

Use of Methanol as a Potential Alternative Fuel in a Power Generation Gas Turbine

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Abstract. Decarbonisation and emissions reduction have become major priorities in industrial power generation. Achieving net-zero greenhouse gas emissions requires adopting alternative fuels such as ammonia, hydrogen, and alcohols, with methanol emerging as a promising candidate. This study investigates the feasibility of using methanol in the SGT5-2000E gas turbine at Killingholme Power Station by modelling the combustion performance of a Siemens Energy Dry Low NO_x (DLN) Hybrid Burner, capable of liquid and gaseous fuel operation. A dual-phase strategy is proposed: initial liquid methanol firing to generate sufficient heat for a Waste Heat Recovery (WHR) system, followed by a transition to evaporated methanol. This approach could reduce fuel consumption by 5–6% and reduce NO_x emissions. Chemical kinetics modelling of evaporated methanol combustion showed a potential 10% NO_x reduction compared to methane, alongside challenges such as increased flashback risk and higher autoignition potential. A key challenge was the increased fuel injection pressure drop due to methanol's higher mass flow. A RANS (Reynolds-Average Navier-Stokes) CFD (Computational Fluid Dynamics) model was developed, showing that non-uniform nozzle modifications most effectively improved mixing, lowered peak flame temperatures, reduced flashback risk, and significantly decreased NO_x emissions. The results highlight the potential for retrofitting turbines for low-carbon bio- and e-methanol combustion, supporting greener energy solutions and longer turbine life. The methanol dual-phase concept shows strong promise for further development.

1 Introduction

Decarbonisation is a critical challenge in the power generation sector. Renewable energy sources, including wind and solar, lack the flexibility provided by dispatchable power sources like gas turbines. Transitioning these engines to operate on green carbon-free fuels such as hydrogen and ammonia, can play a vital role in reducing carbon emissions. Other promising alternatives include carbon-based biodiesels, bio-alcohols, and e-alcohols, all offering significant CO₂ reduction potential. These fuels are already available at large scale, unlike hydrogen and ammonia, which remain distant from widespread use in power generation gas turbines. A recent test on a similar machine to the one analysed in this paper, owned by Uniper, demonstrated the successful replacement of diesel with hydrotreated vegetable oil (HVO) in liquid-fired gas turbines, as reported by Runyon et al. [1].

This study focuses on the Killingholme Power Station as a case example. Currently, the plant operates as an Open Cycle Gas Turbine (OCGT) facility under the capacity market framework, ensuring sufficient electricity supply during peak demand periods. The station consists of four Siemens Energy SGT5-2000E gas turbines equipped with lean-premixed Siemens Energy Hybrid Burners, running on natural gas. It delivers a combined electrical output of approximately

600MW. The performance parameters of this gas turbine are presented in Table 1.

Table 1. Siemens Energy SGT5-2000E gas turbine specification [2].

Simple cycle power output (MW)	198
Gross efficiency (%)	37.6
Pressure ratio	12.8:1
Exhaust mass flow (kg/s)	558
Exhaust temperature (°C)	536

Table 2. Representative burner inlet conditions and total gas turbine mass flows at base load.

Compressor discharge pressure (bar)	11.2
Compressor discharge temperature (K)	608
Fuel (natural gas) temperature (K)	293
Fuel (natural gas) LHV (MJ/kg)	47.1
Fuel (natural gas) net mass flow (kg/s)	9.2
Compressor outlet (air) mass flow (kg/s)	513
Fuel Supply Pressure (bar)	18

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However, engines in Killingholme Power Station are a different variant of SGT5-2000E characterized by power output to the grid of around 150MW. For purposes of this study the representative conditions for the machines located in Killingholme Power Station are presented in Table 2.

This study investigates the use of methanol, in both vapor and liquid phases, as a potential fuel for application in Siemens Energy Hybrid Burners capable of accommodating different fuel states. Abbott et al. [3] previously investigated ethanol as a preliminary candidate among alcohol-based fuels for gas turbines. Their results showed that the existing burner could operate on both natural gas and evaporated ethanol in a lean premixed regime without hardware modifications. They also found that NO_x emissions would remain comparable when operating at equivalent flame temperatures with either natural gas or evaporated ethanol.

