method can be attributed to the location of the largest stripped droplets. As explained in *section 5.5.4* from Chapter 5, the hybrid resolved method transitions the VOF blobs into large Lagrangian droplets across the entire spray height, which results in a more uniform distribution of the centreline SMD profile. However, this is not the case with the hybrid stripping method as the larger Lagrangian droplets are mainly stripped from the tip of the jet column as shown in **Figure 6-12**. As a result, the larger droplets tend to remain within the windward region even further downstream of the injector, which explains the local increase in centreline SMD. This also indicates that the stripping mechanism could be responsible for the underpredicted SMD within the spray core region. However, further analysis is required to rule out any overprediction of the breakup process caused by potential differences in the modelling of the VOF-Lagrangian phase interactions.

Figure 6-13 shows that the Lagrangian droplet diameter predicted by the optimized hybrid stripping method is on average 10% smaller across the entire spray length analyzed ($x/d \leq 60$). However, the discrepancies in average droplet diameter decrease as the droplets travel along the domain to eventually become non-significant in the far-field region with an average relative difference of only 2% ($x/d > 30$). Indeed, the most significant discrepancies are located within the jet column region ($x/d \leq 2$) where the relative difference is on average 37% followed by 15% from the wake region of the jet up to the maximum axial distance reached by the VOF droplet cloud as observed in *section 6.6.1* ($2 < x/d \leq 30$).

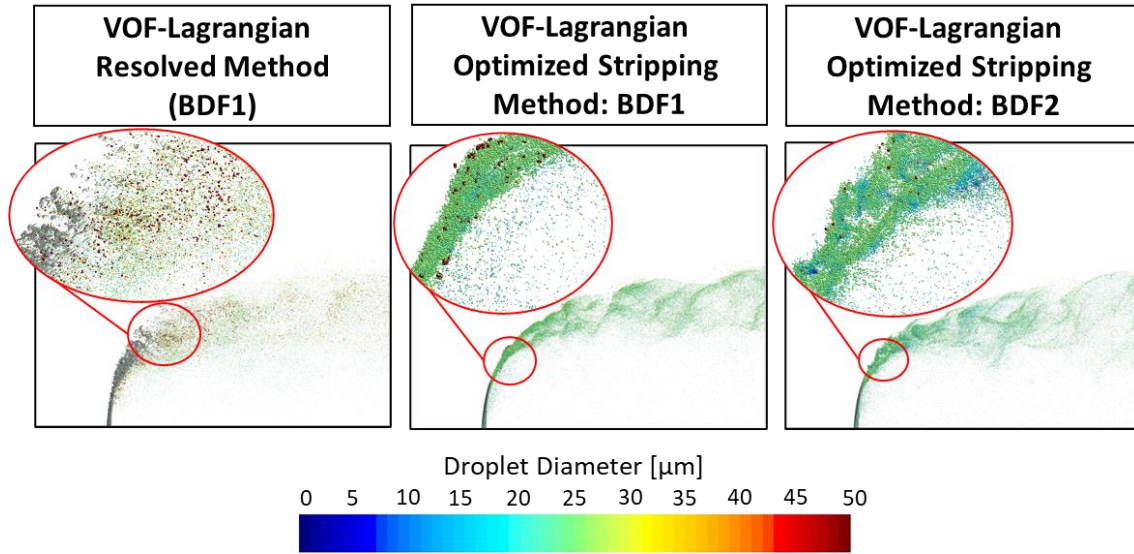


Figure 6-12: Instantaneous Lagrangian droplet diameter D_p for different VOF-Lagrangian transition methods and temporal discretization schemes (3D VOF interface in grey).

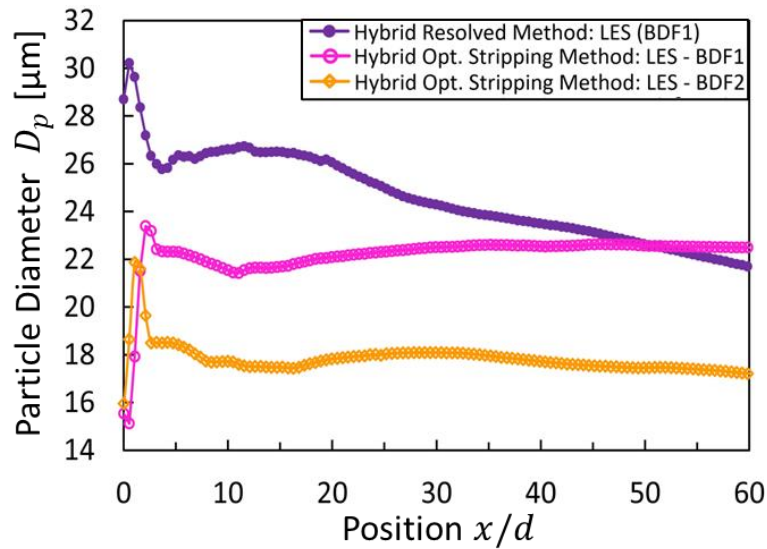


Figure 6-13: Time-averaged axial evolution of the average Lagrangian droplet diameter D_p for different VOF-Lagrangian transition methods and temporal discretization schemes.

The reduction in discrepancies with the axial distance can be attributed to the continuous decrease in droplet diameter predicted by the hybrid resolved method within the far-field region while the hybrid stripping method locally predicts no significant change in the average droplet size. This indicates that the latter predicts the breakup process to occur mainly within the near-field region, which can be attributed to the effect of the stripping transition on the properties of the Lagrangian droplets.

As described in equation (5-16), smaller parent droplets are more likely to breakup unless they become too small compared to the critical radius, which becomes larger with the axial distance due to the slip velocity decreasing as the droplets exchange momentum with the continuous phase. Thus, according to the SSD breakup model, the particles are expected to breakup mostly within the near-field region over a length that is controlled by the size and velocity of the initial Lagrangian particles introduced in the domain. With the VOF-Lagrangian approach, the maximum droplet diameter in the domain is limited by the transition method as the size of the initial parent droplets is directly inherited from the VOF blobs or the stripped droplets. Considering that the hybrid stripping method introduces significantly smaller parent particles in the domain as the VOF blob diameter within the jet column region is on average 30% larger, it inevitably restricts much more the occurrence of breakup further away from the jet column region. This explains why the droplet diameter predicted by the hybrid stripping method does not change significantly after the jet column region ($x/d > 10$) despite locally predicting a higher slip velocity magnitude that should be enhancing the breakup process as shown in **Figure 6-14**. Therefore, the stripped droplet diameter is the main factor limiting the breakup process and is responsible for the overall smaller centreline SMD predicted.

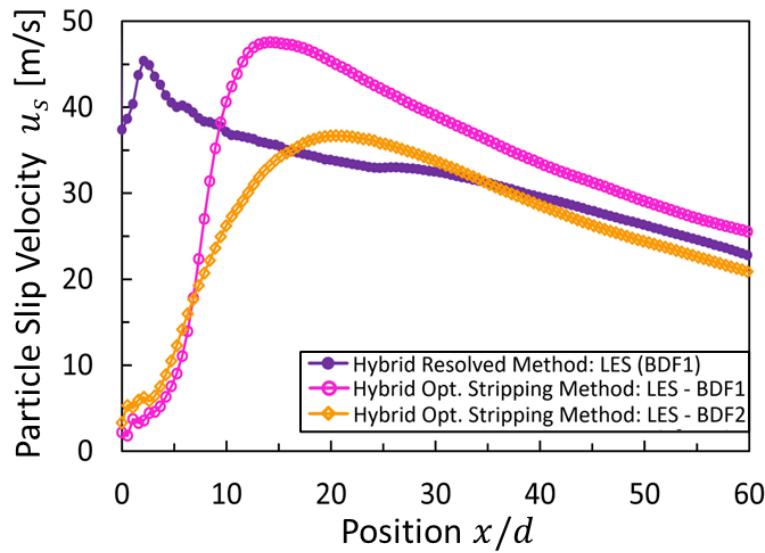


Figure 6-14: Time-averaged axial evolution of the average slip velocity u_s for different VOF-Lagrangian transition methods and temporal discretization schemes.

In addition, the method used to calculate the stripped droplet velocity can also be considered to have a significant impact on the breakup process due to its effect on the

particle slip velocity. Indeed, the slip velocity predicted by the hybrid stripping method is on average 94% smaller within the jet column region ($x/d \leq 2$) due to the stripped droplets inheriting their velocity components directly from the cells filled by the VOF interface [130]. **Figure 6-14** shows that it results in a local average slip velocity close to zero. Although the slip velocity rapidly increases within the wake region of the jet ($2 < x/d \leq 10$) to ultimately become higher than the hybrid resolved method's predictions, it is on average 53% smaller locally which necessarily limits the breakup process as it increases the critical radius size. Therefore, deriving the initial parent droplet velocity from the VOF interface instead of inheriting the VOF blob velocity prevents the droplet diameter from being significantly underpredicted by limiting the breakup process in the near-field region.

Considering the discrepancies in SMD are not caused by an overprediction of the breakup process, the predictive capabilities of the optimized hybrid stripping method could be improved. The stripping criterion could be further optimized to strip larger droplets while simultaneously taking advantage of the lower slip velocity predicted within the near-field region to ensure these larger droplets are also transported further downstream the injector. This is a more favourable outcome compared to the source of discrepancies in droplet velocity because the potential solution can be implemented while maintaining the low cost of the proposed methodology.

In order to provide appropriate recommendations for future work on improving the proposed stripping criterion, it is necessary to analyze its current effectiveness. As explained in *section 6.4*, an additional criterion was introduced to prevent the transition from occurring in the small cells generated at the maximum AMR level. Although the stripping process was successfully restricted to interface cells with an adapted size larger than 50 μm , it did not prevent stripping droplets smaller than 50% of this value considering the average stripped diameter was 19.9 μm with a standard deviation of 3.4 μm . Therefore, the stripping mechanism tends to override the target stripping diameter $(D_{p,s})_{Target}$ imposed to ensure the parcels stripped are physical as indicated by equation (6-9) [130]. This was expected due to the adapted cell size being larger than the actual cell size as mentioned in *section 6.4*, but it does not explain why the average stripped diameter is close to the minimum size anticipated of 25 μm . Despite the unexpectedly

smaller average stripped droplet diameter, the largest droplets stripped often reached the maximum size anticipated of 100 μm . This suggests that the VOF mass that could be stripped $m_{L,S}$ from the larger interface cells tends to be too small to produce a parcel with at least 1 particle.

As detailed in *section 6.4*, the optimized hybrid stripping method proposed consists of limiting $m_{L,S}$ to the target stripping mass $(m_{L,S})_{Target}$ by strategically imposing a small stripping mass flux. Therefore, the stripping criterion could be improved by dynamically adapting the stripping mass flux based on the adapted cell size. The stripping of larger droplets could be promoted without significantly impacting the number of particles by only increasing the mass flux in the interface cells associated with the lowest AMR level. The VOF mass accumulated in those cells could be tracked and replaced in equation (6-11) and equation (6-8) to determine the minimum mass flux value required to strip one particle with the largest possible diameter, which corresponds to 50% of the cell size. In addition, the stripping process could be limited based on the average cell size at the maximum AMR level instead of the adapted cell size, which can be misleading to use when trying to estimate the minimum stripped droplet diameter. However, strictly restricting the stripping transition to the bigger cells might require increasing the stripped mass flux overall. Thus, future work should be done to assess the computational cost of this additional modification to the stripping criterion formulation as it could increase the number of stripped droplets.

Alternatively, the stripping process within the larger cells could be promoted by removing the restriction imposed on the stripped diameter to allow transitioning droplets smaller than 50% of the cell size. However, this approach could be counterproductive to improving the predictive capabilities in the SMD. Indeed, the smeared VOF liquid phase and smaller VOF-Lagrangian interaction area density usually contained within the larger interface cells might not allow the stripping of proportionally large droplets. Therefore, it is recommended to first determine if relaxing the target diameter criterion in the larger interface cells can locally enhance the stripping process without resorting to only stripping significantly small droplets. If the approach is found to be viable, future work then needs to be done on implementing a non-deterministic stripping criterion that can efficiently restrict the minimum droplet size within the larger cells. Once again, this could

be done by tracking the VOF mass accumulated in the larger cells and using equation (6-11) with equation (6-10) to determine the largest droplet diameter that could be imposed to strip one particle.

6.7 Discussion: Temporal Discretization Scheme

The results obtained from changing the temporal discretization with the optimized hybrid stripping method show that using a higher order scheme tends to underpredict the overall SMD, but it does not have a significant impact on the overall predictions in spray trajectory or droplet velocity. Although the discrepancies in centreline SMD and droplet axial velocity both tend to increase and become much more important at higher transverse distance ($y/d > 20$), the relative difference in SMD is an order of magnitude higher. Therefore, the latter will be investigated first followed by the discrepancies in droplet velocity as it can potentially provide a better insight into the effect of the temporal discretization scheme on the interactions between the VOF phases and the Lagrangian droplets as well as the stripping breakup mechanism.

6.7.1 Temporal Discretization Scheme: Effect on SMD

Although the main discrepancies in centreline SMD and droplet axial velocity both occur within the windward region of the spray ($y/d > 20$), the BDF2 scheme predicts a local centreline particle slip velocity smaller by 7% on average. Moreover, it also predicts an average droplet diameter 19% smaller across the entire spray length analyzed ($x/d \leq 60$) despite simultaneously predicting a smaller particle slip velocity on average by 12% as shown in **Figure 6-13** and **Figure 6-14** respectively. Therefore, it is not possible to conclude that the BDF2 scheme underpredicts the overall SMD due to a general overprediction of the breakup process.

As shown in **Figure 6-12**, the BDF2 scheme tends to strip fewer droplets of larger size compared to BDF1. In fact, the maximum particle diameter stripped using the latter was on average 79 μm and often reached the expected maximum value of 100 μm as mentioned in *section 6.6.3*. In comparison, the largest droplets stripped with the BDF2 scheme were on average 37% smaller and their diameter always remained inferior to 50 μm . This suggests the BDF1 scheme predicts the larger cells have enough VOF mass to strip at least one particle, which means the VOF interface is smeared up to the baseline

cells. Despite the differences observed in the stripping mechanism, the stripped droplet properties are not likely the main source of discrepancies in SMD considering the relative difference in the average stripped diameter is less than 1%.

Nevertheless, it is possible to observe in **Figure 6-12** that the BDF2 scheme generates a few groups of significantly small particles with a droplet diameter smaller than $5\text{ }\mu\text{m}$ in both breakup regions. Analyzing the instantaneous images of the spray taken every 10 time-steps during the simulation revealed that the smaller particles stripped near the jet surface get caught in a recirculation zone when using the BDF2 scheme, which causes them to rapidly breakup into extremely smaller droplets. **Figure 6-15** shows the instantaneous position of the Lagrangian droplets scaled at a constant point size and coloured by their diameter. These snapshots were taken every $\approx 0.025\text{ ms}$ over a 0.4 ms period starting approximately 2 ms after activating the VOF-Lagrangian transition model ($\Delta t_{Lag.}$). The test section is represented from the injector (slightly upstream) up to the domain's exit.

Within the time frame selected, there are initially 3 distinct clusters of small droplets located near the jet column, which are circled using different dash styles. As the simulation time progresses, these clusters swirl and elongate behind the jet column until they are sufficiently dispersed transversely to break down into other distinct structures as shown at $\Delta t_{Lag.} = 2.12\text{ ms}$. These clusters of smaller droplets located at higher transverse distances are then transported downstream the injector where they continue to swirl and further break down into distinctive groups of even smaller droplets. These groups tend to remain within the windward and spray core regions as they travel along the domain, which is where the BDF2 scheme significantly underpredicts the centreline SMD.

In addition, some clusters predicted by the BDF2 scheme (such as the one circled in red in **Figure 6-15**) remain trapped within the jet column region for a long time where they continue to swirl and break down into smaller droplets, which either get stuck in the jet column region as well or travel to the far-field region. As a result, small droplets are continuously introduced in the spray at lower transverse distance over a long time, which further contributes to the BDF2 scheme underpredicting the SMD in the spray core and leeward regions.

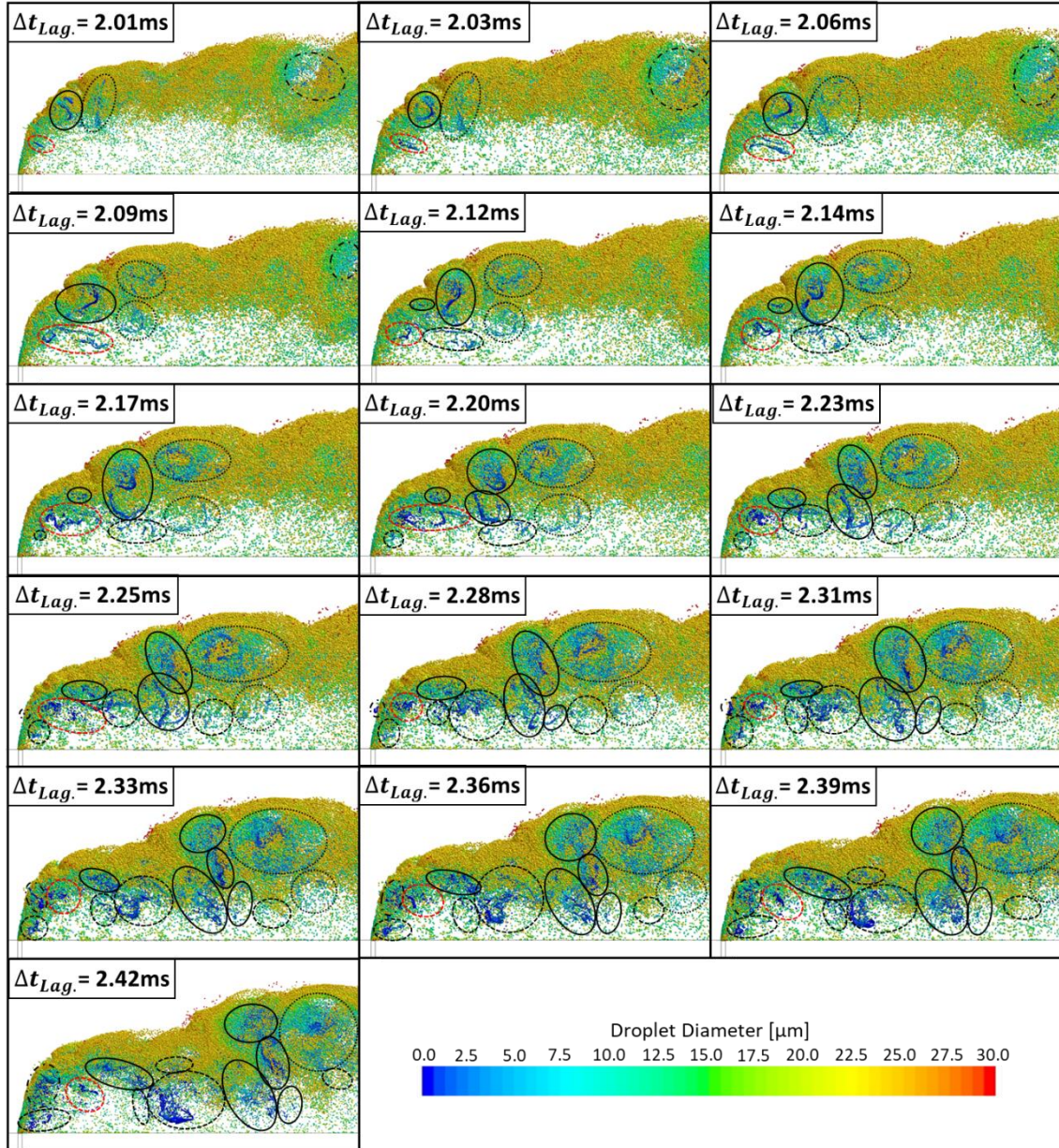


Figure 6-15: Time evolution of the instantaneous Lagrangian droplet diameter predicted by the optimized hybrid stripping method with the BDF2 scheme over a 0.4ms timeframe approximately 2 ms after activating the VOF-Lagrangian transition (images taken every ≈ 0.025 ms).

Figure 6-16 shows that the BDF1 scheme also forms clusters of small droplets within the same period. However, there are fewer groups of these small droplets, and they don't break down as much and they disperse less transversely. Moreover, there are no groups of small droplets swirling behind the jet column region, which indicates that those observed in the far-field region likely originate from a local overprediction of the breakup

process. This is further supported by the sudden apparition of a group of small droplets further away from the injector at $\Delta t_{Lag.} = 2.27$ ms and $\Delta t_{Lag.} = 2.40$ ms. Therefore, the lower order scheme is not likely impacted by the same “onset” swirling breakup mechanism or at least not to the same extent as the BDF2 scheme.

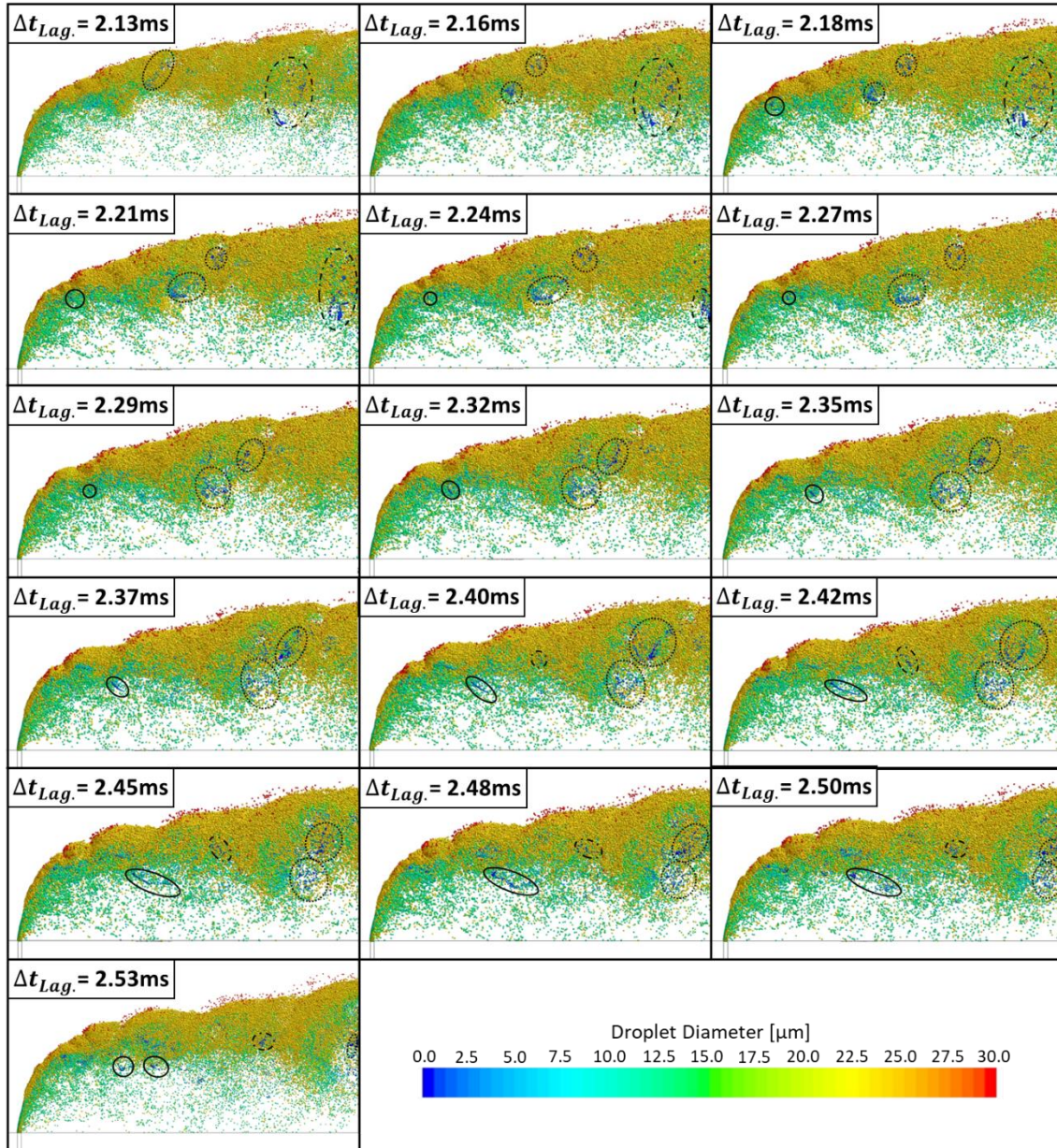


Figure 6-16: Time evolution of the instantaneous Lagrangian droplet diameter predicted by the optimized hybrid stripping method with the BDF1 scheme over a 0.4 ms timeframe approximately 2 ms after activating the VOF-Lagrangian transition (images taken every ≈ 0.025 ms).

It is important to note that the breakup phenomenon observed with the higher order scheme does not occur continuously, which is why there are fewer groups of small droplets initially present in the instantaneous Lagrangian droplet images shown in **Figure 6-15**. However, it has a significant impact on the time-averaged accuracy of the solution considering the standard deviation in centreline SMD is on average 85% higher with the BDF2 scheme despite predicting lower SMD values. Therefore, the latter is likely underpredicting the overall SMD due to periodic fluctuations in the continuous flow field that impact the VOF-Lagrangian interactions and stripping mechanism, especially behind the jet column region.

This aspect can be further investigated by identifying the coherent-vortex structures using the Q-criterion [208] as it allows the visualization of the unsteady characteristics of the turbulent continuous flow field [209, 210]. **Figure 6-17** and **Figure 6-18** show the instantaneous isosurface of the Q-criterion coloured by the vertical (Y axis) and longitudinal (Z axis) velocity components for the BDF1 and BDF2 scheme respectively at the beginning and end of the period used to visualize the instantaneous evolution of the droplet diameter in **Figure 6-15** and **Figure 6-16**. Similar to the previous images, the test section is represented from upstream of the injector to the exit of the domain.

The instantaneous isosurfaces of the Q-criterion reveal that both temporal discretization schemes can capture the intricate vortex structures that characterize the turbulent interactions of jets in crossflows [9, 10]. This is first observed in **Figure 6-17** and **Figure 6-18** by the formation of two large vortex structures upstream of the injector that end up surrounding the jet column with a high longitudinal velocity component of opposite signs, which could be classified as horseshoe vortices [10, 52]. It is also possible to observe that the interactions between the VOF phases are stronger in the near-field region due to the transverse penetration of the liquid jet in the crossflowing gas, which also generates counter-rotating vortices that propagate downstream the jet column. One of the main differences between both temporal discretization schemes is that the BDF2 scheme captures more vortices in the wake of the jet that are moving with higher longitudinal and vertical velocities in both negative and positive directions, which suggests the local continuous flow is swirling at a much higher intensity. These high-velocity swirling vortices are also more numerous in the far-field region, which is where clusters of small

droplets are transported in a swirling flow pattern after breaking up into even smaller droplets as shown in **Figure 6-15**. These findings indicate that the BDF2 scheme enhances the flow unsteadiness, which is likely intensifying the interactions between the Lagrangian droplets and turbulent eddies. This would agree with the results reported in the literature regarding the effect of using higher-order temporal discretization schemes on the flow unsteadiness [130, 205, 206]. In fact, the BDF1 scheme has been reported to diffuse more rapidly the vortices compared to the BDF2 scheme even when using a lower time step [205, 206]. While the numerical errors induced by the former are often dominated by dissipation, the higher-order temporal discretization schemes are more prone to temporal dispersion errors [205, 206].

The higher ratio between the average number of Lagrangian droplets and the average number of stripped droplets per time step achieved with the BDF2 scheme indicates that the breakup process is enhanced by the unsteadiness of the turbulent flow field. Indeed, the BDF2 scheme predicts on average 5.2 times more particles and 49% more parcels than the BDF1 scheme despite only stripping 1.2 times more droplets per time step. Thus, the higher order scheme is likely creating localized zones of high-intensity breakup that generate non-physically small droplets that are transported downstream the injector at a higher speed. Hence why the BDF2 scheme tends to underpredict significantly the SMD across the entire spray length and slightly overpredict the droplet velocity despite predicting a higher particle slip velocity.

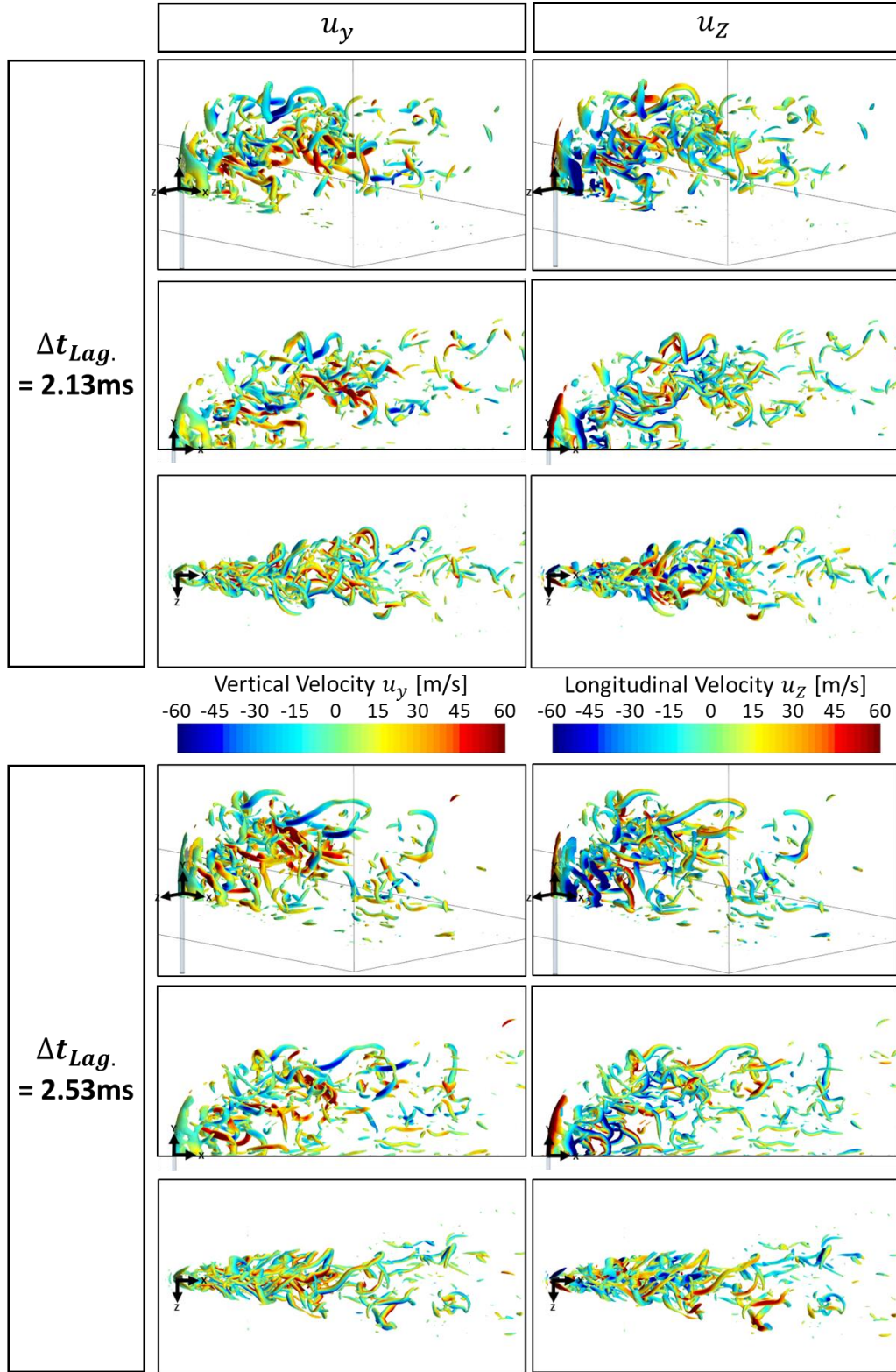


Figure 6-17: Instantaneous isosurface of Q-criterion ($Q = 3.0\text{E}+09 \text{ s}^{-2}$) coloured by the vertical and longitudinal velocity components predicted by the optimized hybrid stripping method with the BDF1 scheme at the start ($\Delta t_{Lag.} = 2.13 \text{ ms}$) and end ($\Delta t_{Lag.} = 2.53\text{ms}$) of the breakup evolution represented in Figure 6-16.

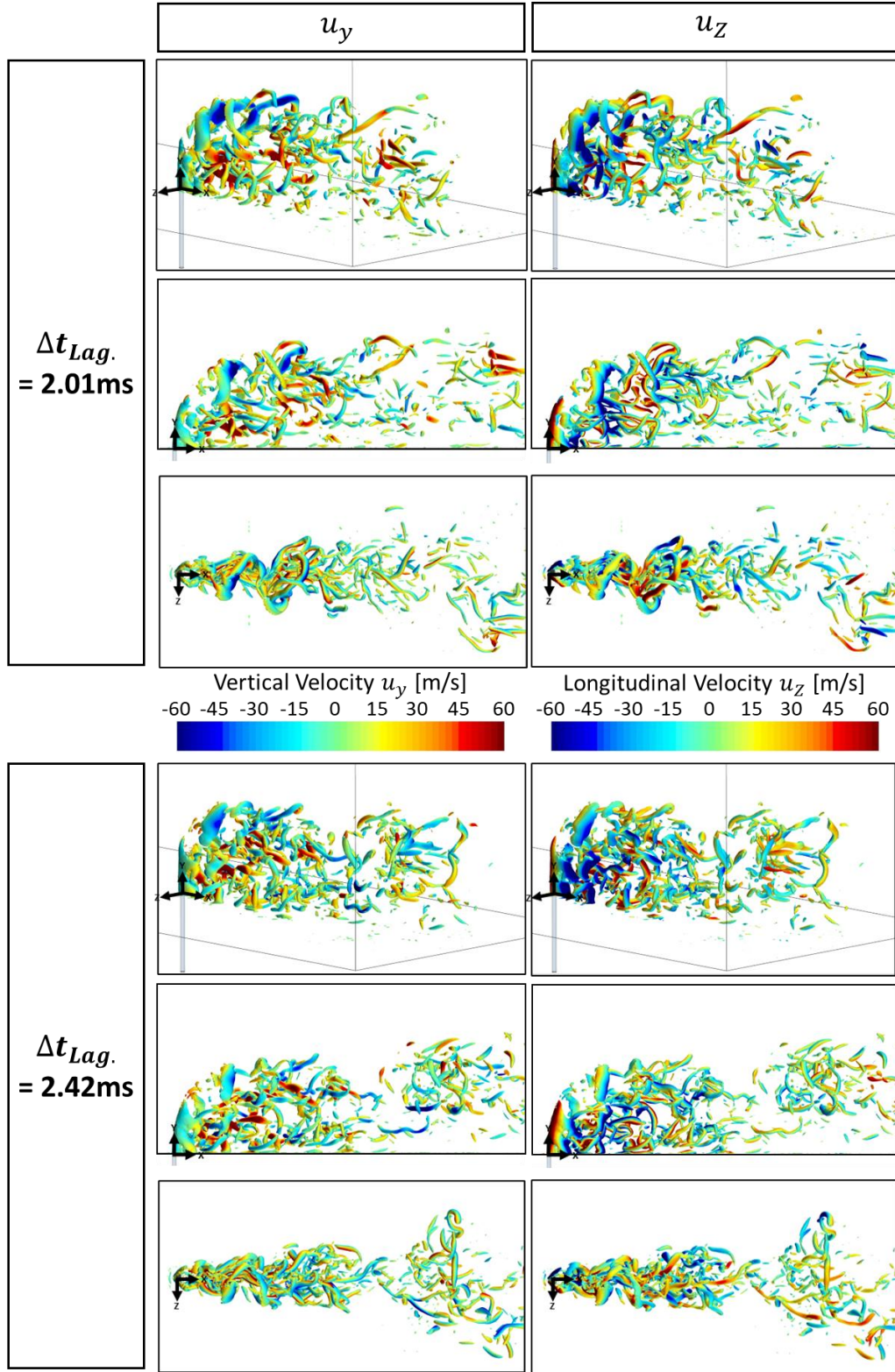


Figure 6-18: Instantaneous isosurface of Q-criterion ($Q = 3.0E+09 \text{ s}^{-2}$) coloured by the vertical (Y axis) and longitudinal (Z axis) velocity components predicted by the optimized hybrid stripping method with the BDF2 scheme at the start ($\Delta t_{Lag.} = 2.01 \text{ ms}$) and end ($\Delta t_{Lag.} = 2.42 \text{ ms}$) of the breakup evolution represented in Figure 6-15.

6.7.2 Temporal Discretization Scheme: Effect on Droplet Velocity

It is also possible to observe in **Figure 6-11** that the continuous phase velocity magnitude within the wake region of the jet predicted by the optimized hybrid stripping method tends to be lower with the BDF1 scheme compared to BDF2. This could explain why the latter tends to predict a slightly higher centreline droplet axial velocity in the spray core region as shown in **Figure 6-6**. Although the BDF2 scheme predicts a slightly higher continuous phase velocity magnitude behind the liquid jet column, the local droplet velocity magnitude is on average 7% lower as shown in **Figure 6-10**. Considering the relative difference in the velocity magnitude of the stripped droplets is only 1%, the stripping mechanism is not sufficiently influenced by the temporal discretization scheme to explain the lower droplet velocities observed when using BDF2. Therefore, the higher continuous phase velocity magnitude predicted by the latter likely indicates the presence of a recirculation zone that has a stronger impact on the Lagrangian droplets formed during the breakup process.

The presence of a stronger recirculation zone in the jet column region when using the BDF2 scheme is further supported by comparing the characteristics of the vortex structures in the turbulent continuous flow field shown in **Figure 6-17** and **Figure 6-18**. Indeed, although both temporal discretization schemes predict the presence of high-intensity vortices within the jet column region, the BDF2 scheme tends to predict a greater number of swirling structures.

6.7.3 Temporal Discretization Scheme: Effect on Spray Trajectory

As shown in **Figure 6-9**, using the BDF2 scheme with the hybrid stripping method decreases the vertical and horizontal jet column penetration on average by 12% and 21% respectively. Although this could explain the slightly lower transverse trajectory predicted using the BDF2 scheme, the relative difference in jet column penetration is more important than those in overall spray trajectory which are non-significant as reported in *section 6.5.1*. This indicates the Lagrangian droplets stripped from the jet column are transported on longer vertical and axial distances when using the BDF2 scheme. Indeed, the maximum spray trajectory predicted with the latter is on average 2.6 times higher than the maximum vertical penetration of its jet column, which represents an absolute difference in the discrepancy of 34% from the BDF1 scheme. Thus, the higher-order

temporal discretization scheme might enhance the interactions between the Lagrangian droplets and the continuous phase.

This is further supported by observing the intensity of the vortices in the near-field region showcased in **Figure 6-18**. Although the vortices within the near-field region are not travelling to higher transverse distances when using the BDF2 scheme, the higher intensity of their vertical velocity components is likely enhancing the transverse dispersion of the Lagrangian droplets. This would explain why there are no significant differences in the spray trajectory despite the BDF2 scheme predicting a lower penetration of the liquid jet column. Furthermore, the BDF2 scheme also enhances their radial dispersion considering the spray width predicted is on average 15% larger than with the BDF1 scheme. This can be attributed to the vortices spreading more longitudinally while maintaining a high intensity across the entire spray length, but especially in the far-field region as shown in **Figure 6-18**.

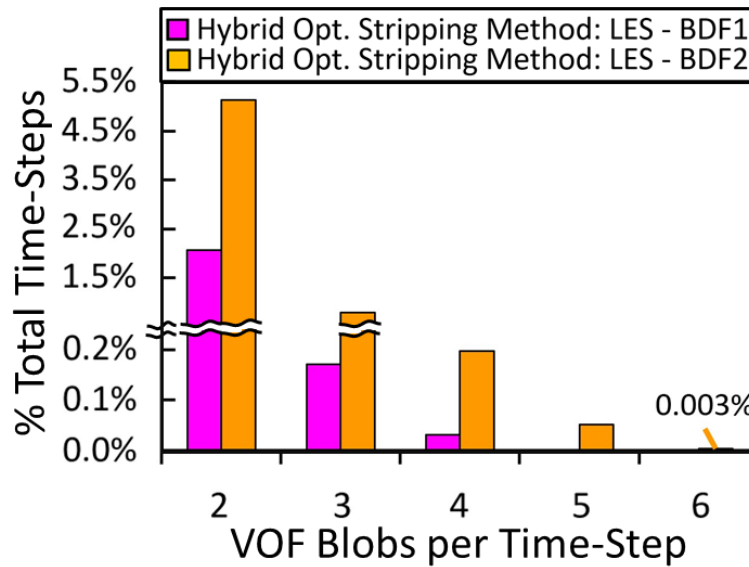


Figure 6-19: Percentage of time-steps during the VOF-Lagrangian transition when more than 1 VOF blob was present in the domain for the optimized hybrid stripping method with different temporal discretization schemes.

The differences in the liquid jet column penetration can be explained by the effect of the temporal discretization scheme on the VOF phase interactions. In addition to having a higher velocity zone behind the jet column region due to the more intense nature of the recirculation flow, the BDF2 scheme also introduces more instabilities at the VOF interface. As shown in **Figure 6-19**, the temporal discretization scheme impacts the

number of blobs detaching from the VOF liquid jet column. In fact, the BDF2 scheme introduces more than 2 blobs per time step on average 6% of the time during the stripping process compared to less than 2% of the time with the BDF1 scheme. In addition, the BDF2 scheme can detach up to 6 VOF blobs from the VOF jet column compared to a maximum of 4 VOF blobs with the BDF1 scheme. As a result, the average number of blobs shed per time step is 5% higher when using the BDF2 scheme with a standard deviation 87% larger. The enhanced blob shedding observed with the BDF2 scheme could reduce the liquid jet column volume, hence the smaller penetration. Indeed, the latter predicts the volume of the liquid jet column to be 13% smaller on average than the BDF1 scheme.

6.8 Computational Cost

As shown in **Figure 6-20**, the optimized hybrid stripping method significantly reduces the computational cost of the VOF-Lagrangian approach. Indeed, its solver CPU time per time step normalized by the number of CPUs (256) Δt_{CPU} is on average 78% smaller than the hybrid resolved method with the same temporal discretization scheme. Although the URANS Lagrangian numerical methodology previously developed and validated remains much more affordable, the computational cost of the VOF-Lagrangian approach is now 6 times higher instead of 30 times higher. Therefore, the optimized hybrid stripping method improves the practicality of using the VOF-Lagrangian approach for low-emission gas turbine applications that would benefit from using LES, such as for combustion modelling.

Normalizing Δt_{CPU} by the average mesh size reveals that the stripping transition model is 1.3 times more expensive than the resolved transition model independently of the interface resolution. This indicates that the discrepancies in computational cost are driven by the higher number of mesh elements required by the hybrid resolved approach to capture a sufficiently fine resolution of the interface in order to shed VOF blobs. As mentioned in *section 6.4*, the optimized hybrid stripping method also allows using a time-step size twice as large, which further improves the computational efficiency of the VOF-Lagrangian approach.

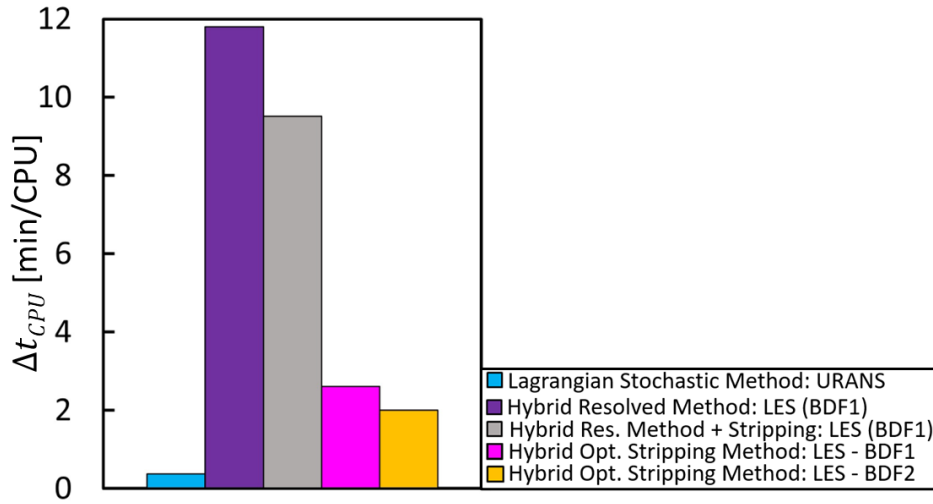


Figure 6-20: Time-averaged solver CPU time per time step Δt_{CPU} for different VOF-Lagrangian transition methods and temporal discretization schemes.

These results agree with the previous findings presented in *section 5.7* of Chapter 5 [44] regarding the higher computational cost of the hybrid resolved method when coupled with the stripping transition model. The higher cost of the stripping transition mechanism can still be attributed to the significantly larger number of particles and parcels that are introduced in the domain. Moreover, it further supports that improving the predictive capabilities of the optimized hybrid stripping method by refining the AMR settings or using a higher-order VOF convection scheme would likely make the proposed methodology more computationally expensive than the hybrid resolved method.

It is also possible to observe in **Figure 6-20** that the computational cost of the optimized hybrid stripping method is lower than the hybrid resolved method regardless of the temporal discretization scheme used. In addition, the BDF2 scheme tends to reduce Δt_{CPU} on average by 23%, which could be surprising considering it predicts on average 4% more mesh elements as well as significantly more particles and parcels as discussed in *section 6.7.1*. There are also no significant differences in the average adapted time-step size that could explain the discrepancies observed in Δt_{CPU} . Thus, it is likely related to the BDF2 scheme requiring on average 34% fewer inner iterations per time step as it indicates a faster convergence of the residuals. This was expected considering higher-order temporal schemes are well known for their improved efficiency and faster convergence [130, 204, 205, 206].

6.9 Conclusion

In summary, the VOF-Lagrangian approach previously developed and validated using a resolved transition method has been optimized to make it more practical for industrial and academic research and development. This was achieved by taking advantage of the stripping transition model, which does not need to capture the dispersed VOF liquid phase in order to introduce Lagrangian droplets in the domain. The impact of the optimized hybrid stripping method proposed on the accuracy of the VOF-Lagrangian approach has been assessed using ambient experimental data at high atomization and turbulence levels from Madabhushi et al. [30].

The predictions in droplet axial velocity were found to be impacted the most by the VOF-Lagrangian transition method due to the effect on the near-field VOF phases interactions of modelling the VOF blobs shedding from the liquid jet column. The predictions could be improved by enhancing the interface resolution of the optimized hybrid stripping method but, at the expense of its affordability. Therefore, the overprediction of the centreline droplet velocity could be considered a limitation of the proposed methodology. Although the lower spray trajectory predicted by the hybrid stripping method can also be attributed to the discrepancies in the VOF phase interactions, it might not be necessary to model the VOF blobs shedding process to improve its predictions. Indeed, capturing a higher penetration of the VOF liquid jet column could be sufficient considering it tends to transport the Lagrangian droplets on a longer vertical distance relative to the column breakup point. Thus, future work could be done to improve the spray trajectory predictions without significantly increasing its computational cost by dynamically adapting the AMR settings based on the position of the VOF liquid interface to further refine the mesh at higher transverse distances. It was also found that the overall SMD tends to be underpredicted because the stripping mechanism tends to override the stripping criterion imposed and restrict the stripping process in the larger cells. Different recommendations have been made to improve the predictive capabilities in SMD that would not have a significant impact on the computational cost, such as dynamically adapting the stripped mass flux based on the cell size to promote the stripping of larger droplets.

Although the hybrid resolved method tends to agree better with the experimental data, the average relative difference between the two methods is less than 15% and their predictive capabilities tend to agree further downstream the injector. Indeed, it was found that the discrepancies in spray trajectory, average droplet diameter and average droplet velocity become non-significant in the far-field region. Moreover, their predictive capabilities are similar when compared to the URANS numerical methodology previously developed and validated with the Lagrangian approach in Chapter 3 and Chapter 4 [42, 43]. Indeed, regardless of the transition method, the VOF-Lagrangian approach tends to better predict the overall droplet axial velocity, improves the SMD predictions in the leeward spray region and better captures the overall shape of its centreline profiles. It also enhances the transverse and radial dispersion of the spray as it models the jet column stripping and/or breakup process. Taking into account the significant reduction in the computational cost of the VOF-Lagrangian approach achieved by using the optimized hybrid stripping method, its trade-off between cost and accuracy is deemed reasonable.

In addition to the different solutions that have already been identified to improve the accuracy of the hybrid stripping method, future work could be done to validate that the conclusions from this study apply to different conditions. However, the outcome is not expected to be drastically different considering the accuracy of the hybrid resolved method was not found to be significantly impacted by the dataset used as presented in Chapter 5 [44]. Therefore, the proposed optimized hybrid stripping method should be a suitable lower-cost alternative over a wide range of conditions for different industrial and academic applications that require using LES to couple atomization modelling with other higher-fidelity models.

The effect of using a higher-order temporal discretization scheme on the predictive capabilities of the VOF-Lagrangian approach was assessed using the optimized hybrid stripping method by comparing the predictions obtained with the BDF1 and BDF2 schemes. The latter was found to amplify the discrepancies with the experimental data mainly for the overall SMD, but also for the droplet velocity at higher transverse distance. Although it did not have a significant impact on the spray trajectory predictions, the BDF2 scheme tends to enhance the transverse and radial dispersion of the Lagrangian droplets relative to the jet column breakup point. These discrepancies can be attributed to

differences in the unsteadiness of the continuous flow that are impacting the overall VOF-Lagrangian interactions as well as the VOF phase interactions in the near-field region. Indeed, the BDF2 scheme tends to capture vortex structures swirling at high velocity and dissipating at a slower rate, which suggests the presence of a stronger recirculation zone in the wake region of the jet. As a result, it tends to create zones of high-intensity breakup that generate isolated groups of non-physically small droplets that are then transported at high velocity in the far-field region where they continue to breakup. The discrepancies observed indicate that higher-order temporal discretization schemes might not be fully compatible with the proposed optimized hybrid stripping method. Restricting the modelling of the VOF liquid phase to the jet column by imposing coarser AMR settings with a 1st order VOF convection scheme might lead to an interface resolution that is too coarse to accurately capture the effect of a more unsteady flow. Refining the AMR settings or using the HRIC convection scheme could improve its predictive capabilities when using a higher-order temporal scheme, but it would go against the objective of the study as it would significantly increase the computational cost. Therefore, it is recommended to limit the temporal discretization scheme to the 1st order for the optimized hybrid stripping method proposed.

6.10 Acknowledgment

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7 Discussion, Conclusion and Future Work

This research focused on the assessment, development, and validation of numerical methodologies for modelling the atomization process of turbulent liquid fuel jets in crossflow (LFJIC) under more representative gas turbine conditions. The work was motivated by the need to improve the practicability, robustness and predictive capabilities of the numerical tools used to guide the design of novel low-emission gas turbine technologies for liquid fuel combustion systems. All the research objectives defined in *section 1.1* were achieved through the work presented in the different chapters as indicated in **Table 7-1**.

Table 7-1: Research objectives addressed in each Chapter.

Research Objectives		Chapters					
		2	Core Research Chapters				7
			3	4	5	6	
1	Compare the predictive capabilities of SSD and deterministic breakup models for LJIC.	X	X				
2	Assess, validate, and develop high and low-fidelity numerical methodologies for turbulent LFJIC that require minimal calibration.		X	X	X	X	
3	Assess, validate, and develop stochastic numerical methodologies that improve the practicability of using higher-fidelity methods to model turbulent LFJIC.				X	X	
4	Ensure the numerical methodologies developed offer a reasonable trade-off between practicability and accuracy.						X
5	Help fill the gaps in knowledge on the different atomization modelling approaches for LFJIC.		X	X	X	X	
6	Disseminate the research outcomes and provide recommendations for Simcenter STAR-CCM+.		X*	X*	X*		X
*Research disseminated in peer-reviewed publications.							

This concluding chapter provides an overall discussion of the main research outputs and addresses the research objectives and limitations. This includes providing guidelines for using the numerical methodologies developed, summarizing the intellectual contribution and real-world impact of the work, and providing recommendations for future work. The 4th research objective is addressed by comparing the predictive capabilities of the

numerical methodologies developed to those reported in the literature for LFJIC. To further support the achievement of the 5th research objective, the novelty, contribution, and impact of the research are highlighted. The 6th research objective is achieved by providing recommendations to improve the atomization modelling capabilities of the numerical CFD software Simcenter STAR-CCM+ based on the main research findings.

7.1 Recommendations for Modelling Turbulent Liquid Jets in Crossflow

Recommended guidelines for using the numerical methodologies developed for modelling LJIC have been established based on the research findings. **Figure 7-1** can be used to determine which methodology is recommended depending on the intended application as described below:

- If the purpose of the work is to assess the effect of different operating conditions or the combustor part designs (heatshield, liner, etc.) on the combustion characteristics (exit temperature, emissions, etc.), then the lower-fidelity URANS Lagrangian methodology should be prioritized due to its lower cost unless otherwise specified (see the next two bullet points).
- If CFD is used to guide the design of a more complex LJIC injector (i.e. not a plain orifice type), the hybrid methodologies should be used considering they allow to capture the effect of the injector geometry and liquid jet column on the spray characteristics. The URANS Lagrangian methodology could be used to model more complex injectors, but the injection settings recommended need to be adapted. This aspect is further discussed in the research limitations (*section 7.5*) and recommendations for future work (*section 7.6*).
- If atomization modelling is coupled with higher-fidelity models that would benefit from using LES to capture complex phenomena (e.g. transient combustion physics, emissions, flashback, acoustics, ignition, etc.), then the developed hybrid methodologies should be used (see the information provided below **Figure 7-1**).

- When the hybrid methodologies are both recommended, the selection of the transition method should be guided by the computational resources available. However, it is recommended to prioritize the resolved transition method if higher levels of accuracy are required.

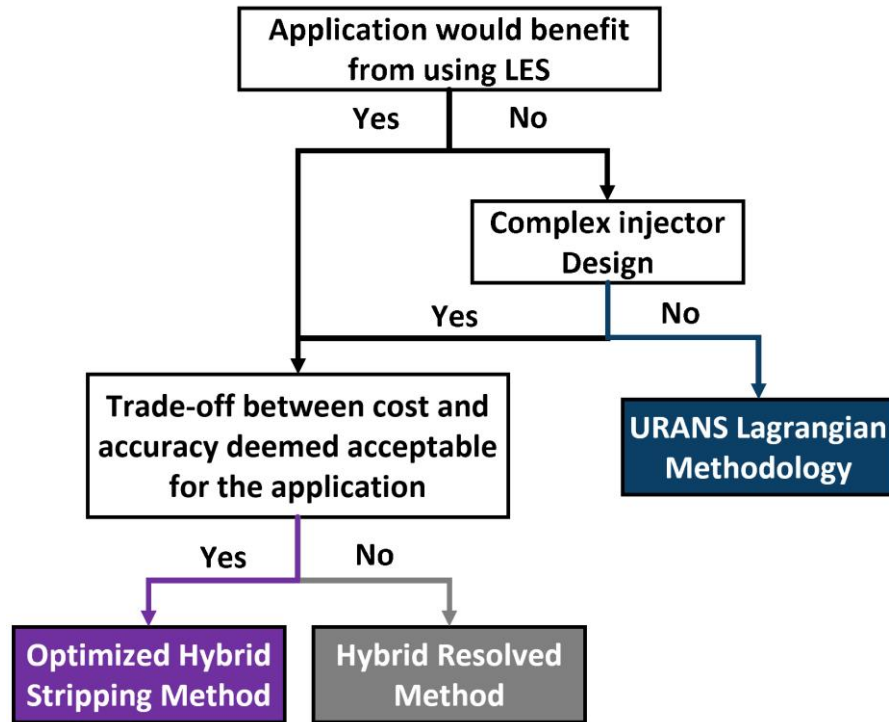


Figure 7-1: Recommended guidelines for modelling turbulent LJIC with the numerical methodologies developed.

The recommended guidelines aim to reduce the risk of unknowingly introducing significant numerical error in the assessment of the combustion characteristics, which can be quite high when coupling atomization with reacting flows. This is due to the effect of evaporation modelling on the droplets, which makes it more challenging to notice the presence of inconsistencies in the spray characteristics. To further augment the level of confidence that can be achieved by using the recommended guidelines, the following research findings must be further emphasized:

- LES should not be used with the Lagrangian approach to model turbulent LJIC due to the state-of-the-art (SOA) subgrid-scale (SGS) models filtering the important unresolved subgrid scale motions. Unless a SGS model specifically developed to address these concerns can be implemented, LES should only be

used to model turbulent LJIC when coupled with the hybrid approach as indicated in **Figure 7-1**.

- The deterministic breakup models should not be used if the empirical constants can not be thoroughly calibrated due to a lack of experimental data or knowledge of the spray characteristics for the injector design and specific conditions studied. In addition to not being practical, the calibration process required is not deemed worth the extra time cost or modelling efforts considering the stochastic methodologies developed from this research were found to achieve similar and often better predictive capabilities for turbulent LJIC. This aspect is further detailed in the *section 7.2*.

The last point is particularly relevant for combustion research involving LFJIC considering discrepancies with the experimental flame characteristics have been attributed to the spray properties predicted by the deterministic breakup models despite their exhaustive calibration [26]. This further supports the decision to recommend the more practical stochastic secondary droplet (SSD) breakup model even if experimental data is available to calibrate the model constants. In such a situation, the available data could be used to further validate the predictions of the stochastic methodology under the specific condition studied before enabling the reacting flow.

Table 7-2 summarizes the models and important settings to impose for recreating the numerical methodologies developed. General recommendations are also included to provide further guidance on how to implement them. Moreover, the values suggested for the transition criteria or injector settings have been generalized to apply to different datasets.

Table 7-2: Numerical models, relevant settings, and recommendations to implement the numerical methodologies developed.

Models	URANS Lagrangian stochastic Methodology	Hybrid resolved method	Optimized hybrid stripping method
Turbulence	• URANS • k-epsilon turbulence • Realizable k-epsilon Two-Layer model • Two-Layer All y+ wall treatment	• LES • WALE SGS model • All y+ Wall Treatment	
Flow	• Implicit Unsteady		
	• Coupled flow solver (implicit) with 2nd order discretization scheme • 2nd order temporal discretization scheme	• Segregated flow solver with 2nd order convection scheme • 1st order temporal discretization scheme • Adaptive Time-Step*	
Lagrangian	• Two-way coupling • SSD breakup model: - Breakup parameter $B_1 = \sqrt{3}$ - Normal velocity coefficient $K_3 = 1$ - Maximum number of child parcels $\geq 10^{**}$ - Target number of particles per parcel $\geq 100^{**}$ • Drag Force with TAB Distortion model (Distorted droplet) • Pressure Gradient Force • Lagrangian courant numbers $\rightarrow$ Imposed using the strategy described in <i>section 4.4.3</i> from Chapter 4 (see equation (4-32))		
	• Turbulent Dispersion Model		
Injector	• Point injection method • injected droplet diameter = injector exit diameter • Parcel stream $\geq 100^{**}$		

Volume-of-fluid (VOF)	N/A	• 1st order face density reconstruction • Surface tension force (CSF model) with semi-implicit treatment	
		• High-Resolution Interface Capturing (HRIC) convection scheme	• 1st order convection scheme
VOF-Lagrangian (Hybrid)	N/A	• Blob Detection Model (minimum liquid volume fraction = 0.5) • VOF-Lagrangian Impingement • Free Surface Adaptive Mesh Refinements (AMR) (hexahedral elements) → Imposed using the settings described in <i>section 6.4</i> of Chapter 6 (see Table 6-2)[†]	
		• Resolved Transition model: - Maximum diameter of transitioning blobs $\geq$ 20% of the nozzle size[‡] - Minimum sphericity of transitioning blobs $\geq$ 0.7[‡] - Minimum liquid volume fraction of transitioning blobs = 0.95[§]	• Optimized stripping Transition model: - Stripped mass flux → Imposed using the strategy described in <i>section 6.4</i> of Chapter 6 (see equation (6-14)) - Stripped diameter = 50% of the adapted cell size - Transition prevented in cells refined to the maximum AMR level → Imposed using the strategy described in <i>section 6.3</i> of Chapter 6 (see Figure 6-1)

*Time-step for the hybrid approach should be imposed to ensure the courant number is lower than 0.7 at the interface.

**Conservative values suggested (see *section 3.4* from Chapter 3 for further details). Higher values would increase the spray discretization, which might increase the accuracy of the solution depending on the operating conditions. However, this would be at the expense of the computational cost.

†The number of AMR levels and minimum adaptation cell size need to be adapted based on the baseline mesh size. For the optimized hybrid stripping method, the number of AMR levels should be fine enough to capture the jet column bending but small enough to obtain an average number of blobs per time step close to 1. Otherwise, the AMR settings need to be coarsened. For the resolved hybrid method, the number of AMR levels should be large enough to capture around 10000 blobs per time step in the domain. Moreover, as recommended in Chapter 5, the upstream swept distance indicated in **Table 6-2** could be reduced to a unity factor similar to the hybrid stripping method.

‡These values will likely need to be adjusted to maximize the frequency of the VOF-Lagrangian transition. Increasing the blob transition diameter might not have any impact on the transition frequency due to the smaller sphericity of the larger blobs. Increasing the blob sphericity might limit the transition process to the far-field region where the smaller VOF blobs are located, which would increase the computational cost due to the larger mass of VOF liquid phase that needs to be modelled in the near-field region. Thus, it is recommended to increase the transition blob diameter while progressively reducing the minimum sphericity criterion to achieve an optimal frequency of the VOF-Lagrangian transition events.

§Reducing this value might increase the frequency of the VOF-Lagrangian transition, but likely at the expense of the solution accuracy considering it will affect the conservation of momentum, mass and energy.

7.2 Predictive Capabilities of Proposed Numerical Methodologies

Each core research chapter includes a discussion of the results that provides a better understanding of the predictive capabilities achieved using the different numerical methodologies developed (Chapter 3 and Chapter 4: URANS stochastic Lagrangian methodology, Chapter 5: Hybrid resolved method, Chapter 6: Optimized hybrid stripping method). Similarities were also established with the research findings from other studies available in the literature on liquid sprays for coaxial and crossflow injectors, which further supports the conclusions of the work and helped identify areas of improvement for future work. Further details regarding these aspects of the analysis can be found in the discussion and conclusion sections of the core chapters.

This section addresses the 4th research objective by comparing the predictive capabilities of the proposed numerical methodologies to the absolute errors extracted from the validation studies available in the literature for LFJIC. The post-processing strategy described in *section 2.5* from Chapter 2 was used to calculate the average absolute error from the validation datasets selected. The resulting error bars obtained for each numerical methodologies developed were then added to the average absolute error graphs previously presented in *section 2.5* (**Figure 2-13** to **Figure 2-15**) as shown in **Figure 7-2** and **Figure 7-3**.

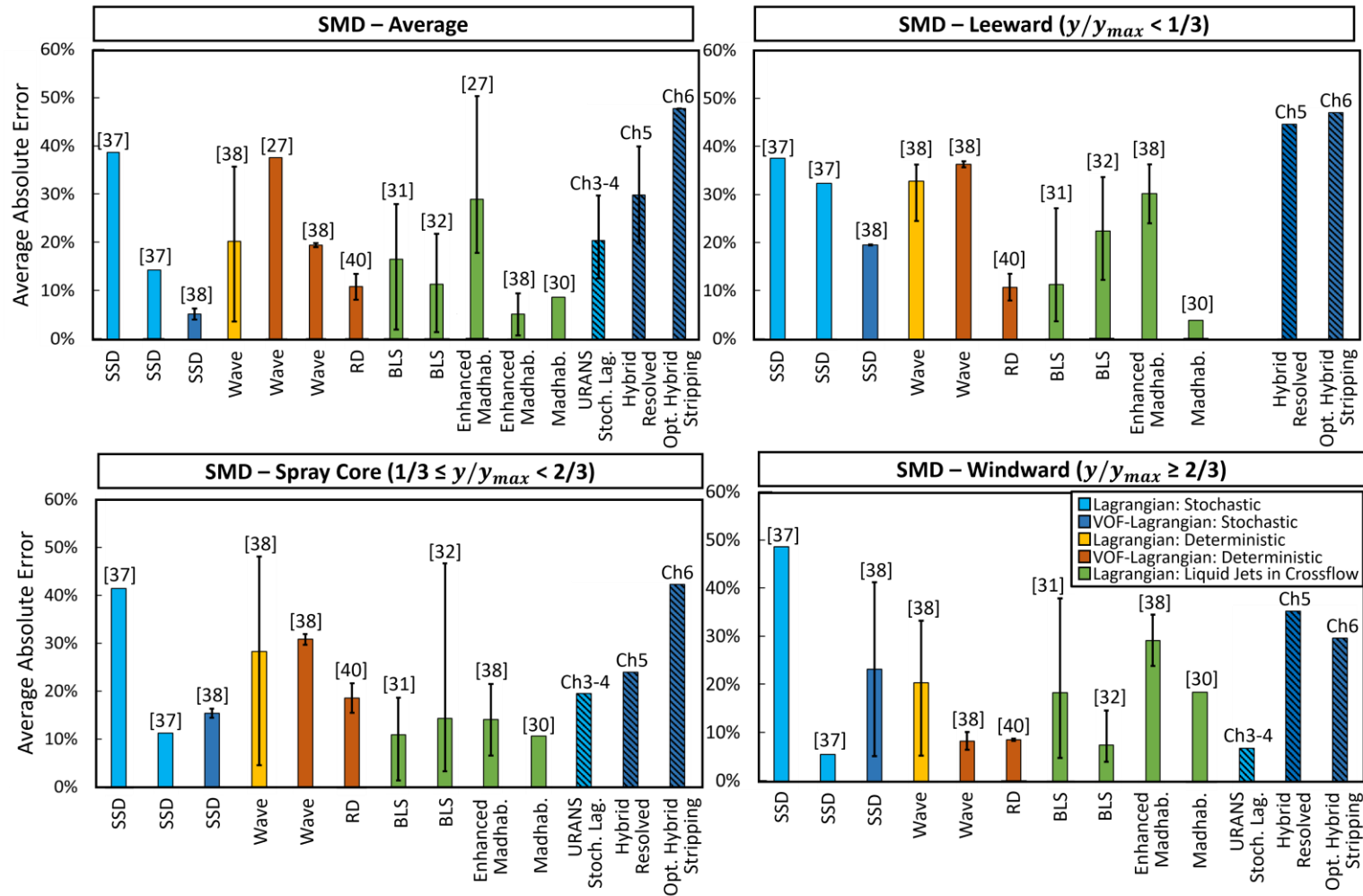


Figure 7-2: Average absolute errors in SMD predicted by the numerical methodologies developed (indicated below hatched bars with chapter above) compared to those reported in the literature for LJIC (reference indicated above plain bars and breakup model indicated below).

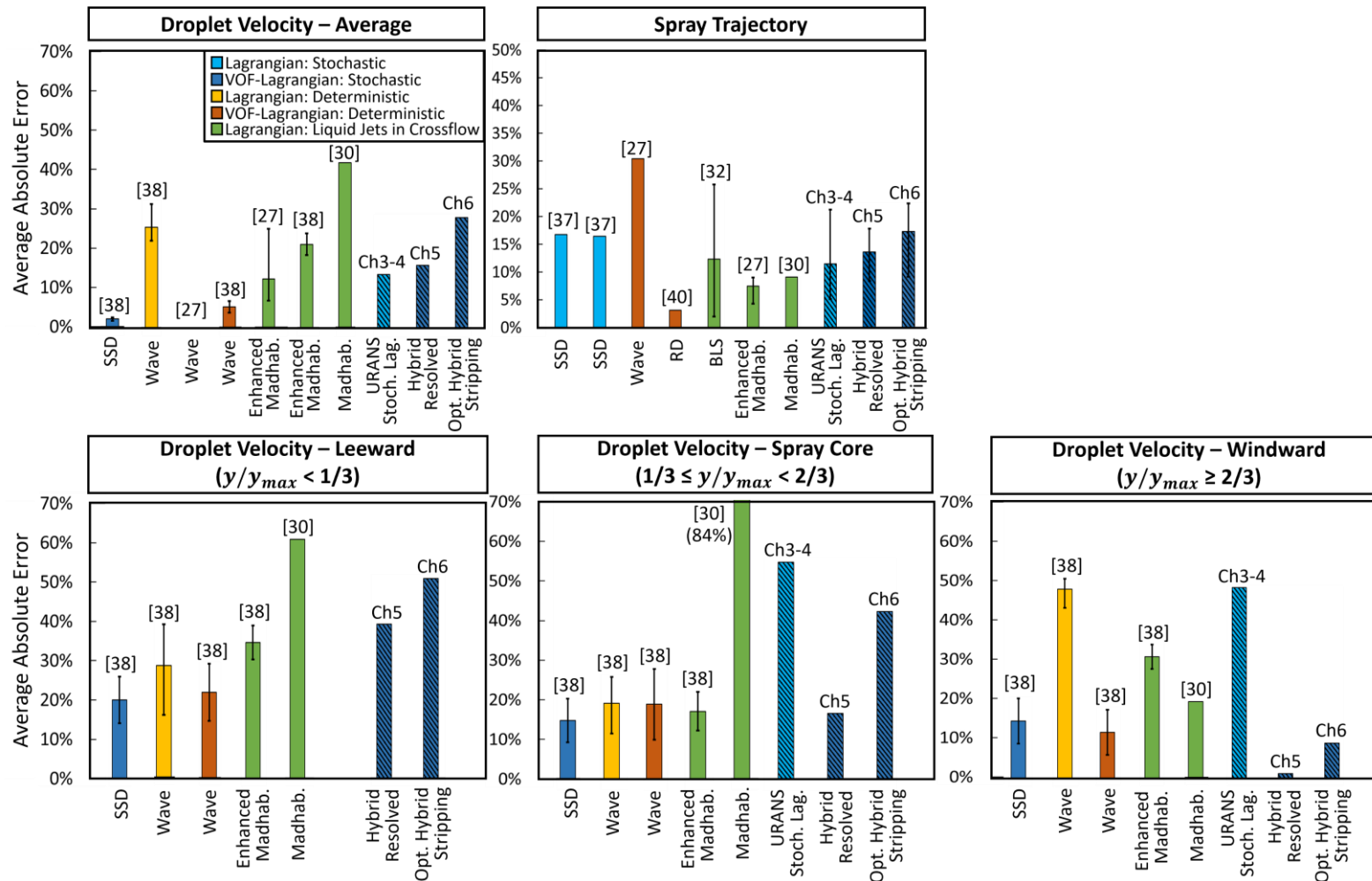


Figure 7-3: Average absolute errors in droplet velocity and spray trajectory predicted by the numerical methodologies developed (indicated below hatched bars with chapter above) compared to those reported in the literature for LJIC (reference indicated above plain bars and breakup model indicated below).

Table 7-3 to **Table 7-5** highlight that the stochastic numerical methodologies developed often achieve better predictive capabilities (i.e. average absolute error achieved in the present work is lower) for the spray characteristics within the windward region, spray core region and on average compared to the validation studies available in the literature for the deterministic breakup models for LFJIC. The first column with the tick marks indicates that the predictive capabilities of the numerical methodologies proposed are better than at least one other study available in the literature for the atomization modelling set-up (approach, breakup model and dataset type) specified. Although this condition might not always be achieved, the absolute error in the present work is often lower than the maximum discrepancies reported in the literature as indicated by the second column with the tick marks. In other words, the last column of these tables indicates that the predictive capabilities of the numerical methodologies proposed are at least better compared to the highest discrepancies reported by similar validation studies available in the literature. Moreover, the predictive capabilities achieved in the present work are sometimes better than all other studies considered for the comparison as shown in **Table 7-4**. The tick marks coloured in blue refer to the URANS stochastic Lagrangian method, dark blue to the hybrid resolved method and purple to the optimized hybrid stripping method.

Table 7-3 shows that the predictive capabilities of the numerical methodologies developed for the spray trajectory, Sauter Mean Diameter (SMD) and droplet velocity are either similar or better than those reported by other Lagrangian validation studies available in the literature on LFJIC. This is also true for the predictions within the spray core and windward regions as shown in **Table 7-5** and **Table 7-4** respectively. In particular, the proposed hybrid methodologies often achieve lower average absolute errors for the droplet velocity across the entire spray height. The URANS stochastic Lagrangian method is also able to achieve better agreement with the experimental data for the spray trajectory, the average droplet velocity and the average SMD as shown in **Table 7-3**. Moreover, it tends to better capture the droplet velocity and SMD within the spray core region as well as the latter within the windward region. Apart from the SMD predictions within the spray core region, similar conclusions can be made regarding the

improved predictive capabilities of the proposed methodologies compared to those specifically developed for LJIC.

Table 7-3: Improvements in predictive capabilities achieved for the average spray characteristics by the proposed numerical methodologies compared to the relevant validation studies available in the literature for LJIC.

Comparison Data	Comparison studies available in the literature			Absolute error of methodology developed is...	
	Approach	Breakup Model	LJIC validation dataset	Better on average than at least 1 comparison study	Within the range of comparison studies
SMD	Lagrangian	LJIC	All†	✓	✓✓
	Lagrangian	All*	Fuel only	✓	✓✓
	Hybrid			✓✓	
Droplet Velocity	Lagrangian	LJIC	All†	✓✓✓	
	Lagrangian	All*	Fuel only	✓✓✓	
	Hybrid			-	-
Spray Trajectory	Lagrangian	LJIC	All†	✓	✓✓
	Lagrangian	All*	Fuel only	✓	✓✓
	Hybrid			✓✓✓	
*Stochastic (SSD), SOA deterministic and deterministic LJIC breakup models †LJIC datasets for any liquid (e.g. water, fuel, emulsions, blends, etc.) ✓: URANS stochastic Lagrangian method (Chapter 3-4) ✓: Hybrid resolved method (Chapter 5) ✓: Optimized hybrid stripping method (Chapter 6)					

Compared to the numerical studies conducted on LFJIC using the hybrid approach with a deterministic or stochastic breakup model, the hybrid resolved methodology developed tends to agree better with the experimental data within the spray core region as well as for the average SMD. The predictive capabilities within the windward region of both hybrid methods proposed also agree with those reported in the literature for the hybrid approach, especially for the droplet velocity considering the significantly lower absolute error achieved as shown in **Figure 7-3**. Despite using the lower-fidelity Lagrangian approach, the URANS stochastic method developed also tends to achieve lower absolute error for the SMD on average and within the spray core and windward regions as seen in **Figure 7-2**. **Table 7-3** and **Figure 7-3** reveal this is also true for the spray trajectory predictions for all methodologies proposed.

Table 7-4: Improvements in predictive capabilities achieved for the spray characteristics in the windward region by the proposed numerical methodologies compared to the relevant validation studies available in the literature for LJIC.

Comparison Data	Comparison studies available in the literature			Absolute error of methodology developed is...	
	Approach	Breakup Model	LJIC validation dataset	Better on average than all comparison studies	Within the range of comparison studies
SMD	Lagrangian	LJIC	All†	✓	✓✓
	Lagrangian	All*	Fuel only	✓	✓✓
	Hybrid			✓	✓✓
Droplet Velocity	Lagrangian	LJIC	All†	✓✓	
	Lagrangian	All*	Fuel only	✓✓	✓
	Hybrid			✓✓	
*Stochastic (SSD), SOA Deterministic and Deterministic LJIC breakup models †LJIC dataset for any liquid (e.g. water, fuel, emulsions, blends, etc.) ✓: URANS stochastic Lagrangian method (Chapter 3-4) ✓: Hybrid resolved method (Chapter 5) ✓: Optimized hybrid stripping method (Chapter 6)					

Table 7-5: Improvements in predictive capabilities achieved for the spray characteristics in the core region by the proposed numerical methodologies compared to the relevant validation studies available in the literature for LJIC.

Comparison Data	Comparison studies available in the literature			Absolute error of methodology developed is...	
	Approach	Breakup Model	LJIC validation dataset	Better on average than at least 1 comparison study	Within the range of comparison studies
SMD	Lagrangian	LJIC	All†		✓✓✓
	Lagrangian	All*	Fuel only	✓✓	✓
	Hybrid			✓✓	
Droplet Velocity	Lagrangian	LJIC	All†	✓✓✓	
	Lagrangian	All*	Fuel only	✓✓✓	
	Hybrid			✓	
*Stochastic (SSD), SOA Deterministic and Deterministic LJIC breakup models †LJIC dataset for any liquid (e.g. water, fuel, emulsions, blends, etc.) ✓: URANS stochastic Lagrangian method (Chapter 3-4) ✓: Hybrid resolved method (Chapter 5) ✓: Optimized hybrid stripping method (Chapter 6)					

In addition, the URANS stochastic methodology developed was found to significantly improve the agreement with the experimental data in the windward region for the SMD compared to the other validation studies conducted on the hybrid and Lagrangian approaches for LJIC. **Table 7-4** also shows that the hybrid numerical methodologies proposed also significantly decrease the absolute errors in the windward region for the droplet velocity.

Regarding the predictive capabilities in the leeward region as defined in *section 2.5* from Chapter 2 ($y < (1/3)y_{max}$), it is not possible to calculate the absolute errors for the URANS stochastic methodology developed due to its underprediction of the spray transverse dispersion. As discussed in Chapter 3 and Chapter 4, the proposed Lagrangian methodology does not tend to capture droplets near the lower wall. This limitation was addressed by developing the hybrid methodologies presented in Chapter 5 and Chapter 6. Although further work needs to be done to improve their predictive capabilities for the SMD within the leeward region, **Figure 7-2** shows that the order of magnitude of their absolute error values agree with those extracted from the existing public studies on the hybrid and Lagrangian approaches for LFJIC. Moreover, they were found to achieve better predictive capabilities for the droplet velocities in the leeward region compared to the LJIC breakup models. This is especially true compared to the results from Madabhushi et al. [30] obtained using their own LJIC breakup model (Madabhushi breakup model) validated using the same dataset.

Therefore, it can be concluded that the stochastic numerical methodologies developed for turbulent LFJIC are often able to achieve similar or better accuracy than the deterministic breakup models used in SOA Computational Fluid Dynamics (CFD) or specifically developed for LJIC. Although their predictive capabilities could be improved in the leeward region, especially for the SMD, recommendations that specifically address these limitations have already been identified in the core research chapters. Thus, the trade-off between practicability and accuracy is deemed reasonable, which confirms the achievement of the 4th research objective presented in **Table 7-1**.

7.3 Novelty, Contribution and Research Conclusions

The novelty of the work presented in the core research chapters resides in the new modelling methodologies developed for turbulent LJIC, the new analysis conducted on the effects of different sub-models and/or boundary conditions, and the validation of the atomization models for LJIC using datasets under more representative gas turbine conditions. The intellectual contribution of the research consists of the new findings and the better understanding gained of the atomization models for LJIC by conducting those new analyses and validation studies. Another important contribution is the improved predictive capabilities achieved by the numerical methodologies developed and their improved practicability due to their ease of implementation and lower computational cost.

This section demonstrates how the 5th research objective described in **Table 7-1** was achieved by summarizing the main elements of the research output described above, which are contributing to fill the gaps in knowledge on atomization modelling for turbulent LJIC. Furthermore, the main research conclusions are provided by articulating the new research findings.

Table 7-6 details the novelty and contribution of the work presented in Chapter 3, which focused on the initial assessment, development, and validation of the URANS stochastic Lagrangian methodology.

Table 7-6: Novelty and contribution of the work presented in Chapter 3.

Novelty	Contribution	
	Contribution to knowledge	Improvements to predictive capabilities
<u>New analysis</u> •Comparison of using the SSD breakup model to non-calibrated SOA deterministic breakup models with the Lagrangian approach for LJIC. •Parametric study of SSD breakup model for LJIC for different boundary conditions. •Effect of time solver (unsteady vs steady RANS) on the predictive capabilities of the Lagrangian approach for LJIC. •Effect of accounting for droplet distortion (TAB distortion model) with SSD breakup model on the predictive capabilities of the Lagrangian approach for LJIC.	<u>Better understanding</u> •The accuracy of SOA deterministic breakup models strongly depends on the calibration of their model constants even for LJIC. Without further calibration, increasing the spray discretization or accounting for the droplet distortion does not improve their predictive capabilities for LJIC. •Better understanding of the effect of the breakup parameter B_1 and normal velocity coefficient K_3 from the SSD breakup model on the spray characteristics predicted for LJIC under different boundary conditions. •Better understanding of the effect of accounting for the spray unsteadiness on the predictive capabilities of the SSD breakup model for LJIC. •Better understanding of the effect of accounting for the droplet distortion on the predictive capabilities of the stochastic and deterministic breakup models for LJIC. <u>New findings/Research conclusions</u> •The SSD breakup model achieves better accuracy than the SOA deterministic breakup models without any calibration of the model constants.	<u>Improvements to prediction methods</u> •Improved predictive capabilities of the Lagrangian approach for LJIC by using the SSD breakup model compared to the non-calibrated SOA deterministic breakup models. •Improved the predictive capabilities of the SSD breakup model for the SMD of LJIC and enhanced the spray radial dispersion in the near-field region by increasing the breakup parameter B_1. •Improved the predictive capabilities of the SSD breakup model for the SMD of LJIC in the spray core and windward regions by using the unsteady RANS solver. •Improved predictive capabilities of the SSD breakup model for the SMD of LJIC in the spray core and leeward regions as well as the overall droplet axial velocity by using the TAB distortion model.

<u>Validation at more representative conditions</u> •Validation of the SSD breakup model at higher pressure and higher gas Weber numbers for LJIC. •Validate the predictive capabilities for the droplet axial velocity of the SSD breakup model for LJIC. <u>New methodologies</u> •Development and validation of a URANS stochastic Lagrangian methodology for turbulent liquid fuel JIC.	•The normal velocity coefficient K_3 does not have a significant impact on the spray characteristics predicted for LJIC regardless of the boundary conditions. •The breakup parameter B_1 impacts the predictions for the spray dispersion as well as the SMD and droplet axial velocity, especially within the windward and spray core regions for LJIC regardless of the boundary conditions. •The unsteady solver impacts the predictions of the SSD breakup model for the SMD and droplet axial velocity in the spray core and windward regions but has no significant impact within the leeward region for LJIC. •The TAB distortion model tends to increase the SMD predicted across the entire spray height as well as the droplet axial velocity within the windward region for LJIC.	<u>Existing public studies</u> •Achieved better agreement with the experimental data for the SMD in the windward region and spray trajectory compared to other studies available in the literature on LJIC conducted using the SSD breakup model or deterministic models for liquid fuels. •Ability to predict more accurately some features of the spray characteristics compared to other studies available in the literature on LFJIC (see <i>section 7.2</i> for further details).
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Table 7-7 summarizes the novelty and contribution of the work presented in Chapter 4 to further develop and validate the stochastic Lagrangian methodology.

Table 7-7: Novelty and contribution of the work presented in Chapter 4.

Novelty	Contribution	
	Contribution to knowledge	Improvements to predictive capabilities
<u>New analysis</u> •Effect of the following models on the predictive capabilities of the Lagrangian approach and on its sensitivity to different boundary conditions for turbulent LJIC: – Turbulence modelling (LES vs URANS). – SOA SGS models (WALE vs Smagorinsky). – Synthetic Eddy Method (SEM) turbulent boundary conditions with different SGS models. – RANS-based turbulent dispersion model and its exact eddy time sub-model.	<u>Better understanding</u> •Better understanding of the sensitivity of the Lagrangian approach to the boundary conditions (operating conditions and gas velocity profile) when using a stochastic breakup model. •Better understanding of the effect of using different turbulence models, SGS models, turbulent boundary conditions, and Lagrangian turbulent dispersion model on the predictive capabilities of the Lagrangian approach. •The SOA SGS models struggle to capture the impact of strong velocity gradients and large Reynolds numbers on the Lagrangian particles from turbulent LJIC due to their filtering of the unresolved smaller-scale motions. As a result, using LES with the Lagrangian approach for turbulent LJIC significantly increases the discrepancies with the experimental data, especially for the spray trajectory and SMD. <u>New findings/Research conclusions</u> •LES tends to overpredict the spray trajectory and underpredict the SMD in the spray core and leeward regions regardless of the gas velocity profile, SGS model or SEM used. The predictive capability of LES for the spray trajectory is also not sensitive to the boundary conditions. However, the SMD predicted by LES in the windward region is sensitive to the gas velocity considering it increases when using a constant profile.	<u>Improvements to prediction methods</u> •Improved the predictive capabilities of the Lagrangian approach for turbulent LJIC and reduced its sensitivity to the boundary conditions by using URANS with a turbulent dispersion model for a wide range of conditions and crossflow gas velocity profiles. •Reduced the sensitivity of the Lagrangian approach coupled with LES to local changes in the velocity field by using the WALE SGS model instead of the Smagorinsky SGS model.

• Sensitivity of the Lagrangian approach to the crossflowing gas velocity profile for turbulent LJIC when using LES with different SOA SGS models and different turbulent boundary conditions. • Sensitivity of the URANS stochastic Lagrangian methodology developed for LJIC to the following elements: – Crossflowing gas velocity profile under different boundary conditions. – Pressure and momentum flux ratio conditions.	• Compared to URANS, LES predicts a higher SMD and lower gas velocity in the windward region and predicts the opposite in the spray core and leeward regions. It also predicts a higher spray trajectory. The effect of using LES instead of URANS on these predictions is not sensitive to the boundary conditions and is independent of the SGS model and SEM. • The SGS models and SEM do not have a significant impact on the predictive capabilities of the Lagrangian approach for the droplet and gas velocities, SMD and spray trajectory of turbulent LJIC. • The effect of the SGS model on the Lagrangian approach is not sensitive to the gas velocity profile or the boundary conditions. However, the spray width predicted by the Smagorinsky SGS model is sensitive to the gas velocity profile. • The effect of the SEM on the predictive capabilities is independent of the SGS model and is not sensitive to the gas velocity profile. However, it is sensitive to the boundary conditions considering the spray width increases under higher-pressure conditions. • The turbulent dispersion model does not have a significant impact on the SMD in the leeward and spray core region but tends to enhance the spray width regardless of the boundary conditions. • The predictive capabilities of the Lagrangian approach for the spray trajectory when using URANS tend to be sensitive to the boundary conditions. However, using the turbulent dispersion model reduces its sensitivity to the boundary conditions.	<u>Proposed methodologies</u> • Significantly improved the agreement with the experimental data achieved by the Lagrangian approach for turbulent LJIC by properly accounting for the upstream gas velocity profile. <u>Existing public studies</u> • Achieved better agreement with the experimental data for the SMD in the windward region and spray trajectory compared to other studies available in the literature on LJIC conducted using the SSD breakup model or deterministic models for liquid fuels.
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<u>New methodologies</u> • Further development and validation of the URANS stochastic Lagrangian methodology for turbulent LFJIC over a wider range of Weber numbers, pressures, and momentum flux ratios.	• The predictive capabilities of the Lagrangian approach for the spray trajectory and SMD in the windward region are sensitive to the gas velocity profile. Using a constant velocity profile increases the values predicted for these spray characteristics independently of the boundary conditions or turbulence model used. The effect of the gas velocity profile on the SMD predicted by the stochastic URANS methodology within the leeward and spray core regions is also sensitive to the boundary conditions. • The stochastic URANS methodology developed is more sensitive to the imposed jet-to-gas velocity ratio than the momentum flux ratio or pressure conditions independently of the gas velocity profile.	• Ability to predict more accurately some features of the spray characteristics compared to other studies available in the literature on LFJIC (see <i>section 7.2</i> for further details).
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Table 7-8 presents the novelty and contribution of the research work presented in Chapter 5, which consisted of developing and validating a novel stochastic methodology for coupling the VOF and Lagrangian approach.

Table 7-8: Novelty and contribution of the work presented in Chapter 5.

Novelty	Contribution	
	Contribution to knowledge	Improvements to predictive capabilities
<u>New analysis</u> • Effect of the modelling approach for LJIC (VOF-Lagrangian vs Lagrangian) on the computational cost. • Effect of the boundary conditions on the computational cost of the Lagrangian and VOF-Lagrangian approaches for LJIC.	<u>Better understanding</u> • Better understanding of the sensitivity of the computational cost of atomization modelling for LJIC to the operating conditions, modelling approach (VOF-Lagrangian vs Lagrangian) and VOF-Lagrangian transition model.	<u>Proposed methodologies</u> • Improved the predictive capabilities of LES for turbulent LJIC by coupling the Lagrangian and VOF approaches.

•Effect of the VOF-Lagrangian transition model on the computational cost of the hybrid approach for LJIC. •Effect of coupling the SSD breakup model with different modelling approaches (VOF-Lagrangian vs Lagrangian) on the predictive capabilities of LES for LJIC. <u>Validation at more representative conditions</u> •Validation of the VOF-Lagrangian approach for LJIC at higher pressure and higher gas Weber numbers. •Validation of the VOF-Lagrangian approach coupled with the SSD breakup model for LJIC at higher pressure, higher Weber numbers and using data for fuel instead of water. •Validate the predictive capabilities for the spray trajectory, SMD and droplet axial velocity within the far-field region ($x/d > 10$) of the VOF-Lagrangian approach coupled with the SSD breakup model for LJIC. <u>New methodologies</u> •Development and validation of a stochastic hybrid VOF-Lagrangian methodology for turbulent liquid fuel JIC.	•Better understanding of the effect of coupling the Lagrangian and VOF approaches with the SSD breakup model on the predictive capabilities of LES for LJIC. <u>New findings/Research conclusions</u> •The VOF-Lagrangian approach has a significantly higher computational cost than the Lagrangian approach for LJIC regardless of the operating conditions or turbulence model used with the latter (LES vs URANS). •The computational cost of the VOF-Lagrangian approach for LJIC increases when imposing a higher momentum flux ratio and/or lower gas pressure. •The VOF-Lagrangian stripping transition model is more computationally expensive than the resolved transition model for the same mesh size. •Compared to the predictions of the Lagrangian approach for LJIC with the SSD breakup model, the VOF-Lagrangian approach enhances the radial and transverse dispersion of the spray, reduces the spray penetration and increases the droplet axial velocity in the windward region while reducing it in the spray core and leeward regions regardless of the operating conditions used.	•Improved the predictions for the SMD within the leeward region and for the overall droplet axial velocity compared to the URANS stochastic Lagrangian methodology previously developed. <u>Existing public studies</u> •Achieved better agreement with the experimental data for the droplet velocity in the windward region compared to other studies available in the literature on liquid fuel JIC. •Ability to predict more accurately some features of the spray characteristics compared to other studies available in the literature on liquid fuel JIC (see section 7.2 for further details).
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Table 7-9 lists the novelty and contribution of the research work done in Chapter 6 to reduce the computational cost of the hybrid approach by proposing an optimized stripping transition method.

Table 7-9: Novelty and contribution of the work presented in Chapter 6.

Novelty	Contribution	
	Contribution to knowledge	Improvements to predictive capabilities
<u>New analysis</u> •Effect of using a higher order temporal discretization scheme (BDF1 vs BDF2) on the predictive capabilities and computational cost of the VOF-Lagrangian approach for LJIC. •Effect of the VOF-Lagrangian transition model on the predictive capabilities and computational cost of the VOF-Lagrangian approach for LJIC. <u>New methodologies</u> •Development and validation of a lower-cost VOF-Lagrangian methodology using a stochastic stripping transition model for turbulent liquid fuel JIC.	<u>New findings/Research conclusions</u> •Compared to the resolved transition model, the optimized hybrid stripping method tends to reduce the spray penetration in the near-field region, increase the droplet axial velocity in the spray core and windward regions and locally decrease the SMD. •The trends in predictive capabilities of the VOF-Lagrangian approach for LJIC are not sensitive to the transition model used. •The BDF2 scheme introduces fluctuations in the continuous flow field, which locally enhances the breakup process when using the optimized hybrid stripping method. As a result, it tends to reduce the SMD and increase the droplet velocity in the windward region compared to the BDF1 scheme. •The BDF2 scheme reduces the computational cost of the VOF-Lagrangian approach with the optimized stripping methodology due to its faster convergence of the residuals.	<u>Improvements to prediction methods</u> •Improved the predictive capabilities of the proposed optimized hybrid stripping method developed for LJIC by using the BDF1 temporal discretization scheme. <u>Proposed methodologies</u> •The predictive capabilities of the proposed optimized hybrid stripping method are either similar to the resolved hybrid method previously developed or deemed reasonable considering the trade-off between cost and accuracy. <u>Existing public studies</u> •Achieved better agreement with the experimental data for the droplet velocity in the windward region compared to other studies available in the literature on liquid fuel JIC. •Ability to predict more accurately some features of the spray characteristics compared to other studies available in the literature on liquid fuel JIC (see <i>section 7.2</i> for further details).

7.4 Research Impact

The increased efficiency and improved predictive capabilities of the proposed numerical methodologies will directly impact the energy and aerospace fields by reducing the production and time cost of developing low-emission technologies with LJIC, as further elaborated below:

- The novel numerical methodologies developed are expected to facilitate and accelerate the development of low-emission gas turbine combustion systems using advanced atomization technologies:
 - The URANS stochastic methodology reduces the time cost of modelling LJIC by improving the practicality of using the lower-fidelity Lagrangian approach as it does not require exhaustive calibration of its model constant or prior knowledge of the spray characteristics.
 - The hybrid methodologies reduce the computational cost of designing novel LJIC injectors by improving the practicality of using the higher-fidelity VOF approach through its coupling with the lower-cost stochastic Lagrangian methodology proposed to account for the effect of the injector geometry and liquid jet column on the spray characteristics.
 - The optimized stripping transition method proposed improves the practicality of using LES to model turbulent LJIC by significantly reducing the computational cost of the hybrid approach.
- The improved practicality and lower computational cost of the numerical methodologies developed should enable further industrial and academic research work on turbulent LJIC that were previously limited by the lack of experimental data, the time cost associated with calibrating the SOA and LJIC deterministic breakup models or the high computational cost of using interface capturing methods to avoid fine-tuning model constants.
- The best practices established for modelling turbulent LFJIC increase the level of confidence in the research and development work of low-emission gas turbine

technologies, thus shortening the design iteration cycle of novel LJIC combustion systems.

- Implementing the recommended best practices would allow a better utilization of the time and computational resources available. Thus, it would enable the study of other complex phenomena requiring higher-fidelity models (e.g. combustion, thermoacoustic, etc.) or that involve a time-iterative process such as the studying the effect on the combustion characteristics (combustion performance, emissions, etc.) of optimizing the design of different combustor parts (e.g. heatshield, liner, etc.) or of using different operating conditions. Easing the strain of modelling atomization on the project resources available would particularly benefit the research work that focuses on studying other aspects of the combustion system that involve turbulent LJIC, especially for applications that require higher-fidelity LES.

7.4.1 Real-World Impact

This research was jointly funded by Siemens Energy and Cranfield University. The author undertook several research placements at Siemens Energy to help implement the numerical methodologies and best practices proposed in *section 7.1*. Thus, the research outcome already has a quantifiable impact on the research and development work of low-emission gas turbines as listed below:

- The research findings from Chapter 3 and Chapter 4 regarding the limitations of the SOA SGS models for turbulent LJIC and the absolute need to calibrate the SOA deterministic breakup models have been used to establish best practices for modelling complex turbulent liquid injectors (both water and fuel) at Siemens Energy.
- The hybrid methodology developed in Chapter 5 is currently being implemented at Siemens Energy Canada Limited to guide the design of novel liquid fuel injectors for low-emission aeroderivative gas turbine combustion systems.
- The URANS Lagrangian stochastic methodology developed from Chapter 3 and Chapter 4 has been used to assess the impact of different boundary conditions on

the combustion exit temperature and emissions of the SGT-A65 conventional industrial gas turbine combustor (Siemens Energy).

- The research findings and methodologies developed from this work have been used at Siemens Energy to establish a best practice guide based on the intent of the simulation (see *section 7.1*).
- Recommendations were made to the development team of Simcenter STAR-CCM+ to implement a user-defined breakup model that would allow more flexibility to further develop stochastic breakup models. The author has participated in the beta testing of the user-defined breakup model, which was made available to all users in fall 2022 through Simcenter STAR-CCM+ version 2210.
- The URANS Lagrangian stochastic methodology developed from Chapter 3 and Chapter 4 was used to design and commission a bespoke high-temperature and high-pressure experimental rig facility for LFJIC. As elaborated in Appendix A, it was designed with versatility in mind to ensure its suitability for a wide range of flow conditions and different injectors, thus enabling a wide variety of experimental research work on turbulent LFJIC at representative gas turbine combustor inlet conditions.

7.5 Research Limitations

This section addresses the limitations of the research work presented, which are mostly related to the validation datasets used and the computational resources required to perform further validation of the higher-fidelity approaches. Recommendations for future work to address these limitations are also suggested in the following section.

- **Validation datasets limited to plain orifice injectors:** As mentioned in Chapter 2, the experimental datasets available in the literature for LJIC are often limited to using plain orifice injectors to gain a better understanding of the fundamental physics involved in the atomization process. Thus, the majority of numerical validation studies and numerical model development work has been conducted using datasets for this type of simple injector, which includes the research presented in this work. Although plain orifice injectors are used in gas turbine combustion systems for

diverse applications, other combustion systems use more complex types such as the pressure-swirl injectors [5, 8]. Therefore, it could be relevant to extend the applicability of the methodologies developed to different injectors, which should be relatively straightforward to do considering their stochastic nature. In particular, this should not be a problem for the hybrid numerical methodologies developed considering they use the higher-fidelity VOF approach to model the primary region, which allows to account for the effect on the spray characteristics of the inner passage of the injector geometry. However, the numerical injection model used by the URANS Lagrangian stochastic methodology developed would need to be adapted considering the point injection method is not likely representative of other injector types. This could be achieved by using a surface injector model to introduce the Lagrangian particles from the centre of the cells located on a surface representing the injector's exit plane [130]. Despite the minor efforts needed to adapt the proposed Lagrangian methodology, such modifications have already been successfully implemented at Siemens Energy to model more complex injection systems. Therefore, all methodologies developed are expected to be suitable to other types of injectors with only minor adjustments required even if their validation has been limited to plain orifice injector datasets in the present work.

- **Validation datasets limited to ambient temperature:** As detailed in *section 2.4* from Chapter 2 and multiple times throughout the core research chapters, only validation datasets at ambient temperatures were used in this work to help fill the significant gaps in knowledge on the baseline predictive capabilities (i.e. ambient temperature) of atomization modelling for LJIC, especially using a stochastic breakup model. This can be attributed in part to the added complexity of evaporation modelling, which impacts the assessment of the atomization modelling approaches by introducing additional uncertainties. Thus, it was deemed preferable to use ambient temperature datasets for the development and validation of atomization models. These research gaps can also be explained by the difficulty of gathering experimental data on the spray characteristics of liquid fuel JIC under high-temperature conditions mainly due to the autoignition risks but also due to the evaporation process. For all these reasons, very few numerical validation studies have been conducted for liquid fuel JIC at high temperatures [21, 39]. Despite the validation of the numerical

modelling approaches being limited to ambient conditions in the present work, the URANS Lagrangian stochastic methodology developed was successfully coupled with a quasi-steady single-droplet evaporation model [211] at Siemens Energy to better evaluate the combustion process of the SGT-A65 aeroderivative gas turbine under different combustor inlet conditions.

- **Computational resources available limiting validation cases for hybrid studies:**

Due to the computational cost of the hybrid VOF-Lagrangian approach studied in Chapter 5 and the limitation on the computational resources available, fewer validation studies could be conducted compared to the previous chapters on the lower-fidelity Lagrangian approach. However, **Table 2-7** from *section 2.4.5* shows that this aspect does not affect the contribution or engineering relevance of the present work considering the existing research gaps on atomization modelling using the hybrid approach for LJIC. Indeed, other validation studies available in the literature seem to have faced similar limitations as very few used more than 2 experimental conditions [36, 39] and were limited to validating the spray trajectory in the near-field region. To further straighten the research findings and conclusions from Chapter 5, two different datasets were used to assess the sensitivity/applicability of the methodology developed to the test section dimensions, injector dimensions, fuel type and experimental conditions. To the best knowledge of the author, no other studies have assessed the predictive capabilities of the hybrid approach using more than one dataset. This also includes the studies conducted using the alternative decoupled VOF-Lagrangian approach developed to reduce the computational cost of hybrid simulations [27, 38]. Moreover, no other studies on the hybrid approach have simultaneously validated the predictions in spray trajectory, SMD and droplet velocity as shown in **Table 2-7** to the best knowledge of the author. Thus, despite the limitations in computational resources, appropriate mitigations were put in place to preserve the novelty and contribution of the research presented in Chapter 5.

7.6 Recommendations for Future Work

This final section addresses the 6th research objective by providing recommendations to augment the atomization modelling capabilities for turbulent LFJIC of the numerical CFD software Simcenter STAR-CCM+, which is widely used by the academic and industrial

gas turbine communities. General recommendations for future research work on modelling LFJIC are also provided based on the main research findings and to address the research limitations discussed in *section 7.5*.

It should be noted that specific recommendations for future work on further developing and improving the predictive capabilities of atomization modelling for turbulent LJIC were presented in the discussion and conclusions sections of the core research chapters (Chapter 3 to Chapter 6). Some of them have already been addressed in this work, such as the recommendation from Chapter 4 to investigate coupling the stochastic Lagrangian methodology developed with higher fidelity approaches to achieve better agreement with the experimental data. This motivated the research and development work on the VOF-Lagrangian approach presented in Chapter 5. The main recommendation for future work stipulated in the latter was to optimize the AMR settings or the VOF-Lagrangian transition model to improve the practicality of the hybrid approach, which inspired the development of the optimized hybrid stripping method proposed in Chapter 6.

7.6.1 Recommendations for Simcenter STAR-CCM+

The four recommendations listed below were provided to the product managers of Simcenter STAR-CCM+ to progress its capabilities in atomization modelling. It is important to note that these recommendations have the potential to improve the predictive capabilities of the numerical methodologies developed, but further validation would be needed. Furthermore, these recommendations could also be extended to other commercial and in-house CFD codes.

1. Adapting the Lagrangian turbulent dispersion model to be used with LES. This could be partially achieved by substituting the RANS turbulent terms (viscosity, kinetic energy, length scales) with the equivalent LES formulation.
2. Implementing a SGS model that accounts for the sub-filtered acceleration of the turbulent Lagrangian droplets, such as the one more recently proposed by Gorokhovski and Oruganti [179].

These two recommendations could potentially be used to improve the predictive capabilities of the Lagrangian approach coupled with LES for turbulent sprays regardless of the injector configuration used (coaxial or crossflow) as suggested in Chapter 4. Thus,

they could benefit the research and development work conducted on a wide range of applications beyond those of interest to the present work.

3. Enabling the compatibility between the VOF-Lagrangian resolved transition model and the higher-order temporal discretization schemes.

This recommendation could be used to further improve the predictive capabilities of the hybrid resolved methodology developed as mentioned in Chapter 5. Despite the effect of the BDF2 scheme on the discrepancies of the optimized hybrid stripping method reported in Chapter 6, the hybrid resolved method could still benefit from the enhanced blob shedding and higher transverse dispersion of the Lagrangian droplets. It could also benefit from the faster convergence of the BDF2 scheme and could reduce its computational cost. This provides further motivation to enable capabilities for higher-order temporal discretization schemes when using the resolved transition model as previously recommended in *section 5.6* of Chapter 5.

4. Enabling user control of the maximum stripped Lagrangian droplet diameter from the VOF-Lagrangian stripping model to allow shedding droplets larger than 50% of the cell size.

This last recommendation could potentially facilitate future work done to improve the SMD predictions of the optimized stripping hybrid method proposed as it would allow injecting larger Lagrangian droplets, which is one of the main aspects to improve as discussed in great detail in Chapter 6. It is important to note that additional validation work would be needed to assess the effect of this strategy on the mass imbalance errors and the numerical stability of the solution.

7.6.2 General Recommendations for Future Work

Future research work on the numerical modelling of LJIC for low-emission gas turbine combustion systems could be done to:

- Validate the applicability of the numerical methodologies developed to other types of injectors. For the hybrid methodologies, this only involves changing the boundary conditions. For the URANS Lagrangian stochastic numerical methodology developed, the injection model would need to be modified based on the injector type as briefly discussed in *section 7.5*. Moreover, a stochastic

methodology would also need to be implemented to impose the particle diameter and cone angle at the nozzle exit. The former could be done by using a log-normal diameter distribution similar to the SSD breakup model's formulation [28] and a rough estimate of the cone angle could be imposed based on the geometric features of the injector's exit. It is important to note that this future work strongly depends on the availability of experimental data on LJIC using injectors different from the plain orifice type. Thus, further experimental work will likely need to be done first to fill the experimental research gaps on using more complex liquid fuel injectors in crossflow.

- Assess the predictive capabilities of evaporation models for liquid fuel JIC using the numerical methodologies developed. This includes the dedicated Lagrangian evaporation model [211] and the Eulerian evaporation framework for the VOF liquid phase [212, 213]. It would also be relevant for engineering development and research work to assess the effect of modelling evaporation on the computational cost of the VOF-Lagrangian approach.
- Use the bespoke high-pressure and high-temperature rig facility designed to help bridge the gaps in knowledge on turbulent LFJIC by conducting experiments investigating the primary and secondary spray breakup, propagation, and evaporation processes under more representative gas turbine conditions. The comprehensive datasets will be generated for a wide range of momentum flux ratios, Weber numbers, pressures and temperatures as detailed in Appendix A, which could be used to further assess, develop, and validate the atomization modelling approaches of turbulent LJIC for diverse applications.
- Further validate and improve the predictive capabilities of the numerical methodologies developed by using the exhaustive datasets generated from the experimental rig facility designed. The high-temperature datasets could also be used to assess their predictive capabilities when coupled with evaporation modelling.

References

- [1] Government of Canada, “Net-zero emissions by 2050,” *Government of Canada*, 05 Apr. 2024. [Online]. Available: <https://www.canada.ca/en/services/environment/weather/climatechange/climate-plan/net-zero-emissions-2050.html>. [Accessed: 2024].
- [2] Crown Commercial Services, “Carbon reduction plan: Policy Paper,” *GOV.UK*, Jan. 02, 2024. [Online]. Available: [https://www.gov.uk/government/publications/carbon-reduction-policy/carbon-reduction-plan#:~:text=This%20Carbon%20Reduction%20Plan%20\(CRP,Greening%20Government%20Commitments%20\(GGC\)](https://www.gov.uk/government/publications/carbon-reduction-policy/carbon-reduction-plan#:~:text=This%20Carbon%20Reduction%20Plan%20(CRP,Greening%20Government%20Commitments%20(GGC)). [Accessed: 2024].
- [3] Reaching ‘net zero’ CO₂ emissions by 2050, “ Commission sets out how to sustainably capture, store and use carbon to reach climate neutrality by 2050”, *European Commission*, 06 Feb. 2024. [Online]. Available: https://ec.europa.eu/commission/presscorner/detail/en/IP_24_585. [Accessed: 2024].
- [4] United Nations: Climate Action, “For a livable climate: Net-zero commitments must be backed by credible action”, *United Nations*. [Online]. Available: <https://www.un.org/en/climatechange/net-zero-coalition>. [Accessed: 2024].
- [5] K. K. Kuo and R. Acharya, *Fundamentals of Turbulent and Multiphase Combustion*. United States of America: Wiley, 2012.
- [6] K. Mahesh, “The interaction of jets with crossflow,” *Annual Review of Fluid Mechanics*, vol. 45, no. 1, pp. 379–407, Jan. 2013, doi: 10.1146/annurev-fluid-120710-101115.
- [7] N. Ashgriz, *Handbook of Atomization and Sprays*. United States of America: Springer, 2011.
- [8] A. H. Lefebvre and D. R. Ballal, *Gas Turbine Combustion: Alternative Fuels and Emissions*, 3rd ed. United States of America: CRC Press, 2010.

- [9] M. Broumand and M. Birouk, “Liquid jet in a subsonic gaseous crossflow: Recent progress and remaining challenges,” *Progress in Energy and Combustion Science*, vol. 57, pp. 1–29, Nov. 2016, doi: 10.1016/j.pecs.2016.08.003.
- [10] A. Coussement, O. Gicquel, and G. Degrez, “Large Eddy Dimulation of a pulsed jet in cross-flow,” *Journal of Fluid Mechanics*, vol. 695, pp. 1–34, Feb. 2012, doi: 10.1017/jfm.2011.539.
- [11] C. W. Hirt and B. D. Nichols, “Volume of Fluid (VOF) method for the dynamics of free boundaries,” *Journal of Computational Physics*, vol. 39, no. 1, pp. 201–225, Jan. 1981, doi: 10.1016/0021-9991(81)90145-5.
- [12] M. Sussman, P. Smereka, and S. Osher, “A level set approach for computing solutions to incompressible Two-Phase flow,” *Journal of Computational Physics*, vol. 114, no. 1, pp. 146–159, Sep. 1994, doi: 10.1006/jcph.1994.1155.
- [13] O. Desjardins, V. Moureau, and H. Pitsch, “An accurate conservative level set/ghost fluid method for simulating turbulent atomization,” *Journal of Computational Physics*, vol. 227, no. 18, pp. 8395–8416, Sep. 2008, doi: 10.1016/j.jcp.2008.05.027.
- [14] C. Baumgarten, *Mixture Formation in Internal Combustion Engines*. Berlin: Springer, 2006.
- [15] M. S. Almanzalawy, L. H. Rabie, and M. H. Mansour, “Modeling of an efficient airblast atomizer for liquid jet into a supersonic crossflow,” *Acta Astronautica*, vol. 177, pp. 142–157, Dec. 2020, doi: 10.1016/j.actaastro.2020.07.031.
- [16] A. Bhandarkar, P. Manna, and D. Chakraborty, “Assessment of droplet breakup models in high-speed cross-flow,” *Atomization and Sprays*, vol. 27, no. 1, pp. 61–79, Jan. 2017, doi: 10.1615/atomizspr.2016015409.
- [17] F. Liu, G. J. Smallwood, and O. L. Gulder, “Numerical study of breakup processes of water jet injected into a cross air flow,” in *ICLASS 2000 Proceedings of the Eighth International Conference on Liquid Atomization and Spray Systems*, Pasadena, California, USA, Jul. 2000, pp. 67-74.

- [18] Y.-Y. Niu, C.-E. Wu, Y.-H. Huang, Y.-J. Chou, and S.-C. Kong, “Evaluation of breakup models for liquid side jets in supersonic cross flows,” *Numerical Heat Transfer. Part A: Applications*, vol. 79, no. 5, pp. 353–369, Nov. 2020, doi: 10.1080/10407782.2020.1847513.
- [19] J. Zhao, Y. Ren, Y. Tong, W. Lin, and W. Nie, “Atomization of a liquid jet in supersonic crossflow in a combustion chamber with an expanded section,” *Acta Astronautica*, vol. 180, pp. 35–45, Mar. 2021, doi: 10.1016/j.actaastro.2020.11.051.
- [20] J. Zhao, W. Lin, C. Yan, Z. Zheng, Y. Tong, and W. Nie, “Mixing enhancement mechanism of combined H₂–Water jets in supersonic crossflows in a combustor with an expanded section,” *International Journal of Hydrogen Energy*, vol. 47, no. 19, pp. 10747–10761, Mar. 2022, doi: 10.1016/j.ijhydene.2022.01.070.
- [21] M. Kamin and P. Khare, “An LES study of kerosene combustion in air crossflow,” in *AIAA 2018 Joint Propulsion Conference*, Cincinnati, Ohio, USA, Jul. 2018, doi: 10.2514/6.2018-4682.
- [22] P. Li, Z. Wang, M. Sun, and H. Wang, “Numerical simulation of the gas-liquid interaction of a liquid jet in supersonic crossflow,” *Acta Astronautica*, vol. 134, pp. 333–344, May 2017, doi: 10.1016/j.actaastro.2016.12.025.
- [23] P. Khare, S. Wang, and V. Yang, “Modeling of finite-size droplets and particles in multiphase flows,” *Chinese Journal of Aeronautics*, vol. 28, no. 4, pp. 974–982, Aug. 2015, doi: 10.1016/j.cja.2015.05.004.
- [24] X. Li and M. Soteriou, “High-fidelity simulation of fuel atomization in a realistic swirling flow injector,” *Atomization and Sprays*, vol. 23, no. 11, pp. 1049–1078, Jan. 2013, doi: 10.1615/atomizspr.2013007395.
- [25] X. Li and M. Soteriou, “Detailed numerical simulation of liquid jet atomization in crossflow of increasing density,” *International Journal of Multiphase Flow*, vol. 104, pp. 214–232, Jul. 2018, doi: 10.1016/j.ijmultiphaseflow.2018.02.016.

- [26] H. Feiz, H. Karim, W. Zhao, J. Song, D. Kubicki, M. Frackowiak, V. Kumar, H. Jadeja, P. Nakod, S. N. Kumar, S. Shrivastava, M. Lambert, and J. G. Lee, “Numerical modelling of combustion of multiple liquid jet in non-uniform crossflow,” in *Proceedings of the ASME Turbo Expo 2023: Turbomachinery Technical Conference and Exposition. Volume 3B: Combustion, Fuels, and Emissions*, Boston, Massachusetts, USA, June 2023, doi: 10.1115/GT2023-104092.
- [27] H. Feiz, W. Zhao, D. Kubicki, M. Frackowiak, V. Kumar, H. Jadeja, P. Nakod, S. Shrivastava, S. K. Nallamothu, M. Lambert, J. G. Lee, and J. Song, “Numerical modeling of liquid jet in non-uniform crossflow using Enhanced Madabhushi model,” in *Proceedings of the ASME Turbo Expo 2022: Turbomachinery Technical Conference and Exposition. Volume 3B: Combustion, Fuels, and Emissions*, Rotterdam, Netherlands, June 2022, doi: 10.1115/GT2022-82766.
- [28] A. H. Lefebvre and V. G. McDonell, *Atomization and sprays*, 2nd ed. United States of America: CRC Press, 2017.
- [29] A. Mashayek, M. Behzad, and N. Ashgriz, “Multiple Injector Model for primary breakup of a liquid jet in crossflow,” *AIAA Journal*, vol. 49, no. 11, pp. 2407–2420, Nov. 2011, doi: 10.2514/1.j050623.
- [30] R. K. Madabhushi, M. Y. Leong, and Hautman, D.J., “Simulation of the break-up of a liquid jet in crossflow at atmospheric conditions,” in *Proceedings of the ASME Turbo Expo 2004: Power for Land, Sea, and Air. Volume 1: Turbo Expo 2004*, Vienna, Austria, June 2004, pp. 697-704, doi: 10.1115/GT2004-54093.
- [31] M. Rachner, J. Becker, C. Hassa, and T. Doerr, “Modelling of the atomization of a plain liquid fuel jet in crossflow at gas turbine conditions,” *Aerospace Science and Technology*, vol. 6, no. 7, pp. 495–506, Nov. 2002, doi: 10.1016/s1270-9638(01)01135-x.
- [32] S. Khosla, and D. S. Crocker, “CFD modeling of the atomization of plain liquid jets in cross flow for gas turbine applications”, in *Proceedings of the ASME Turbo Expo 2004: Power for Land, Sea, and Air. Volume 1: Turbo Expo 2004*, Vienna, Austria, June 2004, pp. 797-806, doi: 10.1115/GT2004-54269.

- [33] S. V. Apte, M. Gorokhovski, and P. Moin, “LES of atomizing spray with stochastic modeling of secondary breakup,” *International Journal of Multiphase Flow*, vol. 29, no. 9, pp. 1503–1522, Sep. 2003, doi: 10.1016/s0301-9322(03)00111-3.
- [34] S. V. Apte, K. Mahesh, M. Gorokhovski, and P. Moin, “Stochastic modeling of atomizing spray in a complex swirl injector using Large Eddy Simulation,” *Proceedings of the Combustion Institute*, vol. 32, no. 2, pp. 2257–2266, Jan. 2009, doi: 10.1016/j.proci.2008.06.156.
- [35] M. Herrmann, “Detailed simulations of the breakup processes of turbulent liquid jets in subsonic crossflows,” in *ICLASS 2009 Proceedings of the 11th Triennial International Annual Conference on Liquid Atomization and Spray Systems*, Vail, Colorado, USA, 2009.
- [36] L. G. Bravo, D. Kim, F. Ham, and K. A. Kerner, “High fidelity simulations of primary breakup and vaporization of liquid jet in cross flow (JICF),” in *2018 AIAA Joint Propulsion Conference*, Cincinnati, Ohio, USA, Jul. 2018, doi: 10.2514/6.2018-4683.
- [37] R. Blanchard and S. Shi, “Validation of a stochastic droplet breakup model applied to a liquid jet in turbulent crossflow,” *Advances in Fluid Mechanics IX, WIT Transactions on Engineering Sciences*, vol. 174, pp. 371–378, Jun. 2012, doi: 10.2495/AFM120331.
- [38] L. Wang, H. Ozogul, T. Kaushik, A. Bhat, and S. Rida, “Towards a detailed liquid fuel injection model for gas turbine combustor CFD,” in *Proceedings of the ASME Turbo Expo 2020: Turbomachinery Technical Conference and Exposition. Volume 4B: Combustion, Fuels, and Emissions*, Virtual, Sep. 2020, doi: 10.1115/GT2020-16044.
- [39] J. Wen, Y. Hu, A. Nakanishi, and R. Kurose, “Atomization and evaporation process of liquid fuel jets in crossflows: A numerical study using Eulerian/Lagrangian method,” *International Journal of Multiphase Flow*, vol. 129, p. 103331, Aug. 2020, doi: 10.1016/j.ijmultiphaseflow.2020.103331.

- [40] M. Heinrich and R. Schwarze, “3D-coupling of Volume-of-Fluid and Lagrangian particle tracking for spray atomization simulation in OpenFOAM,” *SoftwareX*, vol. 11, p. 100483, Jan. 2020, doi: 10.1016/j.softx.2020.100483.
- [41] D. H. Fontes, V. Vilela, L. De Souza Meira, and F. J. De Souza, “Improved hybrid model applied to liquid jet in crossflow,” *International Journal of Multiphase Flow*, vol. 114, pp. 98–114, May 2019, doi: 10.1016/j.ijmultiphaseflow.2019.02.009.
- [42] M. Zghal, X. Sun, P. Q. Gauthier, and V. Sethi, “Validation and assessment of a numerical methodology for turbulent liquid fuel jets in high-speed crossflow,” in *Proceedings of the ASME Turbo Expo 2022: Turbomachinery Technical Conference and Exposition. Volume 2: Coal, Biomass, Hydrogen, and Alternative Fuels; Controls, Diagnostics, and Instrumentation; Steam Turbine*, Rotterdam, Netherlands, June 2022, doi: 10.1115/GT2022-83166.
- [43] M. Zghal, X. Sun, P. Gauthier, and V. Sethi, “Validation of a stochastic breakup model for turbulent jets in high-speed crossflow: Assessment of turbulent interactions and sensitivity to boundary conditions,” *Atomization and Sprays*, vol. 33, no. 4, pp. 25–54, Jan. 2023, doi: 10.1615/atomizspr.2023041220.
- [44] M. Zghal, P. Gauthier, X. Sun, C. Wijesinghe, and V. Sethi, “Validation and assessment of a hybrid VOF-Lagrangian numerical methodology for turbulent liquid fuel jets in high-speed crossflow,” *Journal of Engineering for Gas Turbines and Power*, vol. 146, no. 8, Feb. 2024, doi: 10.1115/1.4064218.
- [45] D. Sedarsky, M. Paciaroni, E. Berrocal, P. Petterson, J. Zelina, J. Gord, M. Linne, “Model validation image data for breakup of a liquid jet in crossflow: part I,” *Experiments in Fluids*, vol. 49, no. 2, pp. 391–408, Jan. 2010, doi: 10.1007/s00348-009-0807-2.
- [46] D. R. Getsinger, L. Gevorkyan, O. I. Smith, and A. R. Karagozian, “Structural and stability characteristics of jets in crossflow,” *Journal of Fluid Mechanics*, vol. 760, pp. 342–367, Nov. 2014, doi: 10.1017/jfm.2014.605.

- [47] R. M. Kelso, T. T. Lim, and A. E. Perry, “An experimental study of round jets in cross-flow,” *Journal of Fluid Mechanics*, vol. 306, pp. 111–144, Jan. 1996, doi: 10.1017/s0022112096001255.
- [48] J. Song, C. C. Cain, and J. G. Lee, “Liquid jets in subsonic air crossflow at elevated pressure,” *Journal of Engineering for Gas Turbines and Power*, vol. 137, no. 4, Oct. 2014, doi: 10.1115/1.4028565.
- [49] R. Payri, J. Gimeno, P. Martí-Aldaraví, and J. S. Giraldo, “Methodology for phase doppler anemometry measurements on a Multi-Hole diesel injector,” *Experimental Techniques*, vol. 41, no. 2, pp. 95–102, Oct. 2016, doi: 10.1007/s40799-016-0154-1.
- [50] A. Braeuer, “Chapter 4 - Shadowgraph and Schlieren techniques,” in *Supercritical fluid science and technology*, 2015, pp. 283–312. doi: 10.1016/b978-0-444-63422-1.00004-3.
- [51] J. Mazallon, Z. Dai, and G. M. Faeth, “Primary breakup of nonturbulent round liquid jets in gas crossflows,” *Atomization and Sprays*, vol. 9, no. 3, pp. 291–312, Jan. 1999, doi: 10.1615/atomizspr.v9.i3.40.
- [52] A. Krothapalli, L. Lourenço, and J.M. Buchlin, “Separated flow upstream of a jet in a crossflow,” *AIAA Journal*, vol. 28, no. 3, pp. 414–420, Mar. 1990, doi: 10.2514/3.10408.
- [53] R. S. Prakash, H. Gadgil, and B. N. Raghunandan, “Breakup processes of pressure swirl spray in gaseous cross-flow,” *International Journal of Multiphase Flow*, vol. 66, pp. 79–91, Nov. 2014, doi: 10.1016/j.ijmultiphaseflow.2014.07.002.
- [54] A. Sinha, R. S. Prakash, A. M. Mohan, and R. V. Ravikrishna, “Airblast spray in crossflow – Structure, trajectory and droplet sizing,” *International Journal of Multiphase Flow*, vol. 72, pp. 97–111, Jun. 2015, doi: 10.1016/j.ijmultiphaseflow.2015.02.008.
- [55] S. Rezayat, M. Farshchi, and M. Ghorbanhoseini, “Primary breakup dynamics and spray characteristics of a rotary atomizer with radial-axial discharge channels,” *International Journal of Multiphase Flow*, vol. 111, pp. 315–338, Feb. 2019, doi: 10.1016/j.ijmultiphaseflow.2018.10.001.

- [56] M. Y. Leong, V. G. McDonell, and G. S. Samuelsen, "Effect of ambient pressure on an airblast spray injected into a crossflow," *Journal of Propulsion and Power*, vol. 17, no. 5, pp. 1076–1084, Sep. 2001, doi: 10.2514/2.5846.
- [57] L. K. B. Li, S. I. Green, M. H. Davy, and D. T. Eadie, "Viscoelastic air-blast sprays in a cross-flow. part 1: penetration and dispersion," *Atomization and Sprays*, vol. 20, no. 8, pp. 697–720, Jan. 2010, doi: 10.1615/atomizspr.v20.i8.30.
- [58] L. K. B. Li, S. I. Green, M. H. Davy, and D. T. Eadie, "Viscoelastic air-blast sprays in a cross-flow. part 2: droplet velocities," *Atomization and Sprays*, vol. 20, no. 8, pp. 721–735, Jan. 2010, doi: 10.1615/atomizspr.v20.i8.40.
- [59] L. Miniero, K. Pandey, D. Fredrich, S. Shcherbanev, U. Doll, A. Giusti, N. Noiray, "Air-blast atomization and ignition of a kerosene spray in hot vitiated crossflow," *Combustion and Flame*, vol. 256, p. 112915, Oct. 2023, doi: 10.1016/j.combustflame.2023.112915.
- [60] P. Kulkarni, S. R. Bhdange, S. D. Deshmukh, and D. Deshmukh, "Combined correlation to predict trajectories of airblast spray and jet in cross-flows-independent of two-phase momentum ratio," *Atomization and Sprays*, vol. 32, no. 9, pp. 1–17, Jan. 2022, doi: 10.1615/atomizspr.2022040375.
- [61] S. Patil and S. Sahu, "Air swirl effect on spray characteristics and droplet dispersion in a twin-jet crossflow airblast injector," *Physics of Fluids*, vol. 33, no. 7, Jul. 2021, doi: 10.1063/5.0054430.
- [62] A. Sinha and R. V. Ravikrishna, "Experimental studies on structure of airblast spray in crossflow," *Sādhanā Academy Proceedings in Engineering Sciences*, vol. 44, no. 5, Apr. 2019, doi: 10.1007/s12046-019-1096-y.
- [63] Z. P. Tan, "The physics of twin-fluid jet-in-crossflow at atmospheric and jet-engine operating conditions," *Physics of Fluids*, vol. 31, no. 4, Apr. 2019, doi: 10.1063/1.5090110.
- [64] K.-C. Lin, K. Kirkendall, P. Kennedy and T. Jackson, "Spray structures of aerated liquid fuel jets in supersonic crossflows," in *AIAA 35th Joint Propulsion Conference and Exhibit*, Los Angeles, California, USA, Jun. 1999, doi: 10.2514/6.1999-2374.

- [65] K.-C. Lin, P. Kennedy, and T. Jackson, “Structures of aerated-liquid jets in subsonic crossflows,” in *AIAA 39th Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2001, doi: 10.2514/6.2001-330.
- [66] C. Ghenai, H. Sapmaz, and C.-X. Lin, “Penetration height correlations for non-aerated and aerated transverse liquid jets in supersonic cross flow,” *Experiments in Fluids*, vol. 46, no. 1, pp. 121–129, Aug. 2008, doi: 10.1007/s00348-008-0547-8.
- [67] B.-F. Bai, H.-B. Zhang, L. Liu, and H.-J. Sun, “Experimental study on turbulent mixing of spray droplets in crossflow,” *Experimental Thermal and Fluid Science*, vol. 33, no. 6, pp. 1012–1020, Sep. 2009, doi: 10.1016/j.expthermflusci.2009.05.002.
- [68] S. M. Choi, S. H. Jang, D. H. Lee, and G. W. You, “Spray characteristics of the rotating fuel injection system of a micro-jet engine,” *Journal of Mechanical Science and Technology*, vol. 24, no. 2, pp. 551–558, Feb. 2010, doi: 10.1007/s12206-009-1206-6.
- [69] S. Rezayat, M. Farshchi, H. Karimi, and A. Kebriaee, “Spray characterization of a slinger injector using a High-Speed imaging technique,” *Journal of Propulsion and Power*, vol. 34, no. 2, pp. 469–481, Mar. 2018, doi: 10.2514/1.b36498.
- [70] H. Zhang, B. Bai, L. Liu, H. Sun, and J. Yan, “Droplet dispersion characteristics of the hollow cone sprays in crossflow,” *Experimental Thermal and Fluid Science*, vol. 45, pp. 25–33, Feb. 2013, doi: 10.1016/j.expthermflusci.2012.09.021.
- [71] S.-S. Lee, W. Kim, and W.-S. Yoon, “Spray formation by a swirl spray jet in low speed cross-flow,” *Journal of Mechanical Science and Technology*, vol. 24, no. 2, pp. 559–568, Feb. 2010, doi: 10.1007/s12206-009-1222-6.
- [72] A. Lynch, R. G. Batchelor, B. Kiel, J. Miller, J. Gord, and M. F. Reeder, “Spray characteristics of a pressure-swirl fuel injector subjected to a crossflow and a coflow,” *Atomization and Sprays*, vol. 21, no. 8, pp. 625–643, Jan. 2011, doi: 10.1615/atomizspr.2012004012.

- [73] H. Zhang, B. Bai, L. Liu, H. Sun, and J. Yan, "Experimental study of the mixing of two impinging pressure-swirl sprays in crossflow," *Experimental Thermal and Fluid Science*, vol. 49, pp. 67–74, Sep. 2013, doi: 10.1016/j.expthermflusci.2013.04.002.
- [74] S.-Y. No, "A review on empirical correlations for jet/spray trajectory of liquid jet in uniform cross flow," *International Journal of Spray and Combustion Dynamics*, vol. 7, no. 4, pp. 283–313, Dec. 2015, doi: 10.1260/1756-8277.7.4.283.
- [75] A. Bellofiore, A. Cavaliere, and R. Ragucci, "Air density effect on the atomization of liquid jets in crossflow," *Combustion Science and Technology*, vol. 179, no. 1–2, pp. 319–342, Jan. 2007, doi: 10.1080/00102200600809563.
- [76] R. D. Ingebo and H. Foster, "Drop size distribution for cross-current break-up of liquid jets in air streams," National Advisory Committee for Aeronautics, NACA TN 4087, 1957. [Online]. Available: <https://ntrs.nasa.gov/citations/19930085138>
- [77] R. D. Ingebo, "Aerodynamic effect of combustor inlet air pressure on fuel jet atomization," *Journal of Propulsion and Power*, vol. 1, no. 2, pp. 137–142, Mar. 1985, doi: 10.2514/3.22771.
- [78] K. D. Kihm, G. M. Lyn, and S. Y. Son, "Atomization of cross-injecting sprays into convective air stream," *Atomization and Sprays*, vol. 5, no. 4–5, pp. 417–433, Jan. 1995, doi: 10.1615/atomizspr.v5.i45.40.
- [79] B. R. Munson, D. F. Young, and W. W. Heubsch, *Fundamentals of Fluid Mechanics*, 8th ed. United States of America: Wiley, 2006.
- [80] P.-K. Wu, K. A. Kirkendall, R. P. Fuller, and A. S. Nejad, "Breakup processes of liquid jets in subsonic crossflows," *Journal of Propulsion and Power*, vol. 13, no. 1, pp. 64–73, Jan. 1997, doi: 10.2514/2.5151.
- [81] S. Tambe, S.-M. Jeng, H. Mongia, and G. Hsiao, "Liquid jets in subsonic crossflow," in *43rd AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2005, doi: 10.2514/6.2005-731.

- [82] K. A. Sallam, C.-L. Ng, R. Sankarakrishnan, C. Aalburg, and K. Lee, “Breakup of turbulent and non-turbulent liquid jets in gaseous crossflows,” in *44th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2006, doi: 10.2514/6.2006-1517.
- [83] A. Osta and K. Sallam, “Effect of nozzle length/diameter ratio on the breakup of round liquid jets in crossflow,” in *46th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2008, doi: 10.2514/6.2008-1040.
- [84] A. Amighi, “Liquid jets in crossflow at elevated temperatures and pressures,” Ph.D. dissertation, Department of Mechanical and Industrial Engineering, University of Toronto, Canada, 2015.
- [85] Siemens Digital Industries Software STAR-CCM+ v2020, “Simcenter STAR-CCM+ User Guide”, *Siemens Digital Industries Software*. [Online]. Available: <https://www.sw.siemens.com/en-US/>. [Accessed: 2020-2021].
- [86] M. Pilch and C. A. Erdman, “Use of breakup time data and velocity history data to predict the maximum size of stable fragments for acceleration-induced breakup of a liquid drop,” *International Journal of Multiphase Flow*, vol. 13, no. 6, pp. 741–757, Nov. 1987, doi: 10.1016/0301-9322(87)90063-2.
- [87] R. R. Lakhamraju, “Liquid jet breakup studies in subsonic airstream at elevated temperatures,” MSc dissertation, Department of Aerospace Engineering and Engineering Mechanics, University of Cincinnati, USA, 2005.
- [88] K. Lee, C. Aalburg, F. J. Diez, G. M. Faeth, and K. A. Sallam, “Primary breakup of turbulent round liquid jets in uniform crossflows,” *AIAA Journal*, vol. 45, no. 8, pp. 1907–1916, Aug. 2007, doi: 10.2514/1.19397.
- [89] K. A. Sallam, C. Aalburg, and G. M. Faeth, “Breakup of round nonturbulent liquid jets in gaseous crossflow,” *AIAA Journal*, vol. 42, no. 12, pp. 2529–2540, Dec. 2004, doi: 10.2514/1.3749.
- [90] C. Aalburg, B. Van Leer, G. M. Faeth, and K. Sallam, “Properties of nonturbulent round liquid jets in uniform gaseous cross flows,” *Atomization and Sprays*, vol. 15, no. 3, pp. 271–294, Jan. 2005, doi: 10.1615/atomizspr.v15.i3.20.

- [91] J. Becker and C. Hassa, “Breakup and atomization of a kerosene jet in crossflow at elevated pressure,” *Atomization and Sprays*, vol. 12, no. 1–3, pp. 49–68, Jan. 2002, doi: 10.1615/atomizspr.v12.i123.30.
- [92] M. Birouk and N. Lekic, “Liquid jet breakup in quiescent atmosphere: a review,” *Atomization and Sprays*, vol. 19, no. 6, pp. 501–528, Jan. 2009, doi: 10.1615/atomizspr.v19.i6.20.
- [93] M. Behzad, N. Ashgriz, and A. Mashayek, “Azimuthal shear instability of a liquid jet injected into a gaseous cross-flow,” *Journal of Fluid Mechanics*, vol. 767, pp. 146–172, Feb. 2015, doi: 10.1017/jfm.2015.36.
- [94] J. A. Schetz and A. Padhye, “Penetration and breakup of liquids in subsonic airstreams,” *AIAA Journal*, vol. 15, no. 10, pp. 1385–1390, Oct. 1977, doi: 10.2514/3.60805.
- [95] R. K. Madabhushi, M. Y. Leong, M. Arienti, C. T. Brown, and V. G. McDonell, “On the breakup regime map of liquid jet in crossflow,” in *ILASS Americas 19th Annual Conference on Liquid Atomization and Spray Systems*, Toronto, Canada, May 2006.
- [96] C. D. Bolszo, V. G. McDonell, G. A. Gomez, and G. S. Samuelsen, “Injection of water-in-oil emulsion jets into a subsonic crossflow: an experimental study,” *Atomization and Sprays*, vol. 24, no. 4, pp. 303–348, Jan. 2014, doi: 10.1615/atomizspr.2014008415.
- [97] M. Eslamian, A. Amighi, and N. Ashgriz, “Atomization of liquid jet in High-Pressure and High-Temperature subsonic crossflow,” *AIAA Journal*, vol. 52, no. 7, pp. 1374–1385, Jul. 2014, doi: 10.2514/1.j052548.
- [98] C. T. Brown, and V. G. McDonell, “Near field behavior of a liquid jet in a crossflow,” in *ILASS Americas 19th Annual Conference on Liquid Atomization and Spray Systems*, Toronto, Canada, May 2006.
- [99] O. Elshamy, and S. M. Jeng, “Study of liquid jet in crossflow at elevated ambient pressures,” in *ILASS Americas 18th Annual Conference on Liquid Atomization and Spray Systems*, California, Irvine, USA, May 2005.

- [100] G. Vich and M. Ledoux, “Investigation of a liquid jet in a subsonic Cross-Flow,” *Fluid Mechanics Research*, vol. 24, no. 1–3, pp. 1–12, Jan. 1997, doi: 10.1615/interjfluidmechres.v24.i1-3.10.
- [101] M. Birouk, B. J. Azzopardi, and T. Stähler, “Primary break-up of a viscous liquid jet in a cross airflow,” *Particle & Particle Systems Characterization*, vol. 20, no. 4, pp. 283–289, Sep. 2003, doi: 10.1002/ppsc.200390034.
- [102] M. Birouk, T. Stähler, and B. J. Azzopardi, “An experimental study of liquid jets interacting with cross airflows,” *Particle & Particle Systems Characterization*, vol. 20, no. 1, pp. 39–46, Feb. 2003, doi: 10.1002/ppsc.200390003.
- [103] C.-L. Ng, R. Sankarakrishnan, and K. A. Sallam, “Bag breakup of nonturbulent liquid jets in crossflow,” *International Journal of Multiphase Flow*, vol. 34, no. 3, pp. 241–259, Mar. 2008, doi: 10.1016/j.ijmultiphaseflow.2007.07.005.
- [104] R. Sankarakrishnan, K. A. Sallam, F. W. Chambers, “Effects of turbulence on the breakup of round liquid jets in gaseous crossflow,” in *Proceedings of the ASME 2005 Fluids Engineering Division Summer Meeting. Volume 2: Fora*, Houston, Texas, USA, June 2005, pp. 281–285, doi: 10.1115/FEDSM2005-77407.
- [105] Y. Zheng and A. W. Marshall, “Characterization of the initial spray from low-weber-number jets in crossflow,” *Atomization and Sprays*, vol. 21, no. 7, pp. 575–589, Jan. 2011, doi: 10.1615/atomizspr.2011003714.
- [106] A. R. Osta and K. A. Sallam, “Nozzle-Geometry effects on Upwind-Surface properties of turbulent liquid jets in gaseous crossflow,” *Journal of Propulsion and Power*, vol. 26, no. 5, pp. 936–946, Sep. 2010, doi: 10.2514/1.49737.
- [107] P.-K. Wu and G. M. Faeth, “Aerodynamic effects on primary breakup of turbulent liquids,” *Atomization and Sprays*, vol. 3, no. 3, pp. 265–289, Jan. 1993, doi: 10.1615/atomizspr.v3.i3.20.
- [108] E. Lubarsky, J. R. Reichel, B. T. Zinn, and R. McAmis, “Spray in crossflow: Dependence on Weber number,” *Journal of Engineering for Gas Turbines and Power*, vol. 132, no. 2, Oct. 2009, doi: 10.1115/1.2904892.

- [109] S. Freitag and C. Hassa, “Spray characteristics of a kerosene jet in cross flow of air at elevated pressure”, in *ILASS Europe 12th Annual Conference on Liquid Atomization and Spray Systems*, Lake Como, Italy, Sep. 2008.
- [110] L. Kong, T. Lan, J. Chen, K. Wang, and H. Sun, “Breakup processes and droplet characteristics of liquid jets injected into low-speed air crossflow,” *Processes*, vol. 8, no. 6, p. 676, Jun. 2020, doi: 10.3390/pr8060676.
- [111] E. Farvardin, M. S. Johnson, H. Alaei, A. Martínez, and A. Dolatabadi, “Comparative study of biodiesel and diesel jets in gaseous crossflow,” *Journal of Propulsion and Power*, vol. 29, no. 6, pp. 1292–1302, Nov. 2013, doi: 10.2514/1.b34743.
- [112] P.-K. Wu, K. A. Kirkendall, R. P. Fuller, M. R. Gruber, and A. S. Nejad, “Spray trajectories of liquid fuel jets in subsonic crossflows,” *Fluid Mechanics Research*, vol. 24, no. 1–3, pp. 128–137, Jan. 1997, doi: 10.1615/interjfluidmechres.v24.i1-3.130.
- [113] K.-C. Lin, P. Kennedy and T. Jackson, “Penetration heights of liquid jets in high-speed crossflows,” in *40th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2002, doi: 10.2514/6.2002-873.
- [114] C. O. Iyogun, M. Birouk, and N. Popplewell, “Trajectory of water jet exposed to low subsonic cross-flow,” *Atomization and Sprays*, vol. 16, no. 8, pp. 963–980, Jan. 2006, doi: 10.1615/atomizspr.v16.i8.70.
- [115] M. Birouk, C. O. Iyogun, and N. Popplewell, “Role of viscosity on trajectory of liquid jets in a cross-airflow,” *Atomization and Sprays*, vol. 17, no. 3, pp. 267–287, Jan. 2007, doi: 10.1615/atomizspr.v17.i3.30.
- [116] C. T. Brown, U. M., Mondragon, V. G. McDonell, and L. Hills, “Investigation of the effect of injector discharge coefficient on penetration of a plain liquid jet into a subsonic crossflow”, in *ILASS Americas 20th Annual Conference on Liquid Atomization and Spray Systems*, Chicago, Illinois, USA, May 2007.

- [117] Y. Song, D. Hwang, and K. Ahn, "Effect of orifice geometry on column trajectories of liquid jets in crossflows," *International Journal of Aeronautical and Space Sciences*, vol. 20, no. 1, pp. 139–149, Jan. 2019, doi: 10.1007/s42405-018-0130-3.
- [118] Gh. Olyaei and A. Kebriaee, "Experimental study of liquid jets injected in crossflow," *Experimental Thermal and Fluid Science*, vol. 115, p. 110049, Jul. 2020, doi: 10.1016/j.expthermflusci.2020.110049.
- [119] J. Stenzler, J. Lee, and D. Santavicca, "Penetration of liquid jets in a crossflow," in *AIAA 41st Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2003, doi: 10.2514/6.2003-1327.
- [120] H. J. Yoon, J. G. Hong, and C.-W. Lee, "Correlations for penetration height of single and double liquid jets in cross flow under high-temperature conditions," *Atomization and Sprays*, vol. 21, no. 8, pp. 673–686, Jan. 2011, doi: 10.1615/atomizspr.2012004212.
- [121] R. Ragucci, A. Bellofiore, and A. Cavaliere, "Trajectory and momentum coherence breakdown of a liquid jet in high-density air cross-flow," *Atomization and Sprays*, vol. 17, no. 1, pp. 47–70, Jan. 2007, doi: 10.1615/atomizspr.v17.i1.20.
- [122] R. Ragucci, A. Bellofiore, and A. Cavaliere, "Breakup and breakdown of bent kerosene jets in gas turbine conditions," *Proceedings of the Combustion Institute*, vol. 31, no. 2, pp. 2231–2238, Jan. 2007, doi: 10.1016/j.proci.2006.07.204.
- [123] L. Li, Y. Lin, X. Xue, W. Gao, and C.-J. Sung, "Injection of liquid kerosene into a high-pressure subsonic air crossflow from normal temperature to elevated temperature," in *Proceedings of the ASME Turbo Expo 2012: Turbine Technical Conference and Exposition. Volume 2: Combustion, Fuels and Emissions, Parts A and B*, Copenhagen, Denmark, June 2012, pp. 877-884, doi: 10.1115/GT2012-69241.
- [124] E. Lubarsky, D. Shcherbik, O. Bibik, Y. Gopala, and B. T. Zinn, "Fuel jet in cross flow - Experimental study of spray characteristics," in *Advanced Fluid Dynamics*, H. W. Oh, Ed. InTech, 2012, pp. 59-80, doi: 10.5772/26045.

- [125] R. S. Prakash, A. Sinha, G. Tomar, and R. V. Ravikrishna, “Liquid jet in crossflow – Effect of liquid entry conditions,” *Experimental Thermal and Fluid Science*, vol. 93, pp. 45–56, May 2018, doi: 10.1016/j.expthermflusci.2017.12.012.
- [126] J. Song, K. Ahn, M.-K. Kim, and Y. Yoon, “Effects of orifice internal flow on liquid jets in subsonic crossflows,” *Journal of Propulsion and Power*, vol. 27, no. 3, pp. 608–619, May 2011, doi: 10.2514/1.b34011.
- [127] P.-K. Wu, K. A. Kirkendall, R. P. Fuller, and A. Nejad, “Spray structures of liquid fuel jets atomized in subsonic crossflows,” in *36th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 1998, doi: 10.2514/6.1998-714.
- [128] P. Sagaut, *Large Eddy Simulation for Incompressible flows*, 2nd ed. Berlin: Springer, 2006.
- [129] T. H. Pulliam and Zingg, D. W., *Fundamental Algorithms in Computational Fluid Dynamics*. Switzerland: Springer, 2014.
- [130] Siemens Digital Industries Software STAR-CCM+, “Simcenter STAR-CCM+ User Guide”, Siemens Digital Industries Software. [Online]. Available: <https://www.sw.siemens.com/en-US/>. [Accessed: 2022-2024].
- [131] S. B. Pope, *Turbulent Flows*. Cambridge: Cambridge University Press, 2000.
- [132] C. T. Crowe, M. Sommerfeld, and Y. Tsuji, *Multiphase Flows with Droplets and Particles*. United States of America: CRC Press, 1998.
- [133] T.-H. Shih, W. W. Liou, A. Shabbir, Z. Yang, and J. Zhu, “A new k-epsilon eddy viscosity model for high Reynolds number turbulent flows,” *Computers & Fluids*, vol. 24, no. 3, pp. 227–238, Mar. 1995, doi: 10.1016/0045-7930(94)00032-t.
- [134] F. Nicoud and F. Ducros, “Subgrid-Scale stress modelling based on the square of the velocity gradient tensor, flow, turbulence and combustion,” *Flow, Turbulence and Combustion*, vol. 62, no. 3, pp. 183–200, Jan. 1999, doi: 10.1023/a:1009995426001.

- [135] B. A. De Freitas Duarte, F. Barbi, M. M. Villar, R. Serfaty, and A. Da Silveira Neto, “Primary atomization of a turbulent liquid jet in crossflow: a comparison between VOF and FGVT methods,” *Journal of the Brazilian Society of Mechanical Sciences and Engineering*, vol. 42, no. 6, May 2020, doi: 10.1007/s40430-020-02365-8.
- [136] M. Herrmann, “A parallel Eulerian interface tracking/Lagrangian point particle multi-scale coupling procedure,” *Journal of Computational Physics*, vol. 229, no. 3, pp. 745–759, Feb. 2010, doi: 10.1016/j.jcp.2009.10.009.
- [137] A. A. Mukundan, G. Tretola, T. Ménard, M. Herrmann, S. Navarro-Martinez, K. Vogiatzaki, J. C. Brändle de Motta, and A. Berlemont, “DNS and LES of primary atomization of turbulent liquid jet injection into a gaseous crossflow environment,” *Proceedings of the Combustion Institute*, vol. 38, no. 2, pp. 3233–3241, Jan. 2021, doi: 10.1016/j.proci.2020.08.004.
- [138] J. Shinjo and A. Umemura, “Simulation of liquid jet primary breakup: Dynamics of ligament and droplet formation,” *International Journal of Multiphase Flow*, vol. 36, no. 7, pp. 513–532, Jul. 2010, doi: 10.1016/j.ijmultiphaseflow.2010.03.008.
- [139] Movaghar, M. Linne, M. Herrmann, A. R. Kerstein, and M. Oevermann, “Modeling and numerical study of primary breakup under diesel conditions,” *International Journal of Multiphase Flow*, vol. 98, pp. 110–119, Jan. 2018, doi: 10.1016/j.ijmultiphaseflow.2017.09.002.
- [140] M. Herrmann, “A balanced force refined level set grid method for two-phase flows on unstructured flow solver grids,” *Journal of Computational Physics*, vol. 227, no. 4, pp. 2674–2706, Feb. 2008, doi: 10.1016/j.jcp.2007.11.002.
- [141] M. Sussman and E. Puckett, “A Coupled Level Set and Volume-of-Fluid method for computing 3D and axisymmetric incompressible two-phase flows,” *Journal of Computational Physics*, vol. 162, no. 2, pp. 301–337, Aug. 2000, doi: 10.1006/jcph.2000.6537.

- [142] S. R. Prakash, S. S. Jain, J. A. Lovett, B. N. Raghunandan, R. V. Ravikrishna, and G. Tomar, “Detailed numerical simulations of atomization of a liquid jet in a swirling gas crossflow,” *Atomization and Sprays*, vol. 29, no. 7, pp. 577–603, Jan. 2019, doi: 10.1615/atomizspr.2019031322.
- [143] X. Li, H. Gao, and M. Soteriou, “Investigation of the impact of high liquid viscosity on jet atomization in crossflow via high-fidelity simulations,” *Physics of Fluids*, vol. 29, no. 8, Aug. 2017, doi: 10.1063/1.4996178.
- [144] M. Rudman, “A volume-tracking method for incompressible multifluid flows with large density variations,” *International Journal for Numerical Methods in Fluids*, vol. 28, pp. 357–378, 1998, doi:10.1002/(SICI)1097-0363(19980815)28:2<357::AID-FLD750>3.0.CO;2-D.
- [145] D. Zuzio, J.-L. Estivalèzes, and B. DiPierro, “An improved multiscale Eulerian–Lagrangian method for simulation of atomization process,” *Computers & Fluids*, vol. 176, pp. 285–301, Nov. 2018, doi: 10.1016/j.compfluid.2016.12.018.
- [146] S. Osher, and R. Fedkiw, *Level Set Methods and Dynamic Implicit Interfaces*. United States of America: Springer, 2003.
- [147] M. Herrmann, “A Eulerian Level Set/vortex sheet method for two-phase interface dynamics,” *Journal of Computational Physics*, vol. 203, no. 2, pp. 539–571, Mar. 2005, doi: 10.1016/j.jcp.2004.08.023.
- [148] Y. Ling, S. Zaleski, and R. Scardovelli, “Multiscale simulation of atomization with small droplets represented by a Lagrangian point-particle model,” *International Journal of Multiphase Flow*, vol. 76, pp. 122–143, Nov. 2015, doi: 10.1016/j.ijmultiphaseflow.2015.07.002.
- [149] R. D. Reitz and R. Diwakar, “Structure of high-pressure fuel sprays,” in *SAE International Congress and Exposition*, Detroit, Michigan, USA, Feb. 1987, doi: 10.4271/870598.
- [150] J. C. Beale and R. D. Reitz, “Modeling spray atomization with the Kelvin-Helmholtz/Rayleigh-Taylor hybrid model,” *Atomization and Sprays*, vol. 9, no. 6, pp. 623–650, Jan. 1999, doi: 10.1615/atomizspr.v9.i6.40.

- [151] P. J. O'Rourke and A. A. Amsden, "The TAB method for numerical calculation of spray droplet breakup," in *1987 SAE International Fall Fuels and Lubricants Meeting and Exhibition*, Nov. 1987, doi: 10.4271/872089.
- [152] G. I. Taylor, "The instability of liquid surfaces when accelerated in a direction perpendicular to their planes", *Proceedings of the Royal Society of London. Series A, Mathematical and Physical Sciences*, vol. 201, no. 1065, pp. 192-196, Mar. 1950, doi: 10.1098/rspa.1950.0052.
- [153] R. D. Reitz and R. Diwakar, "Effect of drop breakup on fuel sprays," in *SAE International Congress and Exposition*, Detroit, Michigan, USA, Feb. 1986, doi: 10.4271/860469.
- [154] K. Y. Huh and A. D. Gosman, "A phenomenological model of diesel spray atomization," in *International Conference on Multiphase Flow*, Tsukuba, Japan, Sep. 1991.
- [155] P. K. Senecal, K. J. Richards, E. Pomraning, T. Yang, , M. Z., Dai, R. M. McDavid, M. A. Patterson, S. Hou, and T. Shethaji, "A new parallel Cut-Cell Cartesian CFD code for rapid grid generation applied to In-Cylinder diesel engine simulations," in *SAE 2007 World Congress and Exhibition*, Detroit, Michigan, USA, Apr. 2007, doi: 10.4271/2007-01-0159.
- [156] A. A. Ranger and J. A. Nicholls, "Aerodynamic shattering of liquid drops," *AIAA Journal*, vol. 7, no. 2, pp. 285–290, Feb. 1969, doi: 10.2514/3.5087.
- [157] D. Kim, F. Ham, S. Bose, H. Le, M. Herrmann, X. Li, M. C. Soteriou, and W. Kim, "High-fidelity simulation of atomization in a gas turbine injector high shear nozzle," in *ILASS Americas 26th Annual Conference on Liquid Atomization and Spray Systems*, Portland, Oregon, USA, May 2014.
- [158] J. Zhao, W. Lin, C. Yan, Z. Zheng, Y. Tong, and W. Nie, "Mixing enhancement mechanism of combined H₂–Water jets in supersonic crossflows in a combustor with an expanded section," *International Journal of Hydrogen Energy*, vol. 47, no. 19, pp. 10747–10761, Mar. 2022, doi: 10.1016/j.ijhydene.2022.01.070.

- [159] A. L. Pillai, J. Nagao, R. Awane, and R. Kurose, “Influences of liquid fuel atomization and flow rate fluctuations on spray combustion instabilities in a backward-facing step combustor,” *Combustion and Flame*, vol. 220, pp. 337–356, Oct. 2020, doi: 10.1016/j.combustflame.2020.06.031.
- [160] Y. Gopala, “Breakup characteristics of a liquid jet in subsonic crossflow,” Ph.D. dissertation, College of Engineering, Georgia Institute of Technology, USA, 2012.
- [161] Y. Gopala, P. Zhang, O. Bibik, E. Lubarsky, and B. T. Zinn, “Liquid fuel jet in crossflow - Trajectory correlations based on the column breakup point,” in *48th AIAA Aerospace Sciences Meeting Including the New Horizons Forum and Aerospace Exposition*, Orlando, Florida, USA, Jan. 2010, doi: 10.2514/6.2010-214.
- [162] V. G. Shaw and E. Gutmark, “Water and fuel jet droplet distributions in low and high temperature subsonic crossflows,” in *AIAA Scitech 2021 Forum*, Virtual, Jan. 2021, doi: 10.2514/6.2021-0082.
- [163] J. Deepe, J. Lee, D. A. Santavicca, and W. Lee, “Effect of Weber number on modulated jets in crossflow,” in *44th AIAA Aerospace Sciences Meeting and Exhibit*, Reno, Nevada, USA, Jan. 2006, doi: 10.2514/6.2006-1223.
- [164] A. R. Karagozian, “Transverse jets and their control,” *Progress in Energy and Combustion Science*, vol. 36, no. 5, pp. 531–553, Oct. 2010, doi: 10.1016/j.pecs.2010.01.001.
- [165] A. B. Liu, D. Mather, and R. D. Reitz, “Modeling the effects of drop drag and breakup on fuel sprays,” in *SAE International Congress and Exposition*, Detroit, Michigan, USA, Mar. 1993, doi: 10.4271/930072.
- [166] A. Sinha and R. Ravikrishna, “LES of spray in crossflow – Effect of droplet distortion,” *International Journal of Spray and Combustion Dynamics*, vol. 9, no. 1, pp. 55–70, Jun. 2016, doi: 10.1177/1756827716652511.
- [167] L. Schiller and A. Naumann, “Über die grundlegenden Berechnungen bei der Schwerkraftaufbereitung,” *Zeitschrift des Vereines deutscher Ingenieure*, vol. 77, no. 12, pp. 318–320, Mar. 1933.

- [168] ANSYS, “Fluent User Theory Guide”, ANSYS. [Online]. Available: <https://www.ansys.com/>. [Accessed: 2021].
- [169] A. Yang, “Preliminary design and performance evaluation of plain orifice fuel injectors for low emission combustors”, MSc dissertation, Centre for Propulsion and Thermal Power Engineering, Cranfield University, UK, 2019.
- [170] P. B. Nihagaye, G. Zhou, and X. Yang, “Modelling spray performance of alternative aviation fuel,” *Energy*, vol. 224, Jun. 2021, doi: 10.1016/j.energy.2021.120086.
- [171] F. X. Tanner, “Liquid jet atomization and droplet breakup modeling of non-evaporating diesel fuel sprays,” in *SAE International Congress and Exposition*, Detroit, Michigan, USA, Feb. 1997, doi: 10.4271/970050.
- [172] M. Gorokhovski, R. Zamansky, C. Le Ribault and T. Deng, “Application of stochastic models to primary air-blast atomization and cavitation,” in *Proceedings of the Summer Program 2012*, Center for Turbulence Research, Stanford University, 2012, pp.325-334. [Online]. Available: <https://ctr.stanford.edu/publications/summer-program-proceedings/proceedings-2012-summer-program>
- [173] J. Heide, M. Karlsson, and M. Altimira, “Numerical analysis of Urea-SCR sprays under cross-flow conditions,” in *WCX™ 17: SAE World Congress Experience*, Mar. 2017, doi: 10.4271/2017-01-0964.
- [174] M. Behzad, N. Ashgriz, and B. Karney, “Surface breakup of a non-turbulent liquid jet injected into a high pressure gaseous crossflow,” *International Journal of Multiphase Flow*, vol. 80, pp. 100–117, Apr. 2016, doi: 10.1016/j.ijmultiphaseflow.2015.11.007.
- [175] A. A. Amsden, J. D. Ramshaw, P. J. O’Rourke, and J. K. Dukowicz, “KIVA: A computer program for two- and three-dimensional fluid flows with chemical reactions and fuel sprays”, Los Alamos National Labs, United-States, Rept LA-10245-MS, 1985. [Online]. Available: <https://www.osti.gov/biblio/5786209>

- [176] M. Gorokhovski and V. L. Saveliev, “Analyses of Kolmogorov’s model of breakup and its application into Lagrangian computation of liquid sprays under air-blast atomization,” *Physics of Fluids*, vol. 15, no. 1, pp. 184–192, Jan. 2003, doi: 10.1063/1.1527914.
- [177] Q. Wang and K. D. Squires, “Large Eddy Simulation of particle deposition in a vertical turbulent channel flow,” *International Journal of Multiphase Flow*, vol. 22, no. 4, pp. 667–683, Aug. 1996, doi: 10.1016/0301-9322(96)00007-9.
- [178] B. Ničeno, M. T. Dhotre, and N. G. Deen, “One-equation sub-grid scale (SGS) modelling for Euler–Euler Large Eddy Simulation (EELES) of dispersed bubbly flow,” *Chemical Engineering Science*, vol. 63, no. 15, pp. 3923–3931, Aug. 2008, doi: 10.1016/j.ces.2008.04.050.
- [179] M. Gorokhovski and S. Oruganti, “Stochastic models for the droplet motion and evaporation in under-resolved turbulent flows at a large Reynolds number,” *Journal of Fluid Mechanics*, vol. 932, Dec. 2021, doi: 10.1017/jfm.2021.916.
- [180] A. D. Gosman and E. Ioannides, “Aspects of computer simulation of Liquid-Fueled combustors,” *Journal of Energy*, vol. 7, no. 6, pp. 482–490, Nov. 1983, doi: 10.2514/3.62687.
- [181] J. K. Dukowicz, “A particle-fluid numerical model for liquid sprays,” *Journal of Computational Physics*, vol. 35, no. 2, pp. 229–253, Apr. 1980, doi: 10.1016/0021-9991(80)90087-x.
- [182] D. J. Brown and P. Hutchinson, “The interaction of solid or liquid particles and turbulent fluid flow fields—A numerical simulation,” *Journal of Fluids Engineering*, vol. 101, no. 2, pp. 265–269, Jun. 1979, doi: 10.1115/1.3448949.
- [183] W. Rodi, “Experience with two-layer models combining the k-epsilon model with a one-equation model near the wall,” in *AIAA 29th Aerospace Sciences Meeting*, Reno, Nevada, USA, Jan. 1991, doi: 10.2514/6.1991-216.

- [184] M. Wolfshtein, “The velocity and temperature distribution in one-dimensional flow with turbulence augmentation and pressure gradient,” *International Journal of Heat and Mass Transfer*, vol. 12, no. 3, pp. 301–318, Mar. 1969, doi: 10.1016/0017-9310(69)90012-x.
- [185] T. Jongen, “Simulation and modeling of turbulent incompressible flows”, Ph.D. dissertation, Laboratoire d’Ingénierie Numérique, École Polytechnique Fédérale de Lausanne EPFL, Switzerland, 1998.
- [186] J. Smagorinsky, “General circulation experiments with the primitive equations: Part I, The basic experiment”, *Monthly Weather Review*, vol. 91, pp. 99-164, 1963, doi: 10.1175/1520-0493(1963)091<0099:GCEWTP>2.3.CO;2.
- [187] E. R. Van Driest, “On turbulent flow near a wall,” *Journal of the Aeronautical Sciences*, vol. 23, no. 11, pp. 1007–1011, Nov. 1956, doi: 10.2514/8.3713.
- [188] B. Vreman, B. Geurts, and H. Kuerten, “Realizability conditions for the turbulent stress tensor in Large-Eddy Simulation,” *Journal of Fluid Mechanics*, vol. 278, pp. 351–362, Nov. 1994, doi: 10.1017/s0022112094003745.
- [189] K. Peszyński, “Building a bridge between industry and theory on the example of a new ventilation system,” *EPJ Web of Conferences*, vol. 213, Jan. 2019, doi: 10.1051/epjconf/201921301001.
- [190] Y. Yang, G. He, and L. Wang, “Effects of subgrid-scale modeling on Lagrangian statistics in Large-Eddy Simulation,” *Journal of Turbulence*, vol. 9, p. N8, Jan. 2008, doi: 10.1080/14685240801905360.
- [191] P. Johnson and C. Meneveau, “Predicting viscous-range velocity gradient dynamics in Large-Eddy Simulations of turbulence,” *Journal of Fluid Mechanics*, vol. 837, pp. 80–114, Dec. 2017, doi: 10.1017/jfm.2017.838.
- [192] M. Jangi, R. Solsjo, B. Johansson, and X.-S. Bai, “On Large Eddy Simulation of diesel spray for internal combustion engines,” *International Journal of Heat and Fluid Flow*, vol. 53, pp. 68–80, Jun. 2015, doi: 10.1016/j.ijheatfluidflow.2015.02.002.

- [193] C.-W. Tsang and C. J. Rutland, “Effects of Sub-Grid Scale (SGS) dispersion modeling on Large-Eddy Simulation (LES) of non-evaporative and evaporative diesel sprays,” in *ILASS Americas 29th Annual Conference on Liquid Atomization and Spray Systems*, Atlanta, Georgia, USA, May 2017.
- [194] J. U. Brackbill, D. B. Kothe, and C. Zemach, “A continuum method for modeling surface tension,” *Journal of Computational Physics*, vol. 100, no. 2, pp. 335–354, Jun. 1992, doi: 10.1016/0021-9991(92)90240-y.
- [195] S. Muzaferija and M. Perić, “Computation of free-surface flows using the finite-volume method and moving grids,” *Numerical Heat Transfer. Part B, Fundamentals*, vol. 32, no. 4, pp. 369–384, Dec. 1997, doi: 10.1080/10407799708915014.
- [196] B. P. Leonard, “The ultimate conservative difference scheme applied to unsteady one-dimensional advection,” *Computer Methods in Applied Mechanics and Engineering*, vol. 88, no. 1, pp. 17–74, Jun. 1991, doi: 10.1016/0045-7825(91)90232-u.
- [197] M. Birouk, B. Nyantekyi-Kwakye, and N. Popplewell, “Effect of nozzle geometry on breakup length and trajectory of liquid jet in subsonic crossflow,” *Atomization and Sprays*, vol. 21, no. 10, pp. 847–865, Jan. 2011, doi: 10.1615/atomizspr.2012004338.
- [198] M. Leong, V. Mcdonell, and G. Samuelsen, “Mixing of an airblast-atomized fuel spray injected into a crossflow of air”, Nasa Glenn Research Center, NASA Report No. CR-2000-210467, 2000. [Online]. Available: <https://ntrs.nasa.gov/citations/20000115866>
- [199] J. F. Widmann, C. Presser, and S. D. Leigh, “Improving phase Doppler volume flux measurements in low data rate applications,” *Measurement Science & Technology*, vol. 12, no. 8, pp. 1180–1190, Jul. 2001, doi: 10.1088/0957-0233/12/8/327.
- [200] M. Lambert, T. Esch, M. Braun, and H. Elasrag, “Enhancement of the Madabhushi Liquid Jet in Crossflow Breakup Model by a ligament breakup mechanism,” in *ILASS–Europe 2019 29th Conference on Liquid Atomization and Spray Systems*, Paris, France, Sep. 2019.

- [201] R. N. Dahms and J. C. Oefelein, “The significance of drop non-sphericity in sprays,” *International Journal of Multiphase Flow*, vol. 86, pp. 67–85, Nov. 2016, doi: 10.1016/j.ijmultiphaseflow.2016.07.010.
- [202] C. A. J., Fletcher, *Computational Techniques for Fluid Dynamics I*, 2nd ed. Berlin: Springer, 1998.
- [203] F. Curtiss and J. O. Hirschfelder, “Integration of stiff equations,” *Proceedings of the National Academy of Sciences of the United States of America*, vol. 38, no. 3, pp. 235–243, Mar. 1952, doi: 10.1073/pnas.38.3.235.
- [204] H. Bijl, M. H. Carpenter, V. N. Vatsa, and C. A. Kennedy, “Implicit time integration schemes for the unsteady compressible Navier–Stokes equations: laminar flow,” *Journal of Computational Physics*, vol. 179, no. 1, pp. 313–329, Jun. 2002, doi: 10.1006/jcph.2002.7059.
- [205] L. Wang and D. J. Mavriplis, “Implicit solution of the unsteady Euler equations for high-order accurate discontinuous Galerkin discretizations,” *Journal of Computational Physics*, vol. 225, no. 2, pp. 1994–2015, Aug. 2007, doi: 10.1016/j.jcp.2007.03.002.
- [206] K. R. Holst, R. S. Glasby, and R. B. Bond, “On the effect of temporal error in high-order simulations of unsteady flows,” *Journal of Computational Physics*, vol. 402, p. 108989, Feb. 2020, doi: 10.1016/j.jcp.2019.108989.
- [207] P. Eliasson and P. Weinerfelt, “High-order implicit time integration for unsteady turbulent flow simulations,” *Computers & Fluids*, vol. 112, pp. 35–49, May 2015, doi: 10.1016/j.compfluid.2015.02.006.
- [208] J. C. R Hunt, A. A. Wray, and P. Moin, “Eddies, stream, and convergence zones in turbulent flows,” *Proceedings of the Summer Program 1998, Center for Turbulence Research Report NTRS-19890015184*, pp.193–208, 1988. [Online] Available: <https://ntrs.nasa.gov/citations/19890015184>
- [209] S. J. Lee and Y. A. Hassan, “Numerical investigation of helical coil tube bundle in turbulent cross flow using Large Eddy Simulation,” *International Journal of Heat and Fluid Flow*, vol. 82, Apr. 2020, doi: 10.1016/j.ijheatfluidflow.2019.108529.

- [210] Y. Dubief and F. Delcayre, “On coherent-vortex identification in turbulence,” *Journal of Turbulence*, vol. 1, p. N11, Jan. 2000, doi: 10.1088/1468-5248/1/1/011.
- [211] D. B. Spalding, “A standard formulation of the steady convective mass transfer problem,” *International Journal of Heat and Mass Transfer*, vol. 1, no. 2–3, pp. 192–207, Aug. 1960, doi: 10.1016/0017-9310(60)90022-3.
- [212] S. S. Sazhin, “Advanced models of fuel droplet heating and evaporation,” *Progress in Energy and Combustion Science*, vol. 32, no. 2, pp. 162–214, Jan. 2006, doi: 10.1016/j.pecs.2005.11.001.
- [213] J. Schlottke and B. Weigand, “Direct numerical simulation of evaporating droplets,” *Journal of Computational Physics*, vol. 227, no. 10, pp. 5215–5237, May 2008, doi: 10.1016/j.jcp.2008.01.042.
- [214] Siemens Energy, “SGT-100 gas turbine,” *Siemens Energy*. [Online]. Available: <https://www.siemens-energy.com/global/en/home/products-services/product/sgt-100.html#/> [Accessed: 2024].
- [215] The National Archives, “UK Civil Aviation Authority Engine type certificate,” Data Sheet No. 1049, Nov. 1994. [Online]. Available: https://webarchive.nationalarchives.gov.uk/ukgwa/20150601211403/http://www.caa.co.uk/docs/1419/SRG_PRO_1049%20iss2.pdf [Accessed: 2024].
- [216] KHRONE, “OPTIBAR PT 2000: Operating and installation manual,” *KHRONE*. [Online]. Available: <https://krohne.com/en/products/flow-measurement/flowmeters/differential-pressure-flowmeters>. [Accessed: 2021].
- [217] *Measurement of fluid flow by means of pressure differential devices inserted in a circular cross-section conduits running full Part 2: Orifice plates*, British Standards EN ISO 5167 - 2:2003, 2003.
- [218] CORNING, “Corning HPFS 7979, 7980, 8655 Fused Silica: Optical materials product information, specialty materials divisions,” Corning, 2014. [Online]. Available: <https://www.corning.com/worldwide/en/products/advanced-optics/product-materials/semiconductor-laser-optic-components/high-purity-fused-silica.html> [Accessed: 2021].

- [219] EMERSON, “Technical: Introduction to regulators,” *EMERSON*. [Online]. Available: <https://www.emerson.com/documents/automation/manuals-guides-complete-technical-section-fisher-en-140704.pdf> [Accessed: 2021].
- [220] HEATING PARTS WAREHOUSE.CO.UK, “Riello R40 G10 Burner, Kerosene”, *HEATING PARTS WAREHOUSE.CO.UK*. [Online]. Available: <https://heatingpartswarehouse.co.uk/product/riello-r40-g10-burner-kerosene/>. [Accessed: 2021].
- [221] WANNER HYDRA-CELL, “P200 Pump Series,” *WANNER HYDRA-CELL*. [Online]. Available: <https://www.hydra-cell.com/metering/product/P200.html>. [Accessed: 2021].
- [222] F. Mayinger and O. Feldmann, *Optical Measurements Techniques and Applications*, 2nd ed. Berlin: Springer, 2001.
- [223] S. Kosch, “Calibration of ILIDS and PDPA droplet sizing systems,” MSc dissertation, Department of Mechanical and Industrial Engineering, University of Toronto, Canada, 2015.
- [224] TSI, “Phase Doppler Particle Analyzer (PDPA)/ Laser Doppler Velocimeter (LDV) Operations Manual,” *TSI*, USA, 2006. [Online]. Available: www.tsi.com. [Accessed: 2021].
- [225] M. P. Tokarev, D. K. Sharaborin, A. S. Lobasov, L. M. Chikishev, V. M. Dulin, and D. M. Markovich, “3D velocity measurements in a premixed flame by tomographic PIV,” *Measurement Science and Technology*, vol. 26, no. 6, Apr. 2015, doi: 10.1088/0957-0233/26/6/064001.
- [226] B. Ihracska, R. J. Crookes, D. Montalvão, M. R. Herfatmanesh, Z. Peng, S. Imran, T. Korakianitis, “Opto-mechanical design for sight windows under high loads,” *Materials & Design*, vol. 117, pp. 430–444, Mar. 2017, doi: 10.1016/j.matdes.2016.12.080.
- [227] CRYSTRAN, “The design of pressure windows,” *CRYSTRAN*, UK, 2014. [Online]. Available: www.crystran.co.uk. [Accessed: 2021].

- [228] TOSOH, “Optical silica glass,” *TOSOH*, USA, 2011. [Online]. Available: <https://www.tosohusa.com/products--services/silica-glass>. [Accessed: 2021].
- [229] HERAEUS, “Quartz glass for optics: Data and properties,” *HERAEUS*, UK, 2011. [Online]. Available: https://www.heraeus.com/en/hca/company_hca/downloads_hca/downloads_fused_silica_1.html. [Accessed: 2021].
- [230] OHARA, “High quality silica glass: OHARA QUARTZ, Synthetic Fused Silica for Optics SK-1320 Series”, *OHARA*, USA. [Online]. Available: <http://www.oharacorp.com/fused-silica-quartz.html>. [Accessed: 2021].
- [231] C. Aligrot, J.-C. Champoussin, N. Guerrassi, and G. Claus, “A correlative model to predict autoignition delay of diesel fuels,” in *SAE International Congress and Exposition*, Detroit, Michigan, USA, Feb. 1997, doi: 10.4271/970638.
- [232] H. H. Wolfer, “Ignition lag in diesel engines”, *Translation Royal Aircraft Establishment*, no. 358, 1950.
- [233] N. Watson, A. Pilley, and M. Marzouk, “A combustion correlation for diesel engine simulation,” in *SAE 1980 Automotive Engineering Congress and Exposition*, Feb. 1980, doi: 10.4271/800029.
- [234] F. W. Stringer, A. E. Clarke, and J. S. Clarke, “The spontaneous ignition of hydrocarbon fuels in a flowing system,” in *Proceedings of the Institution of Mechanical Engineers*, vol. 184, no. 10, Sep. 1969, pp. 212-225, doi: 10.1243/PIME_CONF_1969_184_334_02.
- [235] R. Payri, F. Salvador, J. De La Morena, and V. Pagano, “Using a one-dimensional spray model to improve liquid length and ignition delay estimations for diesel flames,” *Applied Thermal Engineering*, vol. 124, pp. 1090–1102, Sep. 2017, doi: 10.1016/j.applthermaleng.2017.06.102.
- [236] D. N. Assanis, Z. Filipi, S. B. Fiveland, and M. Syrimis, “A predictive ignition delay correlation under Steady-State and transient operation of a direct injection diesel engine,” *Journal of Engineering for Gas Turbines and Power*, vol. 125, no. 2, pp. 450–457, Apr. 2003, doi: 10.1115/1.1563238.

- [237] D. F. Davidson, Y. Zhu, J. Shao, and R. K. Hanson, "Ignition delay time correlations for distillate fuels," *Fuel*, vol. 187, pp. 26–32, Jan. 2017, doi: 10.1016/j.fuel.2016.09.047.
- [238] M. A. Carr, P. A. Caton, L. J. Hamilton, J. S. Cowart, M. Mehl, and W. J. Pitz, "An experimental and Modeling-Based study into the ignition delay characteristics of diesel surrogate binary blend fuels," *Journal of Engineering for Gas Turbines and Power*, vol. 134, no. 7, May 2012, doi: 10.1115/1.4006005.
- [239] D. A. Rothamer and L. Murphy, "Systematic study of ignition delay for jet fuels and diesel fuel in a heavy-duty diesel engine," *Proceedings of the Combustion Institute*, vol. 34, no. 2, pp. 3021–3029, Jan. 2013, doi: 10.1016/j.proci.2012.06.085.
- [240] M. F. Al-Dawody and S. K. Bhatti, "Experimental and computational investigations for combustion, performance and emission parameters of a diesel engine fueled with soybean biodiesel-diesel blends," *Energy Procedia*, vol. 52, pp. 421–430, Jan. 2014, doi: 10.1016/j.egypro.2014.07.094.
- [241] J. Safarov, U. Ashurova, B. Ahmadov, E. Abdullayev, A. Shahverdiyev, and E. Hassel, "Thermophysical properties of diesel fuel over a wide range of temperatures and pressures," *Fuel*, vol. 216, pp. 870–889, Mar. 2018, doi: 10.1016/j.fuel.2017.11.125.

Appendices

Appendix A : Development of an Experimental Rig for Liquid Fuel Jets in Crossflow Under Representative Gas Turbine Conditions

In parallel to the numerical work presented in the core research chapters, the author was actively involved in the development of a high-pressure and high-temperature experimental rig facility to investigate the atomization, propagation, and evaporation processes of liquid fuel jets in crossflow (LFJIC) under representative gas turbine combustor inlet conditions. As recommended in *section 7.6.2*, the datasets generated can be used to further evaluate, calibrate, and validate the numerical modelling methodologies proposed in the thesis.

The work presented in this Appendix stems from a collaborative research effort between the author, Dr. Charith Wijesinghe (Research fellow at Cranfield University) and the thesis supervisors (Dr. Sun and Prof. Sethi) with inputs from the project supervisors at Siemens Energy. Although an overview of the rig facility is presented, the discussion focuses on the main contribution of the author to the project, which includes the following elements:

- Refinement of the experimental test points.
- Design of the air delivery system.
- Design of the test section.
- Design and material selection of the optical windows.
- Design of the liquid fuel injector.
- Design of the water injector inside the test section.
- Preliminary design and commissioning of the exhaust system.
- Selection of the secondary instrumentation (metering fuel pump, airflow meter).
- Design of the instrumentation system (support system for the laser diagnostic equipment, initial positioning of the high-speed camera and laser equipment).

It is important to note that Dr. Charith Wijesinghe contributed significantly to the sourcing process of the elements mentioned above in addition to being responsible for the rig assembly and a vast majority of the other aspects of the rig design and commissioning not listed (e.g. final design of the exhaust system, design of the burner system, design and commissioning of the water and liquid fuel delivery systems, etc.). The thesis supervisors were responsible for the preliminary stages of the project's development, which included the selection of the primary instrumentation (laser diagnostic, high-speed imaging) and the definition of the project outline with the input of Siemens Energy. The elements that have been provided by one of the contributors (i.e. not the direct work of the author) will be specified.

A.1 Experimental Research Gaps

The literature review of the numerical validation studies presented in *section 2.4.2* from Chapter 2 revealed important research gaps in the modelling of liquid jets in crossflow (LJIC). In particular, very few numerical studies have used datasets at high pressure [31, 32, 38, 40] or high temperature [21, 36] to validate the predictive capabilities of the different atomization modelling approaches. Furthermore, even fewer studies have used datasets for liquid fuels [30, 31, 32, 38, 40] and those at high-pressure conditions often had low momentum flux ratios [38, 40] and/or non-turbulent jets [40]. Moreover, as discussed in *section 2.4.5*, it is difficult to find numerical studies that have validated their predictions for a wide range of spray characteristics in both breakup regions. These numerical research gaps can be partially attributed to the lack of experimental data available in the literature for turbulent LFJIC at more representative gas turbine conditions.

As shown in **Figure A-1**, several experimental studies have been done to assess the near-field spray region of turbulent LJIC, which includes the primary breakup regimes and related spray characteristics close to the jet column ($x/d \approx 10$ or inferior). However, they were mainly conducted under standard temperature and pressure (STP) conditions [45, 81, 82, 83, 88, 89, 98, 106, 110, 111, 118]. In addition, the few studies conducted at high pressure were either limited to ambient temperature T_{atm} [48, 75, 84, 91, 97, 121, 124] often for relatively low gas Weber numbers ($We_g < 500$) [75, 84, 97, 122] and/or to lower

pressures ($P_g < 10$ bar) [48, 84, 97, 124] not representative of many gas turbine engines that have larger OPRs (> 10) (e.g. SGT-100 [214], RB211 [215]).

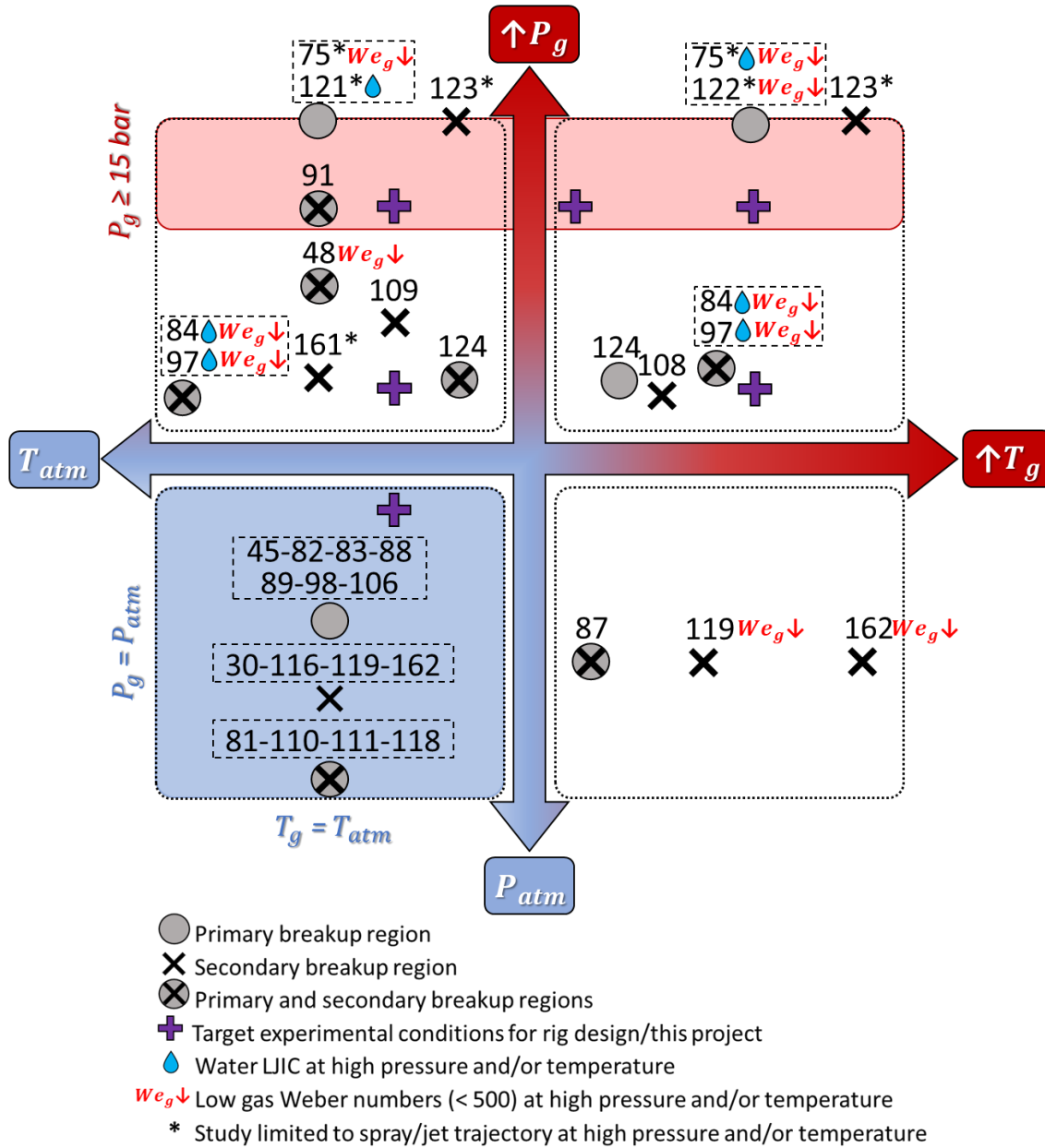


Figure A-1: Main features of the experimental work previously done on liquid jets in crossflow compared to the target conditions for the experimental rig facility (The numbers indicate the experimental studies referenced).

These research gaps also extend to the experimental datasets available in the literature for the secondary breakup region of turbulent LJIC. Indeed, they were mainly obtained at ambient conditions [30, 81, 110, 111, 116, 118, 119, 162] while those at higher pressures are mostly limited to $P_g < 10$ bar [48, 84, 97, 109, 124, 161] and/or ambient temperatures

[48, 84, 91, 97, 109, 124, 161]. Some studies at higher pressure and/or temperature have also restricted the range of gas Weber numbers to $We_g < 500$ [48, 84, 97, 119, 162].

Moreover, regardless of the breakup region studied, many experiments were only carried out using water sprays [45, 84, 83, 97, 98, 106, 110, 116, 118, 125] or opted to restrict the test conditions at the highest pressures and/or temperatures by only injecting water [75, 121] or limiting the gas Weber numbers [48]. Some of the high-temperature experiments were also limited to ambient pressure P_{atm} [87, 119, 162] while those conducted at the highest pressures ($15 \leq P_g \leq 20$ bar) focused on studying the jet column trajectory [75, 121, 122] or provided exhaustive measurements only for lower pressures ($P_g < 10$ bar) [91].

These gaps in knowledge on the physics of LJIC limit the accuracy of the numerical tools commonly used to guide the design of novel low-emission gas turbine combustion systems. Indeed, a vast majority of the existing numerical studies on LJIC have been conducted using deterministic breakup models, which rely on calibrating model constants with experimental data to produce accurate predictions as further demonstrated in Chapter 3. Thus, their accuracy for gas turbine applications can be greatly diminished by a lack of comprehensive experimental datasets available in the literature for the calibration process. Although the stochastic secondary droplet (SSD) breakup model relies less on experimental data, it would also benefit from being validated for liquid fuels as discussed in *section 2.4.2*. The stochastic numerical methodologies proposed in this research could also be further assessed, developed, and validated for higher pressures and temperatures. Therefore, there is a significant need for more research on turbulent LFJIC under representative gas turbine conditions.

Thus, the objective of the work presented in this Appendix was to design and commission a bespoke high-pressure and high-temperature experimental rig facility that will be used to produce comprehensive and exhaustive LFJIC datasets. The numbers in **Figure A-1** refer to the experimental studies cited in this section and the purple crosses represent the test conditions that the experimental rig facility was designed for in order to help fill the gaps in knowledge on LJIC under more representative gas turbine conditions.

A.2 Target Test Conditions

The combinations of air pressures P_g and temperatures T_g selected to fill the gaps in knowledge on turbulent LFJIC for gas turbine applications is presented in **Table A-1**. This results in 6 target test cases as shown in **Table A-2**. The targeted range of gas Weber numbers and momentum flux ratio to be tested with diesel fuel are presented in **Table A-3**.

Table A-1: Target range of air pressure and temperature.

		T_g [K]		
		300	450	600
P_g [bar]	1	X		
	4	X		X
	15	X	X	X

Table A-2: Target test cases classified by the air properties.

Case #	P_g [Bar]	T_g [K]
1	1	300
2	4	300
3	4	600
4	15	300
5	15	450
6	15	600

Table A-3: Target range of momentum flux ratios and gas Weber numbers.

Atomization Levels	Min	Max
Momentum Flux ratio $J = \rho_{jet} u_{jet}^2 / \rho_g u_g^2$	10	50
Gas Weber Number $We_g = \rho_g u_g^2 d / \sigma$	100	2500

The test conditions were refined following the literature review previously presented on the experimental studies of turbulent LJIC and by considering the capacity of the air system as presented in *Appendix A.6.1*. Health and safety considerations also played an important role in the definition of the experimental campaign. As discussed in *Appendix A.8*, the test points were limited at the highest temperature and pressures to avoid autoignition. It should be noted that the experimental studies presented in **Figure A-1**

were conducted with a plain orifice injector likely because the intention was to gain a better understanding of the fundamental physics involved in the atomization and evaporation process of LJIC. Thus, the experimental campaign will also be conducted using a plain orifice injector for the same reasons. However, the rig was designed with versatility in mind to be suitable for a wide variety of LJIC experimental studies, which might involve using different fuels or more complex atomizers such as pressure-swirl injectors.

A.3 Experimental Rig Design

The experimental campaign will be conducted using Cranfield University's pebble bed, which is a heating facility able to deliver air over a wide range of temperatures and pressures representative of gas turbine combustor inlet conditions. The experimental facility with the final rig assembly connected to the pebble bed via the mixing tee/bypass is presented in **Figure A-2**.

As shown in **Figure A-3**, the experimental rig design is composed of an air delivery system, a test section, an exhaust system that includes a back pressure control valve and the burner system, which includes the burner.

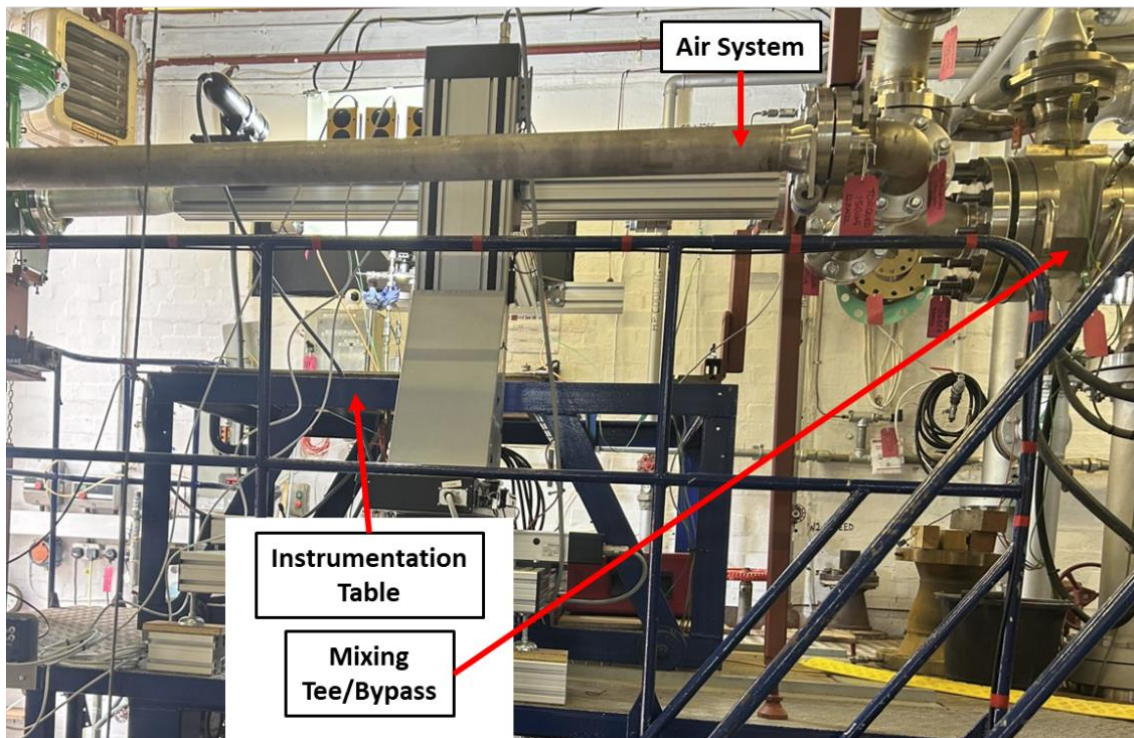
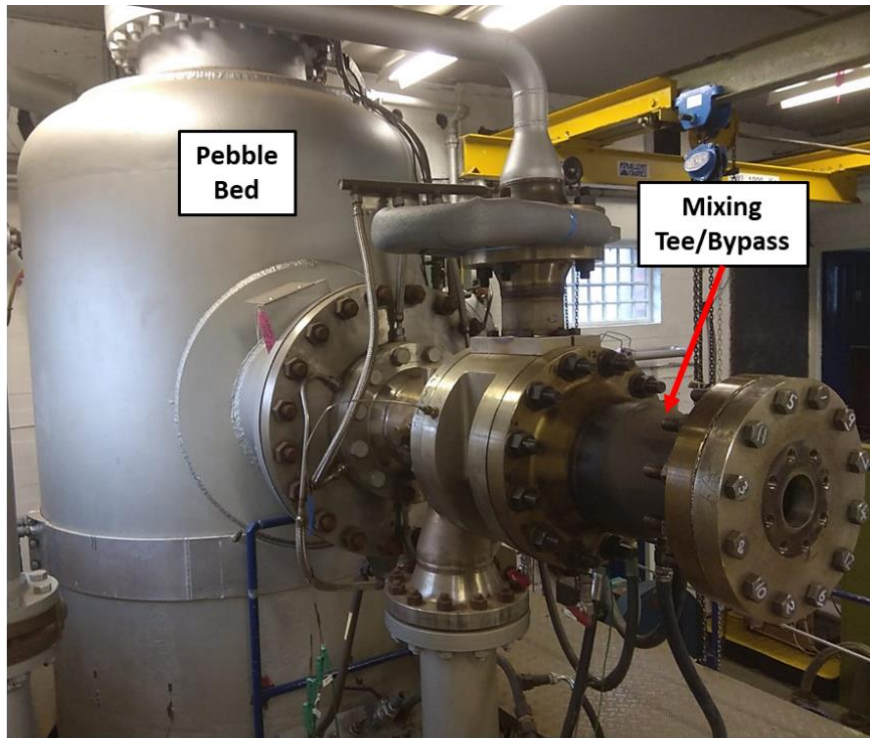


Figure A-2: Experimental facility and final rig assembly.

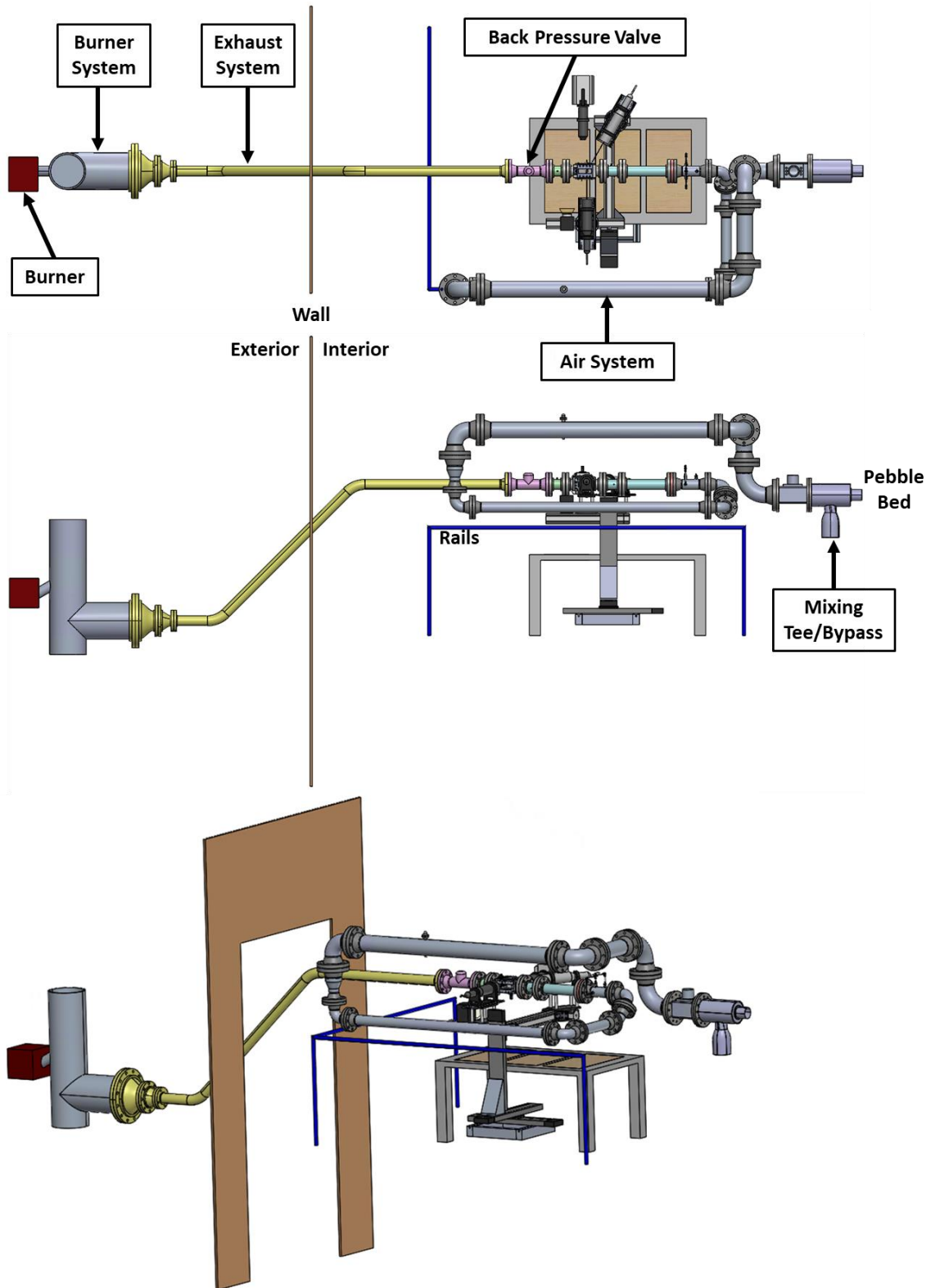


Figure A-3: CAD representation of the designed rig assembly.

A.3.1 Air Delivery System

The upstream air delivery system illustrated in **Figure A-4** consists of a compressor, which brings the air to the required pressure (up to 15 bar), and the pebble bed, which heats the pressurized air to the required temperature (up to 900K at 15 bar). To achieve higher air mass flows, a bypass system is used to mix ambient high-pressure air with hot air at the same pressure. Only a portion of the high-pressure air coming from the compressor goes into the pebble bed and is heated at a higher temperature than the chosen test conditions. The air mass flow capacity of the rig with and without the bypass system for the target cases presented in *Appendix A.2* are shown in **Table A-4**.

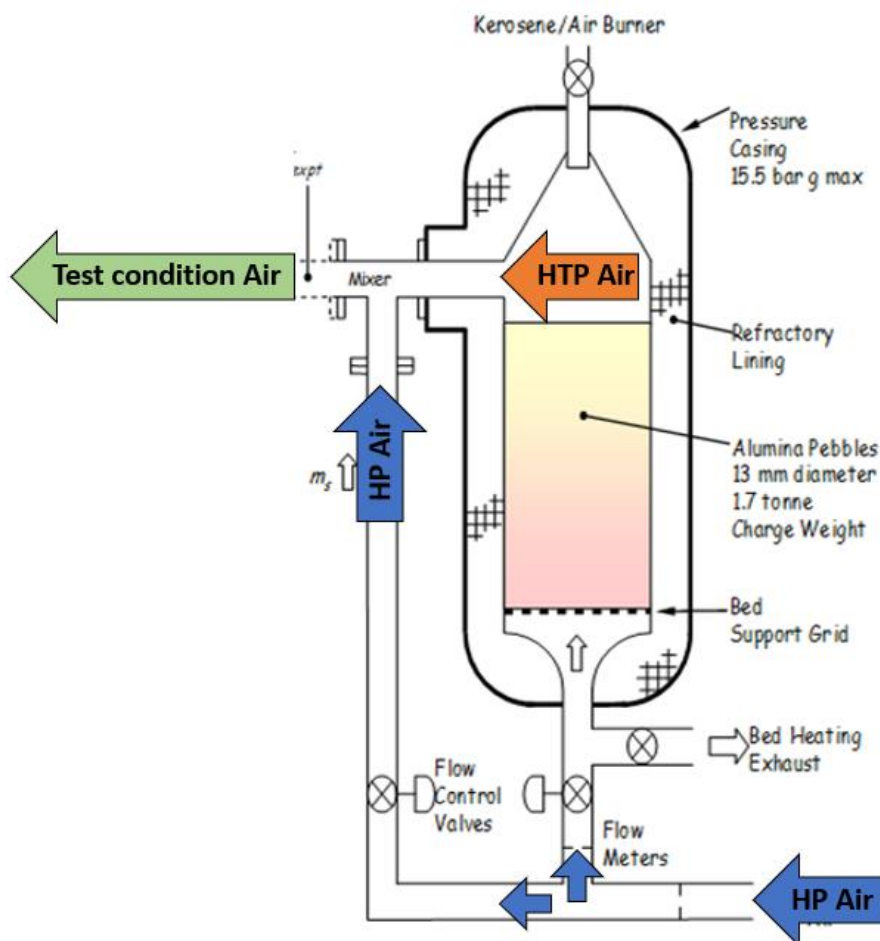


Figure A-4: Air System Schematic. HP: High Pressure; HTP: High Pressure and Temperature (Image courtesy of Cranfield University).

After the mixing tee, the air travels through NPS 5 pipes up to the airflow meter as shown in **Figure A-5**. The diameter of the pipe was selected to fit the outlet diameter of the mixing tee and to reduce the velocity for the flow meter. The airflow meter selected is an

averaging pitot tube, model DN125 from KROHNE. To reduce measurement errors due to turbulence, the pipe length upstream and downstream of the flow meter is 10 times and 5 times the internal pipe diameter respectively, as recommended by the manufacturer [216]. With this configuration, the anticipated level of precision is less than 1% [216].

Table A-4: Air Mass flow capacity of the rig with and without bypass air.

Case #	P_g [bar]	T_g [K]	Maximum air mass flow $\dot{m}_{g_{max,PB}}$ [kg/s]	
			Without Bypass air	With Bypass air
1	1	300	0.68	0.68
2	4	300	1.43	1.43
3	4	600	0.9	1.43
4	15	300	3.81	3.81
5	15	450	2.87	3.81
6	15	600	2.27	3.81

After the flow meter, the pipe diameter is reduced to NPS 3 based on the internal dimension of the test section. In order to reduce the cost of the pipe system, the pipe diameter is reduced directly after the pipe length required downstream of the airflow meter. The maximum pressure drop caused by the circular pipes and fittings upstream of the test section is estimated to be around 2.8%. Before reaching the test section, the flow must be straightened and allowed to develop, which is achieved by using the designed flow straightening system shown in **Figure A-6**.

To straighten the flow, a Zanker flow plate was designed [217]. The design of the Zanker flow plate was incorporated into a flange, which allows to transition from the circular cross-section of the pipes to the rectangular cross-section of the test section. Once the flow goes through the Zanker flow plate, it will stabilize and develop in a long rectangular channel, which has the same cross-section dimensions as the test section. The total length of the rectangular channel upstream of the injection point is approximately 14 times the hydraulic diameter.

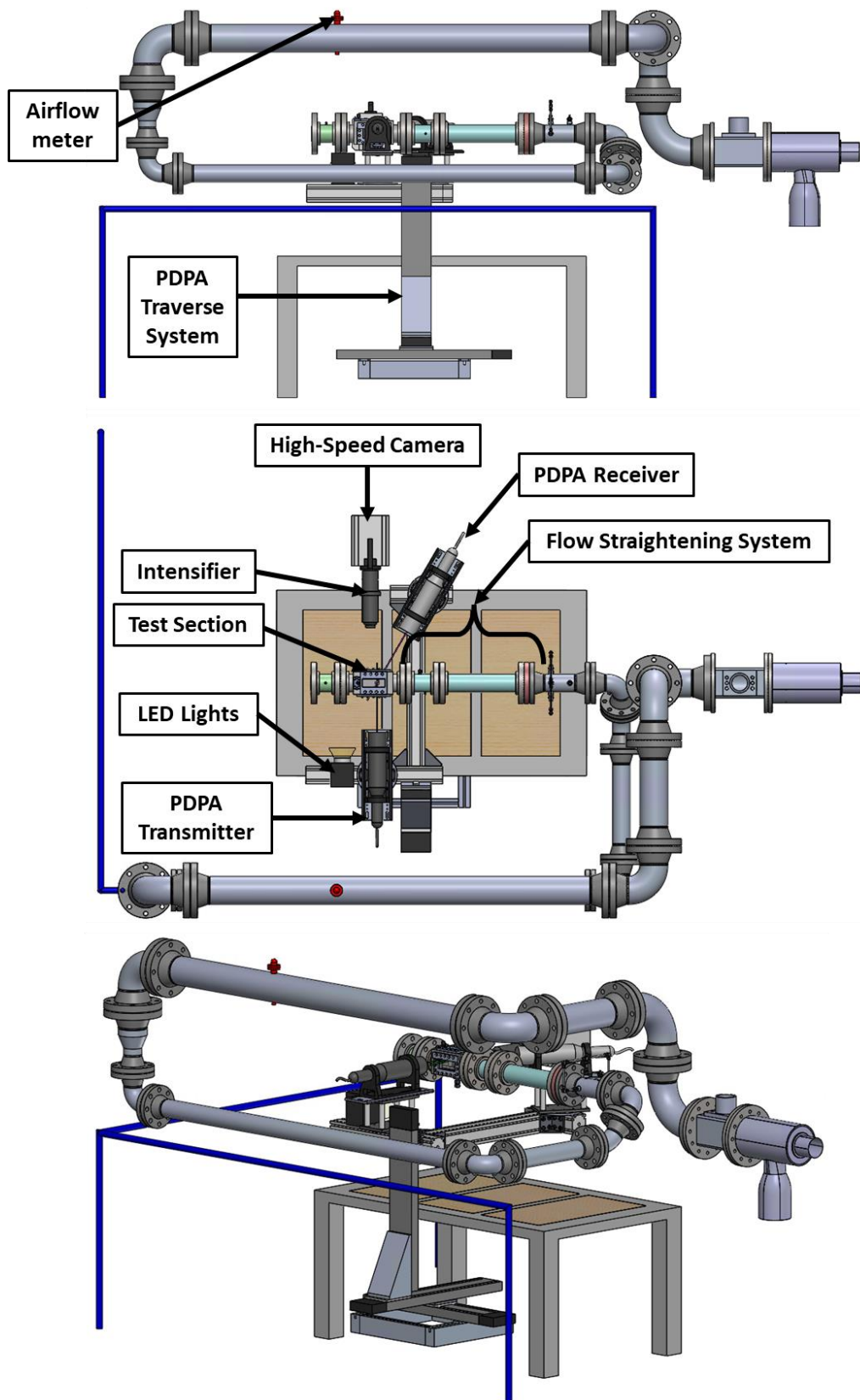


Figure A-5: CAD representation of the upstream rig components designed.

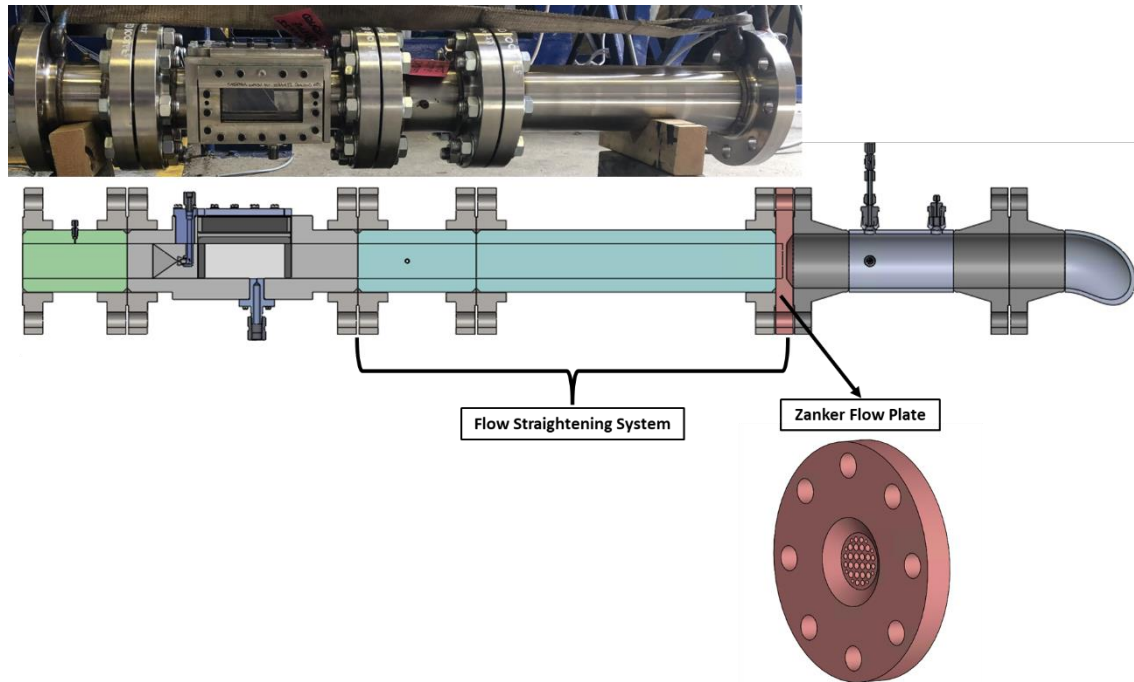


Figure A-6: Flow straightening system with Zanker flow plate (Bottom: Cross-section of the CAD assembly, Top: Partial rig assembly).

The temperature of the air entering the test section is taken by a type K thermocouple inserted inside the rectangular section upstream of the test section. The static pressure is taken by a pressure transducer (PMX309 from Omega). Only one pressure tap is used to measure the pressure in the rectangular channel to avoid disrupting the flow field. For the same reason, the tap hole diameters drilled for the thermocouple and pressure transducer were selected as small as possible (1/16 in. for the thermocouple and 1/4 in. for the pressure transducer).

A.3.2 Test Section

The test section shown in **Figure A-7** was designed to provide 2D optical access through optical windows and to allow for laser diagnostics and high-speed imaging. Different test section designs were considered to incorporate the optical windows and the best design was selected based on the cost and to prevent any significant disruption to the gas flow field. The additional cost of machining the windows into a step to ensure they sit flush with the walls of the test section was justified through numerical simulations that showed the impact of the windows' design on the gas flow field.

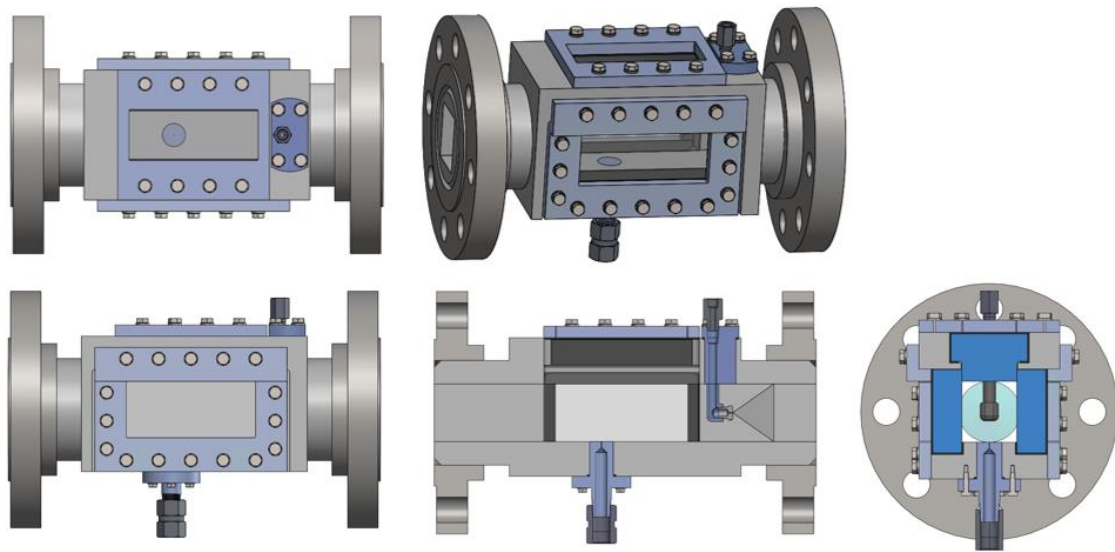


Figure A-7: CAD representation of the test section.

The inner width and height of the test section were selected to avoid fuel impingement on the windows, to respect the pebble bed's capabilities and to stay within the acceptable range of Mach number as detailed in *Appendix A.6*. In addition, the test section design was guided using the URANS Lagrangian stochastic methodology described in Chapter 3 and Chapter 4. The measurement length was selected to avoid autoignition as presented in *Appendix A.8*. As a result, the cross-section width is 45 mm and its height is 50 mm. The total observation length is 115 mm and the measurable length for the spray is 75 mm, which will enable investigation of the secondary breakup and evaporation process.

To prevent autoignition at the highest temperature and pressure, a fine water mist is injected parallel to the flow at the exit of the measurement zone. The water injector is positioned 110 mm away from the liquid fuel injector, which was estimated to be a safe distance considering the risk of autoignition presented in *Appendix A.8*. It should be noted that this fine water mist, which is generated using the small MicroWhirl atomizer from BETE, will not be in operation for all the high-temperature and high-pressure conditions. Indeed, its use is recommended only for a few selected conditions where the jet velocity and/or gas velocity are low or with a high atomization level. For the cases without water injection, a blank will be installed instead of the water injector to avoid any potential disruption of the flow at the outlet.

The laser suppliers were consulted for the design of the test section windows (i.e. material and maximum thickness) to ensure the quality of the measurements. The windows are made of Fused Silica (7980 HPSF Corning grade KrF) and the material grade was selected to ensure low-birefringence, UV-laser resistance, and fluorescence-free. The minimum thickness of the test section windows was estimated using engineering calculations and validated using Finite Element Analysis (FEA) to account for the thermal effects as discussed in *Appendix A.7*. The side windows are 23.5 mm thick and the top window has a 16.5 mm step machined for a total thickness of 38.5 mm. To avoid disrupting the flow field, the windows were designed to sit flush with the test section walls with the gasket installed. The gaskets are made of Thermiculite 815, which is a material resistant to high temperatures and harsh conditions.

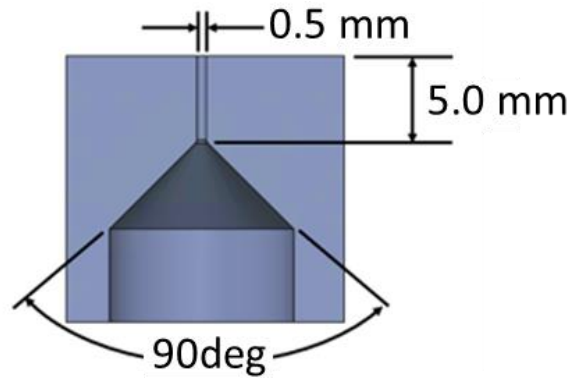


Figure A-8: Plain orifice injector design.

As previously mentioned, the fuel atomizer is a plain orifice injector as shown in **Figure A-8**. The internal dimensions were chosen following an exhaustive literature review. It was found that the orifice diameter d that have been used for LJIC experiments vary between 0.2 mm and 4 mm [48, 75, 80, 81, 82, 83, 84, 87, 91, 97, 99, 106, 109, 112, 113, 119, 121, 122, 123, 218]. However, only a few selected studies used an orifice diameter larger than 1mm [80, 82, 83, 106, 113], which was often to assess the effect of the length to diameter ratio L/d on the spray characteristics or breakup regime. Thus, a mid-value diameter of 0.5 mm was selected. The value of L/d was imposed equal to 10 to achieve a fully developed turbulent velocity profile [83, 106] and the tapered entrance angle to 90° to avoid cavitation [48, 75, 80, 81, 84, 87, 99, 112, 113, 116, 119, 121, 123]. The design of the injector was numerically guided using CFD to ensure there was no flow detachment near the orifice entrance. The external dimensions were chosen so that other

injectors can be easily fitted inside the test section for future experimental work on more complex injectors.

A.3.3 Exhaust System

A rectangular channel was added after the test section to measure the mixture's temperature without changing the cross-section area. After the rectangular channel, a back pressure valve designed by Dr. Charith Wijesinghe was installed to maintain the pressure within the test section by varying the flow according to any fluctuations upstream [219].



Figure A-9: Burner system being tested.

The exhaust system after the test section was designed to ensure health and safety compliance and environmentally safe disposal of exhaust products. Water is injected after the back pressure valve to prevent autoignition from occurring further downstream of the test section. The safe disposal of the gas-liquid mixture is assured downstream of the test section by burning the air and diesel mixture as shown in **Figure A-9**. This allows to dispose entirely of the diesel droplets and vapour without contaminating a significant amount of water, which would have been the alternative option if a wet scrubber was selected. Moreover, without a coalescer filter or cyclone separator, using a fuel burner will prevent releasing diesel vapour into the atmosphere. The burner model selected is Riello R40 G10 kerosene burner [220]. The burner is used far away from the test section, outside of the test house to minimize any effects on the upstream conditions.

A.3.4 Fuel and Water Injection Systems

The fuel is stored in a heated tank and supplied to the test section through a high-pressure delivery system, both located outside of the test facility to comply with safety regulations. For the fuel injection system shown in **Figure A-10**, a metering pump (P200 series from Hydra-Cell) was selected to be suitable for the plain orifice injector test conditions as well as for a more complex atomizer provided by Siemens Energy. For the plain orifice injector, the pump can supply fuel at an injection pressure of 1.3 bar to 50.6 bar at a corresponding maximum volumetric flow rate of 200ml/min up to 2417ml/min. The pump has 3 diaphragms making it virtually pulseless at lower pressure [221]. For higher injection pressure, dampers will be used. Although the pump is a metering pump, an over-gear flow meter will be used to double-check the flow values it measures.

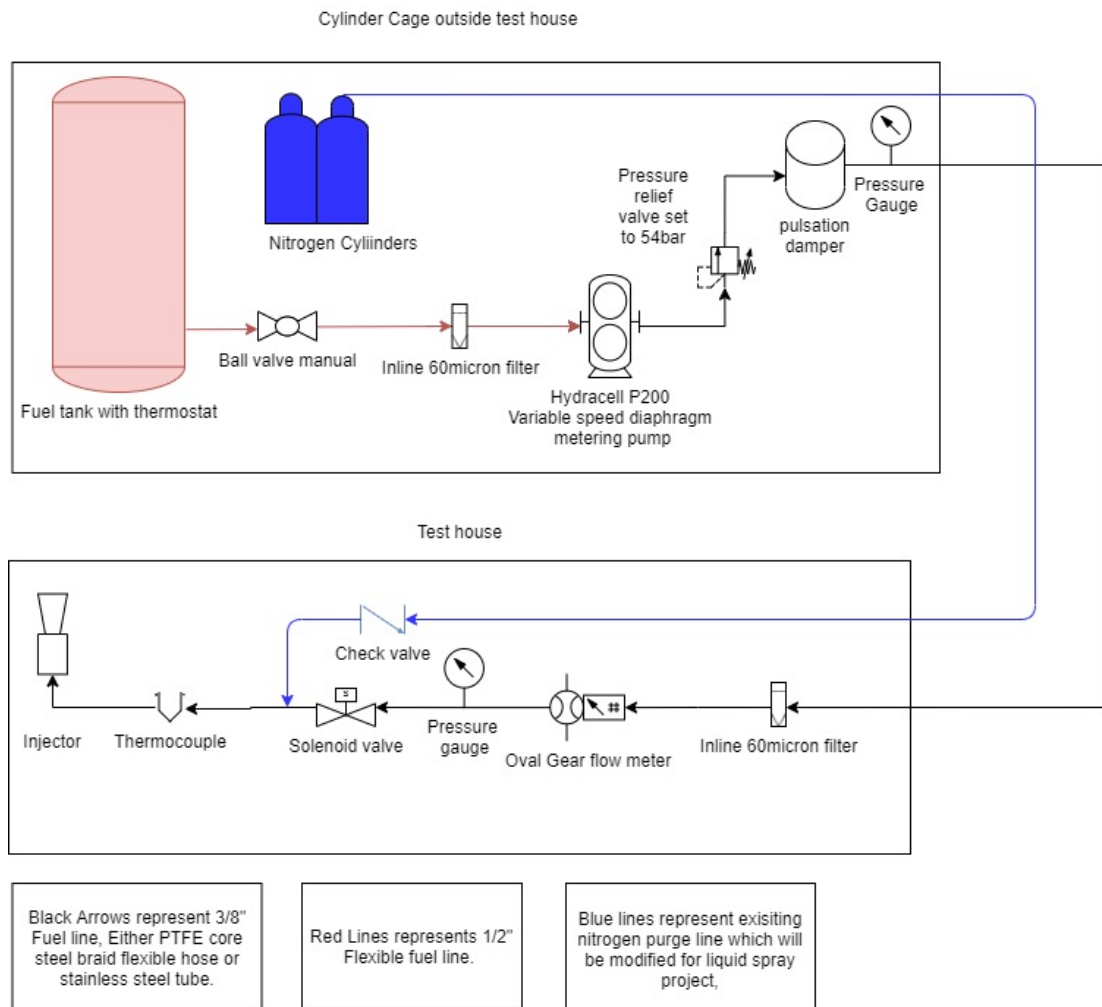


Figure A-10: Fuel Injection System Schematic (Design and image courtesy of Dr. Charith Wijesinghe).

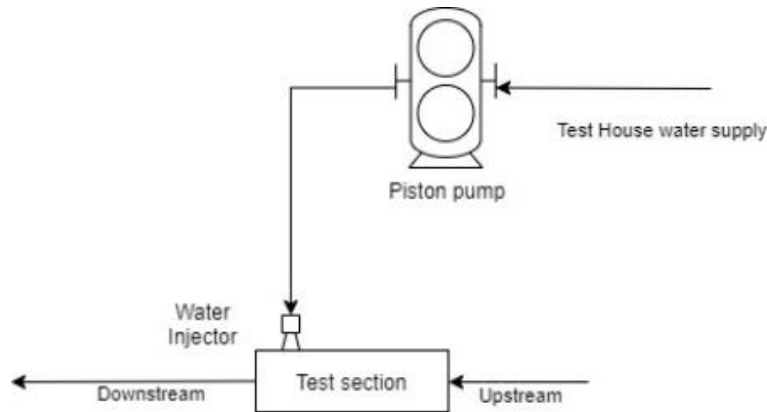


Figure A-11: Water Injection System Schematic (Design and image courtesy of Dr. Charith Wijesinghe).

The water pump used for the water injection system illustrated in **Figure A-11** is from the manufacturer Interpump Group and the model is Modello WS151 Series 47. The maximum pressure of the water pump is 150 bar and the maximum volume flow rate is 15L/min.

A.4 Instrumentation and Measurements

The experimental approach consists of assessing the primary breakup, secondary breakup, spray propagation and evaporation processes of liquid fuel sprays using optical instrumentation and laser diagnostics. The laser supplier (TSI) was consulted during the development of the instrumentation system to ensure the quality of the measurements.

A shadowgraph imaging technique is used to visualize the spray as shown in **Figure A-12**. The High-Speed camera selected by the thesis supervisors is a Phantom v2012 from AMETEK with an LED light array pointed toward the lens. To fully capture the observation length of the test section, the 100 mm lens of the high-speed camera was positioned 570 mm away from the centre of the fuel injector and the LED lights at an opposite distance of 225 mm.

The Laser-Induced Fluorescence (LIF) method will be used to measure fuel concentration, spray penetration and distribution through the centre of the injectors as well as the distribution of vapour and mass flux. For the LIF measurements, the wavelength output is 266nm and the high-speed camera will be used with an intensified camera attachment. The intensifier model selected is the HiCATT 25 mm dual-stage

intensifier attachment (Gen2 and Booster) from Lambert, with a 1:1 relay lens, S20 photocathode, 3ns gating and a 300kHz repetition rate.

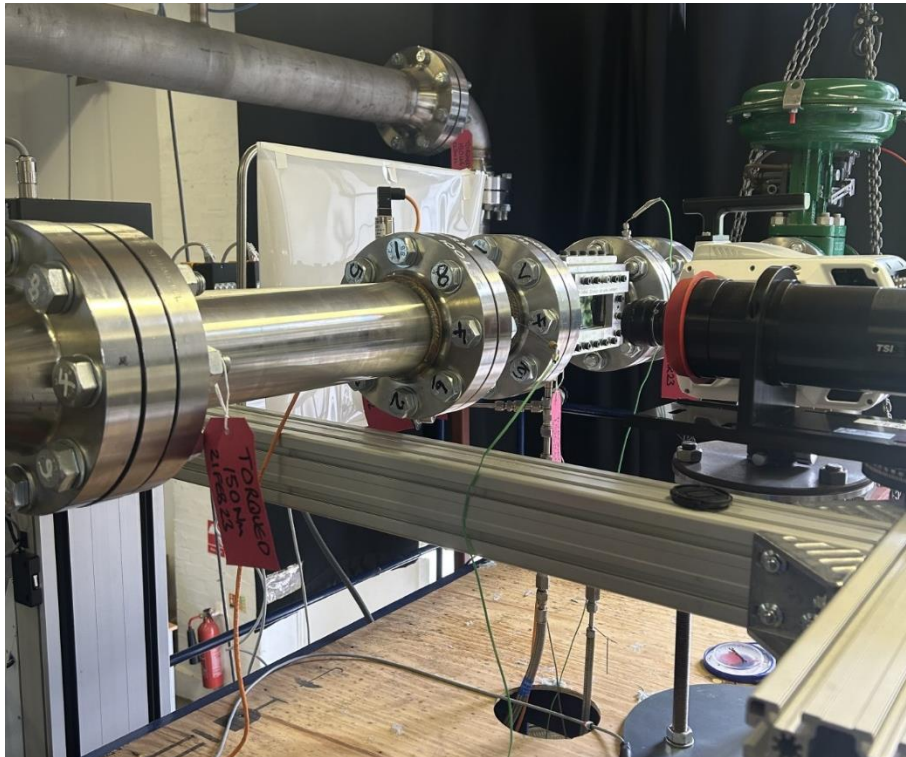


Figure A-12: Instrumentation set-up for the shadowgraph images.

The Phase Doppler Particle Analyzer (PDPA) method will be used to measure the size, velocity and distribution of the droplets. The output wavelengths of the two-component transmitter and receiver probe are 514.5nm and 488nm. The receiving probe and transmitting probe can adopt a “back-scatter” or “forward-scatter” configuration [222, 223, 224] as seen in **Figure A-13**.

The back-scatter arrangement has the advantage of having the probes placed on a single side of the test section, thus reducing the complexity of the support system that needs to be designed. However, “direct forward-scatter arrangement provides the strongest signal. In practice, to avoid reflections, an off-axis forward-scatter location for the receiver is often preferred” [224]. Thus, an off-axis forward scatter configuration was selected for the PDPA measurements. The scattering angle, which is a function of the liquid properties, was imposed equal to the recommended value for diesel fuel (30°) [224]. The focal length of the receiver and transmitter probe are 300 mm and 250 mm respectively.

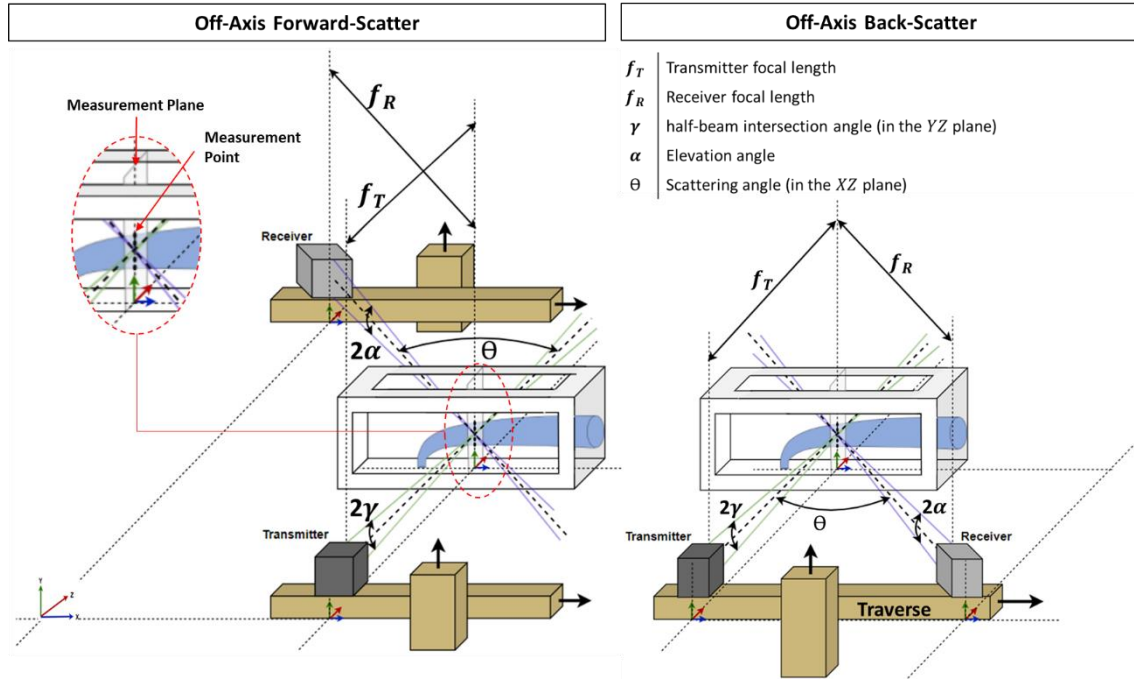


Figure A-13: Possible PDPA configurations for liquid jets in crossflow.

The measurement planes for PDPA are perpendicular to the flow direction. The spray characteristics are measured when a droplet passes through the intersection point of the laser beams. Moving the lasers vertically at a constant scattering angle creates multiple beam intersection points on a single cross-section plane of the spray, as shown in the left image of **Figure A-13**. The characteristics of the spray can be obtained by taking the measurements on multiple cross-section planes. This can be done by moving the laser horizontally without changing the scattering angle.

A support system for the PDPA probe has been designed for easy and safe operation with remote control capabilities to optimize the measurement time, as shown in **Figure A-14**. The support system consists of a 3D traverse system attached to BOSCH rails on which the PDPA probes are fixed. This setup allows to remotely move horizontally and vertically the transmitter and receiver probes without affecting the scattering angle. Moreover, the system was designed to alternate faster between both measurement techniques (i.e. remove the need to install/uninstall the PDPA and shadowgraph instrumentation). To do so, the system does not interfere physically with the High-speed camera, which is fixed to the floor by a tripod (not shown in **Figure A-14**), and the LED light arrays are fixed to the BOSCH rails. Once the PDPA measurements are taken, the

support system moves the probes out of the view of the high-speed camera while simultaneously positioning the LED light array in front of its lens.

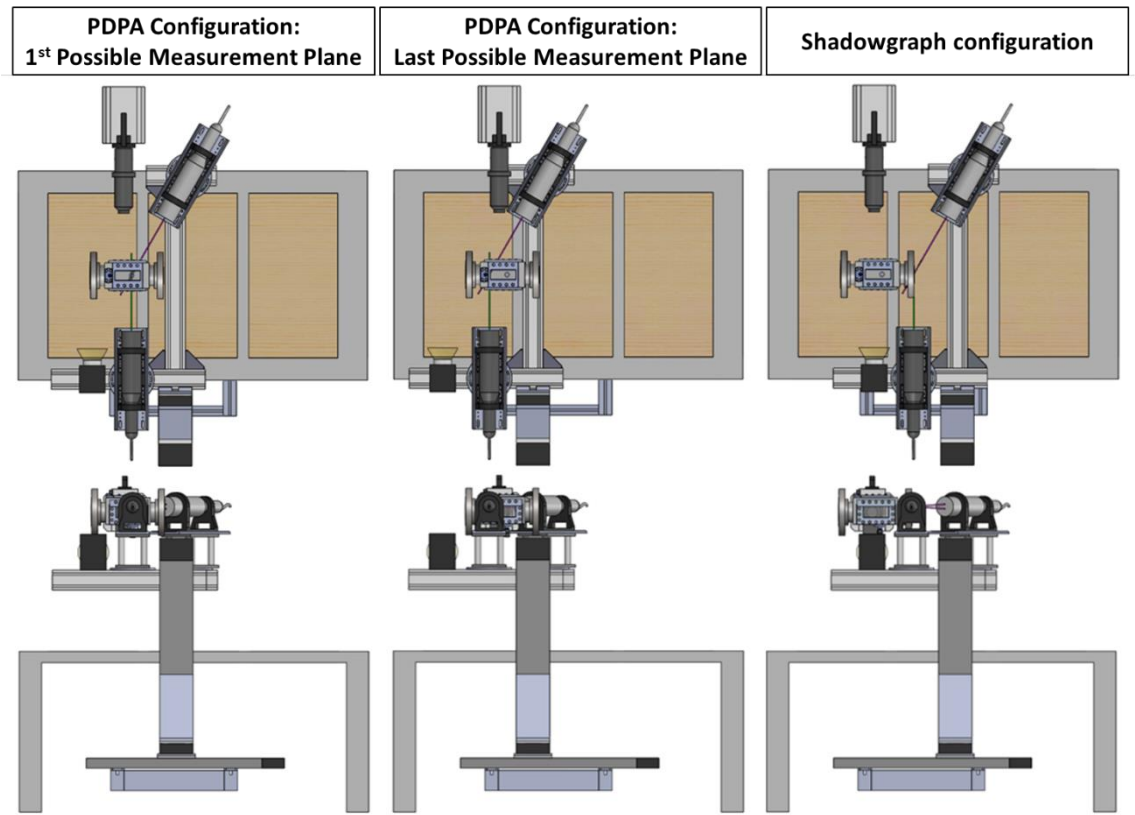


Figure A-14: PDPA support system configurations (represented at a lower height than reality and LED light arrays connection to BOSCH rails not represented).

Particle Image Velocimetry (PIV) will be used to visualize the velocity field without the spray. The measurements will be taken on several cross-sections parallel to the airflow direction. The laser used for PIV is the same as the one used for LIF, but the wavelength output for the former is higher at 532nm. The measurements with PIV will be taken before injecting any liquid fuel spray inside the test section. Since the laser beam enters through the top window of the test section, a support system for the PIV laser can be used without needing to remove the PDPA and shadowgraph equipment.

A.5 Data Processing

The datasets generated will be processed to extract correlations for the jet trajectory, column breakup length and the centreline profiles of the droplet velocity and Sauter Mean diameter (SMD). The droplet velocity and diameter are measured when the droplet passes through the intersection point of the PDPA laser beams. Combining the measurement

points taken on a single cross-section plane allows extracting centreline profiles, similar to those used in the core research chapters to validate the numerical modelling methodologies.

The instantaneous shadowgraph images will be used to identify the different spray primary breakup characteristics by comparing the results with the turbulent LJIC regimes identified in the literature, as discussed in *section 2.1.3*. They will also be processed to obtain time-averaged spray images to extract the mean jet trajectories and derive empirical correlations.

The instantaneous velocity vector map measured with PIV on multiple cross-section planes will be processed to extract the gas velocity profiles. Their combination can provide an approximation of the 3D analytical gas velocity profile distribution [e.g. 225], which will be used to impose the airflow boundary condition in the numerical simulations for the validation work.

To further validate the numerical modelling methodologies developed, the centreline profiles, spray trajectories and breakup characteristics predicted will be compared to the corresponding experimental data, similar to the work presented in the core research chapters.

A.6 Test Section Design

As previously mentioned, the cross-section dimensions of the test section were selected to avoid fuel impingement on the windows, respect the pebble bed's capabilities and stay within the acceptable range of Mach number.

A.6.1 Design Considerations: Subsonic Conditions

The range of gas Weber number and momentum flux ratios presented in **Table A-2** must be covered during the experiments while the Mach number in the test section remains equal or inferior to 0.3. This ensures the airflow characteristics are representative of industrial gas turbine combustor inlet conditions [8]. Thus, for each combination of air pressures and temperatures presented in **Table A-1** and **Table A-2**, the maximum allowable velocity that can be achieved in the test section while maintaining subsonic

conditions is given by equation (A-1). Because the gas Weber number is a function of the gas velocity, it is also limited by the Mach number as shown in equation (A-2).

$$u_{g_{max},Ma} = Ma_{max} \sqrt{\gamma R_G T_g} \quad (A-1)$$

$$We_{g_{max},Ma} = \frac{(u_{g_{max},Ma})^2 \rho_g d}{\sigma} \quad (A-2)$$

Where Ma_{max} is the maximum Mach number (i.e. 0.3), γ is the specific heat ratio for air at the specified pressure and temperature, R_G is the gas constant for air (287J/kgK [79]) and T_g is the air temperature.

The restriction imposed by the Mach number implies that the gas Weber numbers at lower pressure will be limited below the upper limit of the target range presented in **Table A-3**. In other words, it will not be possible for test case 1 to test case 3 to cover the full range of gas Weber numbers (100 to 2500) in order to remain within the acceptable range of Mach numbers. At higher pressures, the maximum gas Weber number is far superior to the upper limit of 2500 presented in **Table A-3**. However, to guide the rig design, its value was limited to the latter. This test restriction on the maximum gas Weber number is expressed by equation (A-3).

$$We_{g_{max}} = \min (We_{g_{max,test}}, We_{g_{max},Ma}) \quad (A-3)$$

Where $We_{g_{max,test}}$ is the maximum gas Weber number targeted in the present research (i.e. 2500). For the cases where the maximum gas Weber number to be tested is limited to $We_{g_{max,test}}$, the maximum velocity that can be achieved inside of the test section is smaller than $u_{g_{max},Ma}$ and must be calculated using equation (A-4) instead. When the gas number is not limited to $We_{g_{max,test}}$ the Mach number is the only restriction imposed on the velocity. Thus, for cases 1 to 3, equation (A-1) and equation (A-4) give the same value.

$$u_{g_{max}} = \sqrt{\frac{We_{g_{max}} \sigma}{\rho_g d}} \quad (A-4)$$

For each test case presented in **Table A-2**, the maximum gas velocity and gas Weber numbers that can be achieved while maintaining subsonic conditions are presented in

Table A-5. It is important to note that the actual experimental Weber number is subjected to other considerations such as safety requirements due to autoignition risks.

Table A-5: Maximum gas velocity and gas Weber number for $Ma \leq 0.3$ for each test case.

Case #	P_g [Bar]	T_g [K]	$We_{g_{max}}$	$u_{g_{max}}$ [m/s]
1	1	300	224	104.1
2	4	300	886	104.1
3	4	600	863	145.4
4	15	300	2500	90.3
5	15	450	2500	110.6
6	15	600	2500	127.8

The limitations imposed by the Mach number on the maximum gas velocity inside the test section also impact the maximum mass flow $\dot{m}_{g_{Max}}$ allowable to maintain subsonic conditions as shown in equation (A-5). Where H is the internal height of the test section and W is the width. As discussed in *Appendix A.3.1*, the maximum mass flow is also limited by the air system's capacity, as seen in equation (A-6).

$$\dot{m}_{g_{Max}} = u_{g_{max}} \rho_g H W \quad (A-5)$$

$$\dot{m}_{g_{Max}} = u_{g_{max}} \rho_g H W \leq \dot{m}_{g_{maxPB}} \quad (A-6)$$

Where $\dot{m}_{g_{maxPB}}$ is the maximum mass flow that can be delivered by the air system with the bypass, as presented in **Table A-4**. Since the latter and the maximum velocity are known, it is possible to calculate the maximum cross-section area that the test section can have. Alternatively, for a fixed height or width, the corresponding maximum width or height can also be calculated. The maximum width W_{max} of the test section for a fixed height is calculated using equation (A-7). The variation of its value based on the height selected is shown in **Figure A-15** for each test case.

$$W_{max} = \frac{\dot{m}_{g_{maxPB}}}{u_{g_{max}} \rho_g H} \quad (A-7)$$

As it is possible to observe in **Figure A-15**, the maximum allowable width of the test section decreases with an increasing test section height. Furthermore, test case 4 has the most limiting conditions on the width.

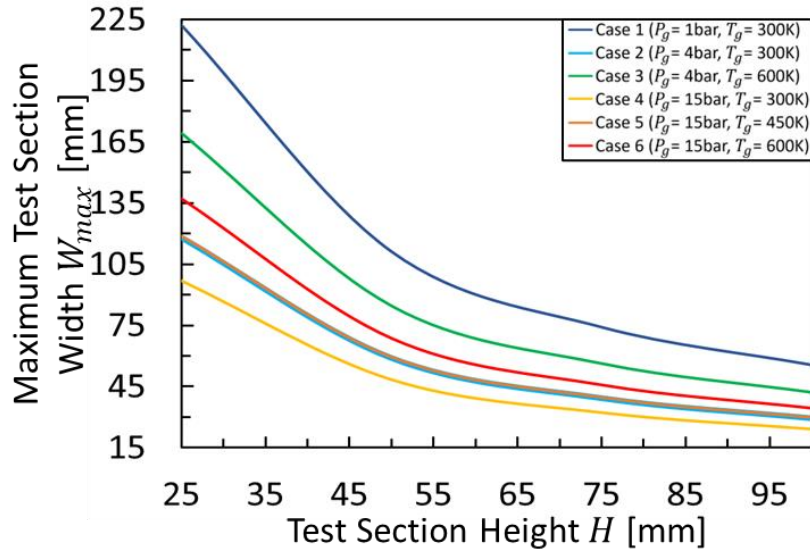


Figure A-15: Maximum width of the test section as a function of the selected height.

Another important aspect to consider when selecting the test section width is that droplet impingement on the walls must be avoided. Therefore, W might need to be larger than the value calculated using equation (A-7). To prepare for this eventuality, it is useful to express the maximum gas Weber number as a function of an imposed width instead of the imposed height H . However, the limitations imposed on W_{max} by the Mach number and the capacity of the air system must still be respected. These additional considerations on $We_{g_{max}}$ are expressed in equation (A-8), which can be used to determine the maximum gas Weber number that can be achieved based on the test section dimensions. It is important to note that this equation does consider the maximum target values presented in **Table A-3**. The variation of the maximum gas Weber number as a function of any given width for $H = 50$ mm is shown in **Figure A-16**.

$$We_{g_{max}} = \min \left(\frac{\rho_g d}{\sigma} \left(\frac{\dot{m}_{g_{max,PB}}}{W \rho_g H} \right)^2, We_{g_{max,Ma}} \right) \quad (A-8)$$

As it is possible to observe in **Figure A-16**, W_{max} must be smaller than 68.5 mm to cover the full range of We_g presented in **Table A-3** when the test section height is limited to 50 mm. For $H > 50$ mm, it is not possible to achieve $We_g = 2500$ for any test cases. To ensure that all higher-pressure test cases can achieve the upper limit of the range presented in **Table A-3**, the maximum width must be limited to 48.5 mm. Moreover, increasing W_{max} above 59.1 mm reduces the value of $We_{g_{max}}$ that can be achieved under the

conditions of test case 2. Considering the design limitations highlighted in **Figure A-15** and **Figure A-16**, the initial width of the test section was set to 45 mm for an initial height of 50 mm. These dimensions respect the limitations imposed by the Mach number, the capacity of the air system and the maximum gas Weber numbers targeted for the project (i.e. 2500).

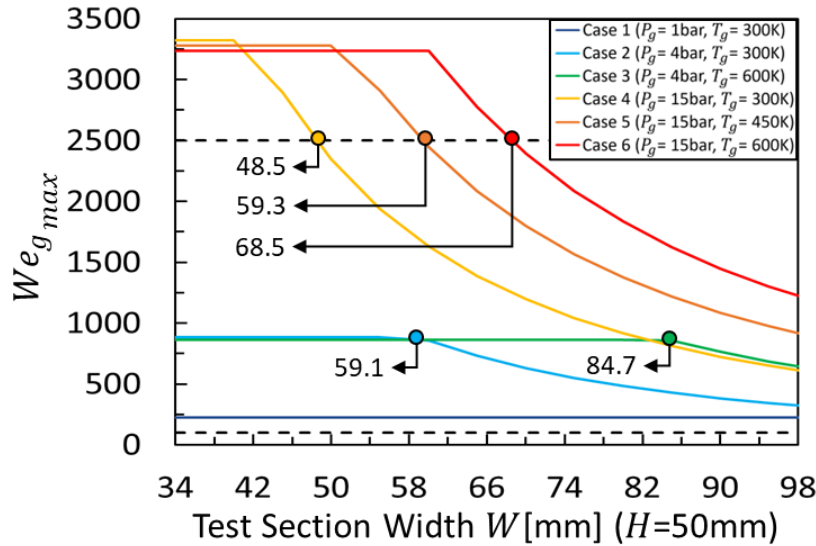


Figure A-16: Variation of the maximum gas Weber number as a function of any given width for a fixed height of 50 mm.

A.6.2 Design Considerations: Wall-Impingement Risks

As previously mentioned, it is also important that the dimensions selected do not cause droplets to impinge on the optical windows' walls, as this would cause problems for the laser diagnostics. To assess the risk of wall-impingement for the selected dimensions, correlations for the droplet trajectory and width can be used along with numerical simulations.

To avoid droplet impingement on the top window, H must be higher than the predicted windward spray trajectory for the selected observation length L_{test} , which was set to 75 mm to prevent autoignition as detailed in *Appendix A.8*. Empirical correlations proposed in the literature to predict the spray trajectory of LJIC are presented in *section 2.1.4* from Chapter 2. To perform a conservative assessment of the wall-impingement risk, the test condition resulting in the highest spray penetration for each empirical correlation presented in **Table 2-2** was used to generate the curves shown in **Figure A-17**. For a vast

majority of these correlations, this was achieved by using test case 1 (ambient pressure and temperature) with the maximum momentum flux ratio ($J = 50$) and minimum gas Weber number ($We_g = 100$). A few other correlations also predict that a high spray trajectory will be achieved at higher pressures and/or temperatures (test case 5 or test case 6) often with $J = 50$ and $We_g = 100$. Thus, the two extreme conditions (i.e. test case 1 and test case 6) were selected to perform the numerical validation of the test section design.

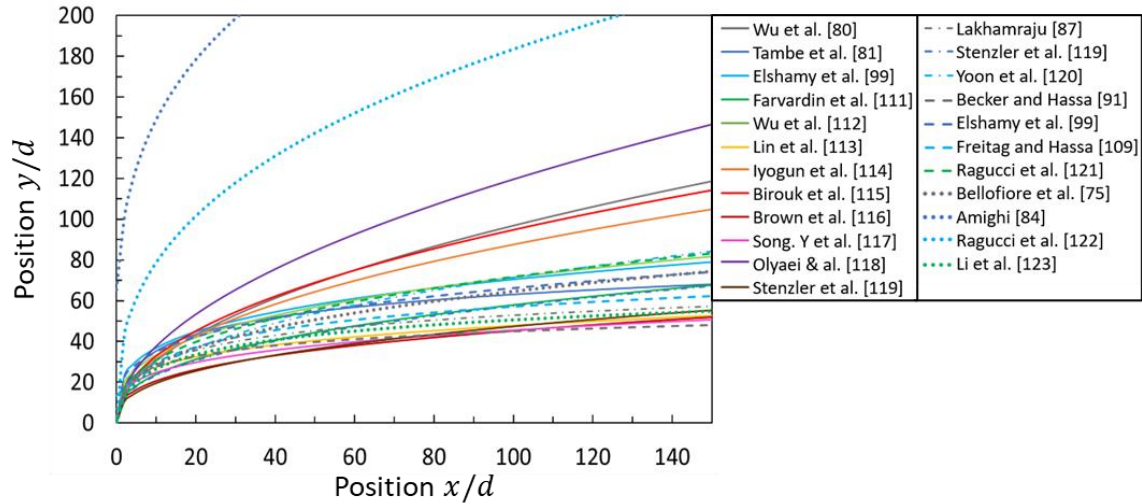


Figure A-17: Maximum spray trajectory predicted for the target test conditions by different empirical correlations available in the literature (derived from conditions at: Solid lines – STP, Dashed-dotted lines – HTSP, Dashed lines – STHP, Dotted lines – HTP).

To avoid droplet impingement on the side windows, W must be larger than the predicted width of the spray for L_{test} . Empirical correlations proposed in the literature to predict the spray width of LJIC are presented in *section 2.1.4* from Chapter 2. As previously mentioned, the few experimental studies that have measured the spray width reported that it only depends on the momentum flux ratio and increases with the latter. Thus, for each correlation presented in **Table 2-4**, the maximum momentum flux ratio targeted ($J = 50$) was used to predict the maximum curves for the spray width, which are presented in **Figure A-18**.

To the best knowledge of the author, there are no correlations available in the literature for the spray width derived from experiments at high temperatures. The few empirical correlations presented in *section 2.1.4* were obtained from experiments conducted under ambient conditions or standard temperatures at high pressures (STHP) [91]. This is probably due to the complexity of including an optical access in the cross-section plane.

However, higher temperatures are more likely to evaporate the small droplets located on the periphery of the spray, thus reducing the spray width. Therefore, the extreme test conditions selected previously to assess the maximum spray trajectory are deemed suitable to perform a conservative numerical assessment of the wall-impingement risks on the side windows.

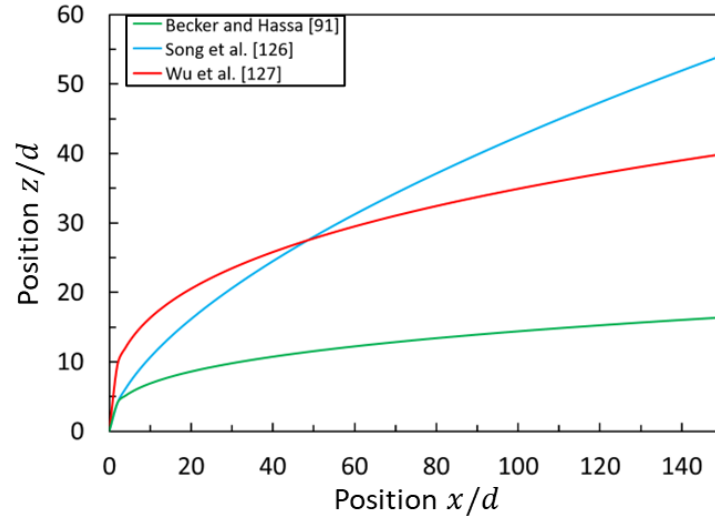


Figure A-18: Maximum half spray width predicted for the target test conditions by different empirical correlations available in the literature.

The test conditions deemed the most likely to have droplets impinging on the windows based on the assessment of the empirical correlations conducted in the previous section are further detailed in **Table A-6**. It is also important to consider that the velocity profile of the airflow inside the test section can be fully developed, constant or intermediate. One of the main research findings from Chapter 4 was that the air velocity profile can have a significant impact on the spray trajectory predicted. Thus, the two extreme scenarios (i.e. fully developed and constant velocity profiles) were studied for each condition to ensure the test section design is conservatively assessed. The fully developed velocity profile was calculated using the method described in *section 4.4.2* from Chapter 4 for rectangular channels.

The numerical domain is shown in **Figure A-19**. To improve convergence, the length before the injection was set to 40 mm and the length after the injection was slightly longer than L_{test} . The same polyhedral mesh was used for all simulations, which included a volumetric refinement of 0.4 mm in the spray region. The resulting mesh shown in **Figure A-20** has 2.65 million elements and achieves wall y^+ values inferior to 5, thus allowing

capturing the two-way coupling interactions near the walls. It should be noted that using a finer mesh was found to create instability issues as it increases the liquid volume fraction in the cells located in the jet column region.

Table A-6: Test conditions used for the numerical simulations guiding the test section design.

Conditions	Velocity Profile	P_g [bar]	T_g [K]	J	We_g	u_g [m/s]	u_{jet} [m/s]
STP	Fully Developed	1	300	50	100	69.5	18.5
	Constant						
HTP	Fully Developed	15	600	50	100	25.6	18.5
	Constant						

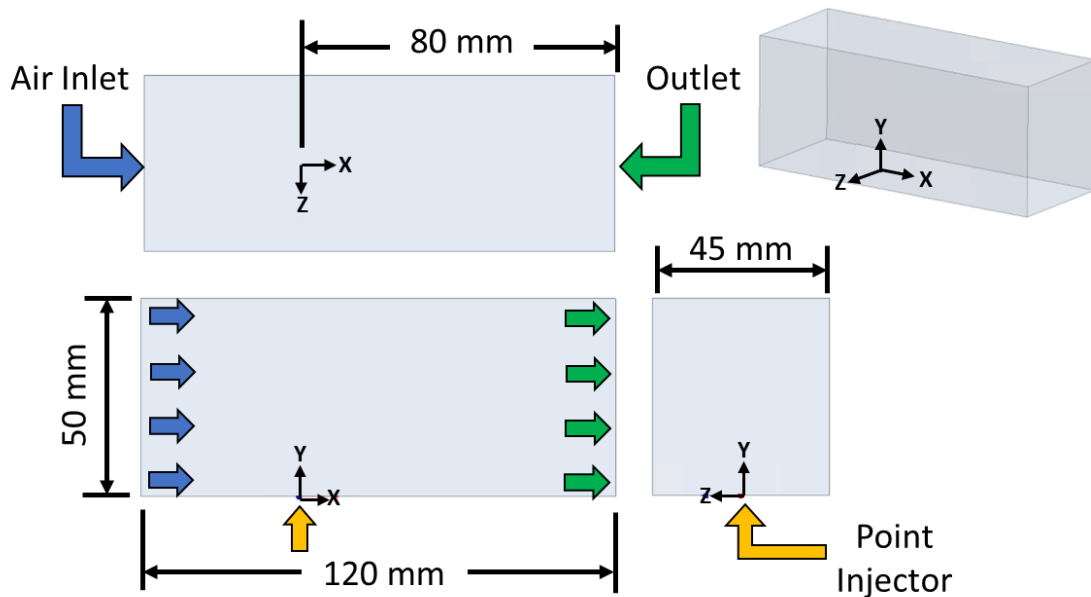


Figure A-19: Numerical domain used to guide the test section design.

The numerical set-up follows the URANS Lagrangian stochastic numerical methodology developed in Chapter 3 and Chapter 4, which is summarized in **Table 7-2** from *section 7.1*. It should be noted that the test section design was developed and commissioned well before undertaking the work from Chapter 6 and Chapter 5 due to the experimental project's timeline. However, it is recommended for future design work to also use the optimized hybrid method as it allows to perform a more conservative assessment of the wall-impingement risks on the side windows. Despite this limitation, the URANS

Lagrangian stochastic methodology is deemed more suitable to assess the wall-impingement risks on the top windows as it was found to predict more accurately the spray trajectory. In addition, the normal velocity coefficient of the SSD model was set to 1 to enhance the radial dispersion of the droplet as recommended in Chapter 3. To further evaluate the wall-impingement risks conservatively, droplet evaporation and heat transfer were not modelled in order to obtain the maximum predictions in spray trajectory and width.

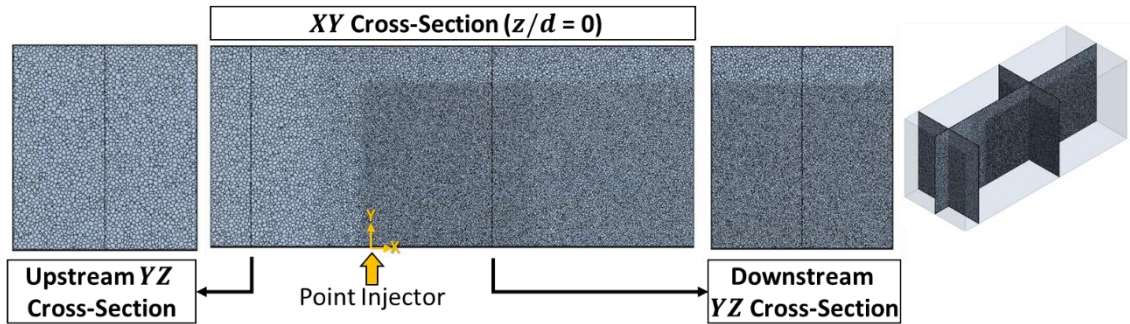


Figure A-20: Numerical grid used to guide the test section design.

Preliminary RANS simulations were conducted to impose the maximum number of child parcels (12), the target number of particles per parcel (1000) and parcel streams (300), which control the spray discretization. The maximum Co_{max} and minimum Co_{min} Lagrangian Courant numbers were calculated using the method described in Chapter 3 and Chapter 4. The time-step imposed varied between 1-2 μs and was selected for each condition to achieve a courant number less than 1 in the spray region. The number of inner iterations imposed varied between 30-80 to ensure a minimum convergence of the residuals to the 2nd order of magnitude. The CFL number of the coupled solver varied between 10-40 and was selected to provide a stable solution. It was observed that the high temperature and pressure (HTP) conditions required a smaller CFL, smaller Lagrangian Courant numbers and more inner iterations than the standard temperature and pressure (STP) conditions. The simulations were run for at least two times the residence time of the droplets inside the numerical domain before starting the time-averaging process. The latter was also run for at least twice the residence time.

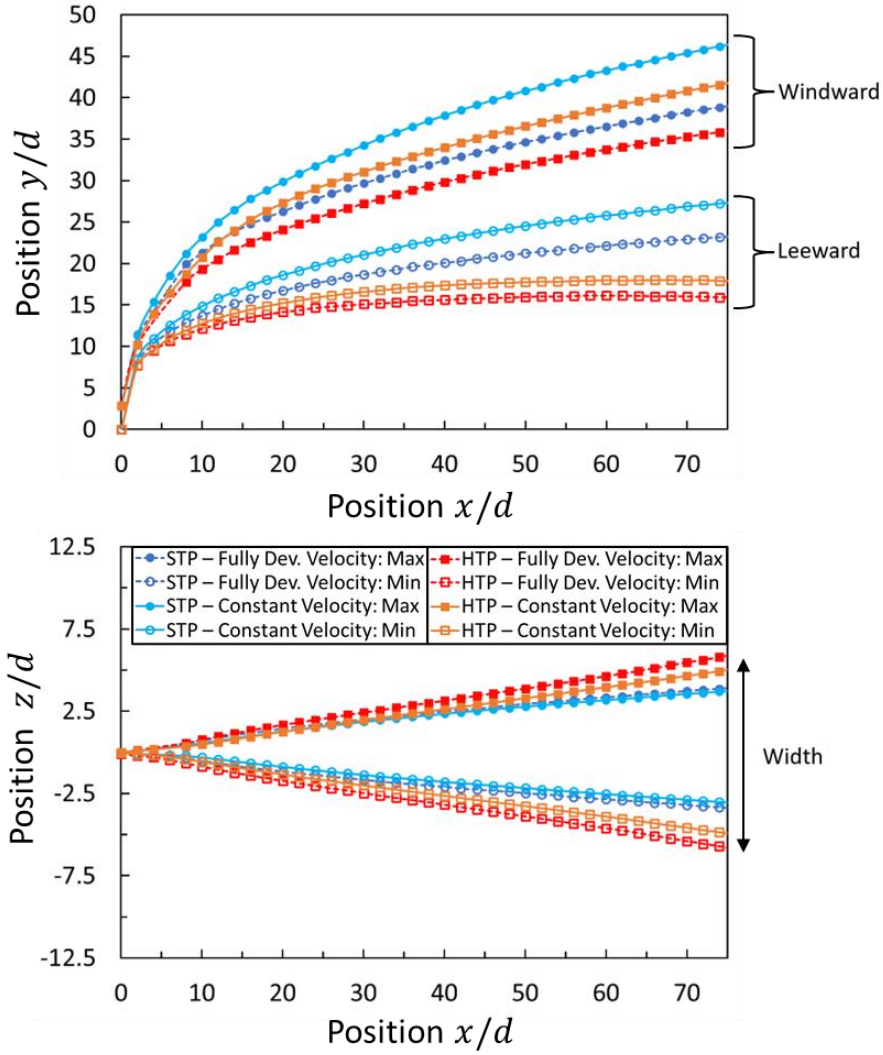


Figure A-21: Time-averaged spray trajectory (top) and width (low) at STP ($P_g=1$ bar, $T_g=300\text{K}$, $J=50$ and $We_g=100$) and HTP (HTP: $P_g=15$ bar, $T_g=600\text{K}$, $J=50$ and $We_g=100$) conditions predicted inside the test section for different velocity profiles (Dashed lines: Fully developed velocity profile, Solid lines: Constant velocity profile, Solid symbols: Maximum curve, Hollow symbols: Minimum curve).

It is possible to observe in the bottom graphic of **Figure A-21** that the velocity profile does not have a significant impact on the spray width at STP conditions. However, the spray width at the end of the measurement zone ($x = 75$ mm) is 17% larger with a fully developed velocity profile when using the HTP condition. Furthermore, the HTP conditions have the highest wall-impingement risk on the side windows despite having the same J and We_g values. Indeed, the spray width predicted at $x = L_{test}$ is 60% larger at HTP condition compared to STP condition when both use a fully developed velocity

profile. This is likely due to the choice of not modelling the evaporation process to obtain predictions that correspond to the “worst” case scenario. Therefore, the numerical predictions indicate that the safety gap between the spray plume and the side windows will be approximately 17 mm for $W = 45$ mm, which is deemed very conservative.

The top graphic of **Figure A-21** shows that using a constant velocity profile predicts a higher spray penetration regardless of the experimental conditions, which agrees with the previous findings from Chapter 4. Indeed, the maximum spray trajectory at the end of the measurement zone is on average 15% smaller when using a fully developed gas velocity profile compared to a constant profile. Moreover, the maximum spray trajectory predicted at $x = L_{test}$ is higher by 11% with the STP condition compared to the HTP condition. Thus, the STP condition has the highest wall-impingement risk on the top window despite having the same J and We_g values. Therefore, the numerical predictions indicate that the safety gap between the spray plume and the top window will be approximately 3 mm for $H = 50$ mm.

Different strategies could be used to increase the safety gap between the maximum spray plume and the top wall, such as reducing the length of the optical windows. However, a longer observation length allows for observing the secondary breakup and evaporation process that occurs at higher temperatures and pressures. Moreover, the test points that have the highest risks of wall-impingement on the top window (i.e. STP conditions) have been more widely studied in the literature as presented in *Appendix A.1*. Thus, avoiding these test points during the experiments would not have a significant impact on the ability of the rig facility developed to fill the gaps in knowledge on LFJIC at representative combustor inlet conditions. Therefore, it was deemed more important to maximize the measurement length regardless of the wall-impingement risks at STP condition. It is important to note that atmospheric conditions should still be tested, but by implementing the following recommendations to mitigate the wall-impingement risks: the experimental campaign for the STP tests conducted at the highest momentum flux ratios should be halted if droplet impingement on the top window becomes a major issue during the experiments. In such a scenario, the windows would be cleaned by either disassembling the test section from the rig to remove them or by running hot air inside of the test section to evaporate any fluid film/droplets. For these reasons, it is recommended to limit the STP

test points to lower momentum flux ratio values. These recommendations also imply that the highest risk of wall-impingement shifted to the HTP conditions, which increases the safety gap between the spray plume and the top window to approximately 8 mm for $H = 50$ mm.

Another option to avoid wall-impingement on the top window at STP condition while maintaining $L_{test} = 75$ mm would be to increase the test section height by reducing its width, as shown in **Figure A-15**. However, this would increase the risk of wall-impingement on the side windows for all test conditions. Although this is not deemed an issue for the plain orifice injector considering the large safety gap predicted, it could prevent adapting the test section in the future to conduct experiments with pressure-swirl atomizers. Moreover, not enough research has been done on the factors influencing the spray width of LJIC, which limits the numerical validation work for this spray characteristic. Thus, it is preferable to keep the current test section height to ensure the test section design is polyvalent and to avoid unknowingly increasing the risk of wall-impingement on the side windows even with a plain orifice injector.

Therefore, for an observation length of 75 mm, the test section dimensions $H = 50$ mm and $W = 45$ mm were deemed the most optimal. The resulting wall-impingement safety gap predicted is around 4-8 mm for the top window and approximately 17 mm for each side window. It should also be noted that the inlet airflow is more likely to be fully developed due to the flow straightener and long channel located upstream of the test section. Thus, the safety gap with the top window is probably closer to 11-14 mm in reality than the 4-8 mm gap predicted using a constant velocity profile under STP and HTP conditions respectively. It is also worth noting that the windward spray trajectories predicted with a fully developed velocity profile tend to agree better with the empirical correlations derived from experiments conducted at similar temperatures and/or pressures as seen in **Figure A-22**. Furthermore, the numerical predictions tend to be within the range of spray trajectories predicted using the correlations available in the literature regardless of the velocity profile imposed, which increases the level of confidence in the present assessment of the wall-impingement risk.

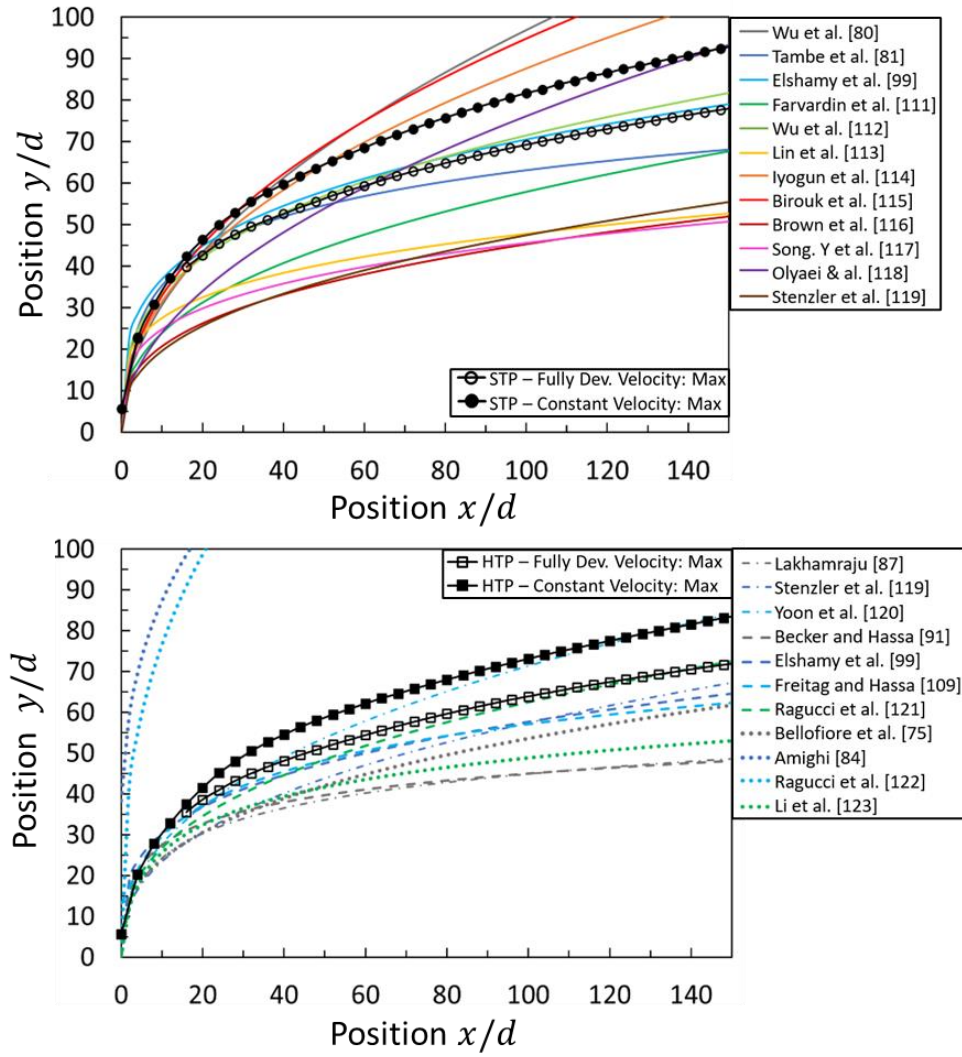


Figure A-22: Comparison of the windward spray trajectories predicted by the empirical correlations available in the literature (derived from: Solid lines – STP conditions, Dashed-dotted lines – HTSP conditions, Dashed lines – STHP conditions, Dotted lines – HTP conditions) to the time-averaged results obtained at STP (top: $P_g = 1$ bar, $T_g = 300$ K, $J = 50$ and $We_g = 100$) and HTP conditions (top: $P_g = 15$ bar, $T_g = 600$ K, $J = 50$ and $We_g = 100$) for different velocity profiles (Hollow symbol: fully developed, Solid symbol: constant).

A.7 Optical Windows Design

Another key design consideration for the test section was the support of the optical windows, which are subjected to large pressure and temperature gradients during the experiments except for test case 1. As previously mentioned, different test section designs were considered to support the windows and down-selected based on their impact on the

gas velocity profile (i.e. if the windows are sitting flush with the test section walls), supplier cost (e.g. thicker windows are more expensive) and manufacturing cost (i.e. machining optical windows is expensive). For each test section design considered as well as each subsequent design iteration of the chosen concept, the minimum thickness of the optical window t_{min} required to support the pressure load was estimated conservatively. This was done by using the maximum values obtained from different equations found in the literature for windows supported under high load, as expressed in equation (A-9).

$$t_{min} = \max(t_{min1}, t_{min2}, t_{min3}) \quad (A-9)$$

Where t_{min1} and t_{min2} are minimum thicknesses calculated from equations found in the literature for circular-supported windows while t_{min3} is for rectangular supported windows. The expression for t_{min1} and t_{min2} are given in equation (A-10) [226] and equation (A-11) [227] respectively.

$$t_{min1} = \left(\frac{1}{2}D_0\right) \sqrt{SF \frac{K_w \Delta P}{\sigma_{max}}} \quad (A-10)$$

$$t_{min2} = \left(\frac{1}{2}D_0\right) \sqrt{SF \frac{K_w \Delta P}{\min(S_y, S_f)}} \quad (A-11)$$

Where σ_{max} is the allowable stress, S_f is the rupture strength and S_y is the offset yield strength. It is recommended to impose the generalized constant K_w equal to 0.75 and the safety factor $SF \geq 2$ [226]. However, the latter was imposed equal to 4 as it was found to be a commonly used value [226, 227], which is more conservative. To reflect that the windows considered are not circular, the unsupported glass length D_0 is defined as the unsupported length of the window L_{ow} as shown in **Figure A-23**. The minimum thickness t_{min3} for a supported rectangular window is given by equation (A-12) [227] and also depends on its unsupported width W_{ow} . The latter corresponds either to the inner height H or width W of the test section based on the location of the window (i.e. side or top window).

$$t_{min3} = L_{ow} \sqrt{\frac{1}{2}SF \left(\frac{K_w \Delta P}{\min(S_y, S_f)} \right) \left(\frac{1}{1 + (L_{ow}/W_{ow})^2} \right)} \quad (A-12)$$

The differential pressure across the window ΔP is the difference between the higher pressure inside the test section and the ambient pressure outside of the test section. To be

conservative, the differential pressure was imposed equal to 15 bar, which is the targeted maximum pressure for the experimental campaign.

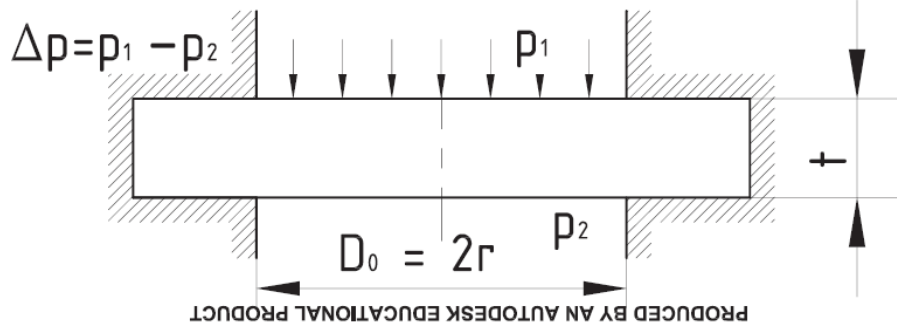


Figure A-23: Pressure forces acting on the unsupported length of a supported optical window (Reprinted from [226] with permission from Elsevier).

A similar strategy was used to estimate conservatively the allowable stress σ_{max} . This was achieved by considering the minimum value obtained from different equations found in the literature for supported windows under high load as expressed in equation (A-13).

$$\sigma_{max} = \min(\sigma_{max1}, \sigma_{max2}) \quad (A-13)$$

Where σ_{max1} and σ_{max2} are the allowable stress of supported windows calculated using equation (A-14) [226] and equation (A-15) [227] respectively. The former also depends on the ultimate strength S_{ut} , which is equal to S_f for brittle material.

$$\sigma_{max1} = \min\left(\frac{S_y}{SF}, \frac{0.4S_{ut}}{SF}\right) \quad (A-14)$$

$$\sigma_{max2} = \min\left(\frac{S_y}{SF}, \frac{S_f}{SF}\right) \quad (A-15)$$

For each optical window, the maximum allowable stress and minimum thickness were calculated using different properties of fused silica glass found in the literature and in catalogues from manufacturers [218, 226, 227, 228, 229, 230]. From all the material properties considered, Tosoh SGM Optical Silica Glass ESL-1000 yields the smallest maximum allowable stress at 4.9 MPa, which results in the smallest thickness for all designs evaluated. These thicknesses were considered for the initial design of the windows.

For the FEA analysis, the material properties used were from Corning HPFS 7980 Fused Silica glass considering this material was ultimately selected. To calculate the maximum allowable stress, it is important to note that equation (A-14) is significantly more

conservative compared to equation (A-15) because the safety factor SF gets multiplied by 2.5. Although this aspect was deemed acceptable to obtain a first estimation of the windows' thickness, it was ultimately deemed too conservative when using FEA to guide the final design iterations. Thus, the maximum allowable stress considered for the FEA simulation was imposed equal to 13.5MPa.

A.8 Autoignition Risks

For test cases 4 to 6, the fuel will be exposed to elevated temperatures and pressures, which contribute to reducing the autoignition delay [231]. To avoid autoignition, the residence time of the fuel droplets inside the test section $\tau_{R,p}$ must be inferior to the autoignition delay time $\tau_{autoignition}$, as expressed in equation (A-16). The latter can be predicted using the Arrhenius-type equation given below [232].

$$\tau_{R,p} < \tau_{autoignition} \quad (A-16)$$

$$\tau_{autoignition} = A_{ign}(P_g^{-n_{ign}})\exp\left(\frac{B_{ign}}{T_g}\right) \quad (A-17)$$

Where A_{ign} , B_{ign} and n_{ign} are model constants that depend on the fuel properties, test conditions and set-up [231]. The model constants available in the literature for Diesel fuel No.2 are presented in **Table A-7**.

Table A-7: Model constants for the autoignition delay time equation available in the literature for Diesel fuel No.2.

Model constants	Watson et al. [233]	Stringer et al. [234]	Aligrot et al. [231]		Payri et al. [235]	Assanis et al. [236]
			(1)	(2)		
A_{ign}	3.45	0.045	1.0199E-04	$\exp(0.0349CN - 18.1888c_{paraf} - 6.3883)$	$0.26P_{inj}^{-0.138}$	$2.4\phi_{eq}^{-0.2}$
n_{ign}	1.02	0.757	0.3931	$0.1097v_L - 0.2903$	0.89	1.02
B_{ign}	2100	5473	8522	$10.583CN + 5951.9c_{paraf} + 6940.8$	2510.9	2100

Where CN is the Cetane number, c_{paraf} is the paraffin content, v_L is the kinematic viscosity of the fuel (diesel fuel No. 2 at 288K), P_{inj} is the injection pressure of the fuel and ϕ_{eq} is the equivalence ratio. To use the datasets generated for future numerical validation work, the properties of the fuel that will be used during the experiments were measured. However, the rig design and development work were done prior to having

selected the diesel fuel supplier. Thus, properties for Diesel fuel No.2 available in the literature were used instead to estimate the autoignition time. For the Cetane number and paraffin content included in the correlation from Aligrot et al. [231], the values suggested by the author were selected (i.e. $CN = 42.8$ and $c_{paraf} = 0.1888$). These values are close to those suggested in more recent work [237, 238, 239]. For each test case, the equivalence ratio was calculated using equation (A-18) [5].

$$\phi_{eq} = \frac{FAR_{max}}{FAR_{st}} \quad (A-18)$$

Where FAR_{st} is the stoichiometric fuel-air ratio (FAR) and FAR_{max} is the maximum FAR that can occur for the given condition. The stoichiometric FAR is calculated as 0.066993 based on the chemical formula of Diesel No.2 (i.e. $C_{14}H_{24}$ [240]). The maximum FAR was then calculated for each extreme combination of momentum flux ratio and gas Weber number allowable in the test section by using equation (A-19).

$$FAR_{max} = \max \left[\left(\frac{\dot{m}_{jet}}{\dot{m}_g} \right)_1, \left(\frac{\dot{m}_{jet}}{\dot{m}_g} \right)_2, \left(\frac{\dot{m}_{jet}}{\dot{m}_g} \right)_3, \left(\frac{\dot{m}_{jet}}{\dot{m}_g} \right)_4 \right] \quad (A-19)$$

Where $\dot{m}_{jet}$ is the fuel mass flow and $\dot{m}_g$ is the air mass flow. Each mass flow ratio represents the FAR for one of the 4 extreme combinations of momentum flux ratio and gas Weber numbers. The first ratio corresponds to $J = 10$ and $We_g = 100$, the 2nd ratio is for $J = 10$ and $We_g = We_{g_{max}}$, the 3rd ratio corresponds to $J = 50$ and $We_g = 100$ and the last ratio is for $J = 50$ and $We_g = We_{g_{max}}$. The value of $We_{g_{max}}$ is given for each test condition in **Table A-5**. The resulting values for the maximum FAR and corresponding equivalence ratio of each test case are presented in **Table A-8**.

Table A-8: Maximum FAR and maximum equivalence ratio for each test case.

Case #	FAR_{max}	ϕ_{eq}
1	0.0164	0.25
2	0.0083	0.12
3	0.0117	0.17
4	0.0043	0.06
5	0.0052	0.08
6	0.0060	0.09

The maximum values of FAR_{max} and ϕ_{eq} occur at the atmospheric conditions of test case 1, where autoignition is not likely to occur. However, to be conservative, these values were used to evaluate the autoignition risk and a safety factor of 1.5 was applied

($\phi_{eq} \approx 0.4$). **Table A-9** presents the autoignition time for test cases 3, 5 and 6 calculated using the different model constants available in the literature as shown in **Table A-7**.

Table A-9: Estimation of autoignition and heating-up time for high-pressure and high-temperature cases.

Case #	P_g [bar]	T_g [K]	Autoignition time [ms]							Droplet lifetime† [ms]
			Watson et al. [233]	Stringer et al. [234]	Aligrot et al. [231]			Payri et al. [235]	Assanis et al. [236]	
					(1)	(2)	(2*)			
3	4	600	28	130	87	150	57	38	21	4-77 (35)
5	15	450	23	No auto-ignition	No auto-ignition	No auto-ignition	No auto-ignition	40	19	4-81 (36)
6	15	600	7	48	52	66	9.9	10	6	3-52 (23)
*Calculated with the fuel kinematic viscosity suggested by the authors [231].										
† Values shown as: Min-max (average)										

The droplet lifetime, which represents the droplet heat-up time under steady-state evaporation, was calculated using the methodology presented by Lefebvre and McDonell [7]. The droplet heat-up time can be calculated using either the initial droplet diameter or the average diameter during the heat-up period, which is a function of the initial size [7]. Thus, for a given initial droplet diameter, two different values of droplet lifetime can be obtained. For each extreme combination of momentum flux ratio and gas Weber number, the initial droplet diameter was predicted using the empirical correlations for the SMD presented in **Table 2-1** from *section 2.1.4*. To be conservative, the droplet lifetime was calculated for each extreme combination by using the maximum, minimum and averaged SMD values obtained from the correlations. Thus, for each extreme combination, six different values of droplet lifetime were obtained in total, meaning that 24 values were calculated per test case. In **Table A-9**, the lower and upper limits of the droplet lifetime represent the minimum and maximum values obtained for the given test case. The average value indicated corresponds to the smallest average droplet lifetime calculated from all the extreme combinations.

As it is possible to observe in **Table A-9**, the model constants proposed in the literature lead to great discrepancies in the autoignition delay. While some correlations predict the autoignition time to be in the order of 50 ms, many others predict it is in the order of 10 ms. These discrepancies can be explained by the properties of diesel fuel varying greatly based on the supplier location, the supplier itself and even the batch year [241]. To make

a conservative assessment of the autoignition risks, the minimum value calculated for each test case was taken into consideration for the following analysis.

For all test cases presented in **Table A-9**, the lower limit of the droplet lifetime is predicted to be inferior to the smallest autoignition time. This occurs at higher gas Weber numbers when the atomization level is high and is expected to generate smaller droplets as discussed in *section 2.1.4*. This indicates that autoignition is likely to occur for those conditions and that extra measures should be taken to decrease the risk. Therefore, a water injector was installed downstream of the measurement zone to quickly cool down the fuel-air mixture. Furthermore, it is recommended to not conduct HTP experiments for $We_g \geq 2000$ with the conditions of test case 6 considering the minimum autoignition time and droplet lifetime are in the same order of magnitude.

The autoignition times calculated were then used to determine the optimal position of the water injection system and the maximum length of the optical windows. The maximum residence length $L_{residence}$ must be inferior to the autoignition length $L_{autoignition}$, which can be estimated using equation (A-20).

$$L_{residence} < [L_{autoignition} = (u_p)\tau_{autoignition}] \quad (A-20)$$

Where u_p is the velocity of the droplets inside the test section, which can be estimated conservatively by using the minimum value of the jet velocity u_{jet} . It can also be estimated using the minimum value of the gas velocity u_g or the minimum average value of both velocities ($u_{avg} = 0.5(u_{jet} + u_g)$). **Table A-10** presents the minimum autoignition lengths for test cases 3, 5 and 6.

Table A-10: Minimum autoignition lengths for test cases 3, 5 and 6.

Case #	P_g [bar]	T_g [K]	$\tau_{autoignition}$ [ms]	u_p [m/s]*		$L_{autoignition}$ [mm]
4	4	600	21	u_g	49	1149
				u_{jet}	8	192
				u_{avg}	29	670
5	15	450	19	u_g	22	428
				u_{jet}	8	160
				u_{avg}	15	294
6	15	600	6	u_g	26	154
				u_{jet}	8	50
				u_{avg}	17	102
* Minimum values shown for u_{jet} , u_g and u_{avg}						

The autoignition lengths calculated with the jet velocity are smaller than the observation lengths that have been used in the literature for high-temperature experiments [e.g. 48, 119]. Thus, using the jet velocity to determine the maximum test section length might be too conservative. On the other hand, the gas velocity is deemed not conservative enough based on the significantly longer lengths calculated. Therefore, the intermediate option (i.e. calculating the autoignition length using the minimum average velocity) was considered instead to guide the test section design.

Regardless of how the droplet velocity is calculated, the autoignition length is the smallest for test case 6 at 102 mm when using the minimum average velocity. Compared to the other test cases, test case 6 limits the observation length significantly. Thus, it was decided to prioritize having a longer measurement zone by limiting the test points of test case 6. This decision was also justified by the fact that the test points at the minimum velocities, which have the highest autoignition risk, are mainly in the non-turbulent jet regime. Considering the latter is not the region of interest for future experimental studies on LJIC, not including those test points in the experimental campaign has no significant impact on the value of the datasets produced.

Therefore, the measurement length of 75 mm selected to avoid droplet impingement on the optical windows is deemed suitable compared to the autoignition length, as it results in a safety factor of 1.4. The distance from the fuel injector to the water injection nozzle $L_{water\ injection}$ was set to 110 mm. This is the closest position away from the injector that allows the insertion of a water nozzle inside the test section without compromising the structural integrity of the windows.

As previously mentioned, further precautions should be taken with test case 6 by limiting the test points selected for the experimental campaign and injecting water for a few conditions. To be conservative, it is recommended to exclude the test point with an autoignition length calculated using u_{jet} inferior to a specified safety length L_{safety} defined below.

$$L_{safety} = (SF) L_{water\ injection} \quad (A-21)$$

Where SF is the factor of safety, which was set to 1.5. Thus, it is not recommended to test the combinations of momentum flux ratios and gas Weber numbers shown in **Figure A-24** that have $L_{autoignition} < 165$ mm under the conditions of test case 6 due to their higher risk of autoignition. It is also recommended to activate the water injector near the test section exit for combinations of We_g and J that have an autoignition length $L_{autoignition}$ calculated with u_{jet} inferior to the position of the back pressure valve (where water is also sprayed).

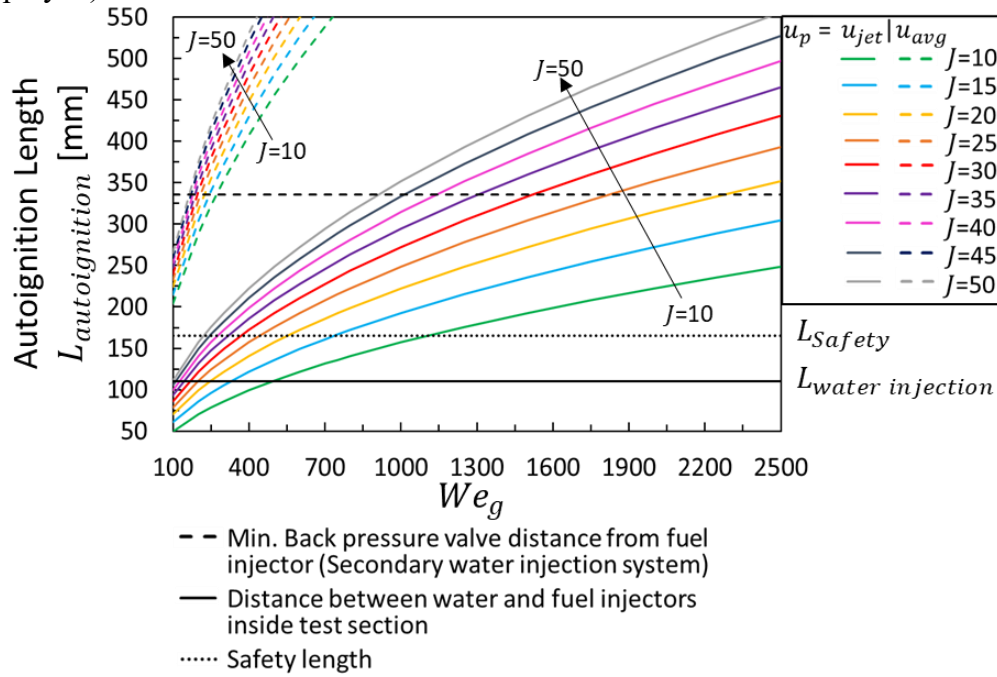


Figure A-24: Autoignition length for potential test points as a function of the momentum flux ratio and gas Weber number for test case 6.

A.9 Conclusion and Future Work

The bespoke experimental rig facility designed could be used for further studies on LFJIC at representative gas turbine conditions over a wide range of pressures, temperatures and atomization levels. The rig was designed with versatility in mind to make sure it could be suitable for a wide variety of spray research projects. In fact, the rig can accommodate different fuels, different types of atomizers as well as different measuring techniques and instrumentation. Future work using the experimental rig facility developed should be done to:

1. Conduct high-quality experiments to generate LFJIC datasets with the custom generic plain orifice injector designed for the test points selected.

2. Investigate the primary breakup, secondary breakup, spray propagation and evaporation processes of turbulent LFJIC using the generated datasets.
3. Extract empirical correlations to predict the Sauter-Mean Diameter (SMD), spray trajectory and column breakup point.
4. Perform additional evaluations, validations, and development work of the numerical modelling approaches previously presented in the core research chapters using the post-processed data obtained from experiments.