However, the higher flame speed of ethanol is increasing flashback risk. Nonetheless, comparisons with similar burner systems operating on natural gas/hydrogen blends, as shown by Blaette et al. [4], indicated that a sufficient flashback margin remains. A modest firing temperature reduction could restore this margin, supporting the feasibility of ethanol operation under controlled conditions.

Caputo [5] further studied ethanol use at the same power plant, using a detailed burner model and evaluating ethanol/water/methanol blends to partly address alcohol taxation. A perfectly stirred reactor model showed a 69% increase in NO_x emissions compared to methane, with only slight reductions from contaminants. Despite technical feasibility, evaporated ethanol operation offered limited emissions benefits due to higher NO_x levels, greater flashback risk, and slightly poorer fuel–air mixing.

This paper explores methanol's potential as an alternative fuel, focusing on its unique chemical and thermodynamic properties. Methanol combustion produces more water vapor, promoting reaction quenching and reducing NO_x emissions, as reported by Kliemke and Johnke [6]. Methanol's complete miscibility with water and low heating value help lower flame temperatures and improve thermal efficiency, but its low lower heating value (LHV) requires higher fuel mass flow to maintain base-load performance. This study builds on earlier feasibility assessments to evaluate methanol's combustion performance in the same burner configuration and identify operational advantages and challenges.

1.1 Methanol as a Fuel

Methanol is a promising alternative to fossil fuels, with lower CO₂ emissions and wide flammability limits, but its environmental impact depends heavily on the production method. When derived from renewable feedstocks and supported by carbon capture and storage (CCS), methanol's life-cycle emissions can be significantly reduced. For renewable fuels like biofuels and e-fuels, only production-related emissions matter, and methanol can cut CO₂ emissions by 50% to nearly

100% compared to natural gas based on data available in [7], highlighting its strong potential for near-term power sector decarbonisation.

Compared to hydrogen, methanol offers much higher volumetric energy density, a safer flammability range, and simpler storage at ambient conditions (20°C, 1bar), whereas hydrogen needs high pressures (up to 700bar) or cryogenic temperatures (−253°C) [7]. Although methanol's lower LHV (about 2.5 times less than methane) demands higher volumetric flow rates to match energy output, leading to greater pressure losses, these challenges can be managed with fuel system modifications for efficient and safe operation.

1.2 Availability of Methanol

Fuel availability is crucial for the viability of alternative fuels, particularly for industrial gas turbines, which consume several kilograms per second. As of 2023, global methanol production was around 0.8 million tons per year [8], with significant growth expected due to expanding renewable methanol initiatives. Currently, 220 renewable methanol projects are underway worldwide, projected to boost production to 19.5 million tons by 2027 and 47.2 million tons by 2030, mainly from renewable and low-carbon sources [8]. Power-to-Fuel technologies will drive this growth, with e-methanol reaching 20.6 million tons, bio-methanol 16.5 million tons, and low-carbon ("blue") methanol 10.1 million tons annually by 2030. According to the Methanol Institute, this expansion reinforces methanol's potential as a fossil fuel alternative, particularly for peak-load power generation where fuel flexibility and availability are essential.

1.3 Methanol use in Gas Turbines – Past Experience

Methanol's historical use in power generation gas turbines is notable, with several experimental and numerical studies examining its combustion, particularly in diffusion flames. A key early study by von KleinSmid et al. [9] in 1981 involved a 26MW gas generator operating on methanol alongside a Jet A fired machine. Methanol combustion reduced NO_x emissions by 75% compared to Jet A and 59% compared to natural gas, without requiring additional equipment like water injection. It also lowered exhaust temperatures, allowing a 10% power increase without compromising turbine lifespan. However, its lower energy density demanded larger storage and fuel handling systems to maintain equivalent heat input.

The latest study by Siemens Energy, reported by Clifford et al. [10], investigated the 20MW SGT-A20 aeroderivative engine operating in diffusion-mode liquid fuel systems through both simulations and experiments. Simulations compared methanol with diesel, while experiments tested methanol against kerosene on a newly commissioned engine. Modelling showed that methanol increased power output by 10.8% and efficiency by 4.2%, driven by higher exhaust mass flow and altered exhaust composition. To accommodate

methanol's higher pressure drop and flow requirements, injector modifications were made doubling the number of injection holes and enlarging the fuel passages increasing flow capacity by 1.95 times [10]. These adjustments maintained droplet sizes comparable to Viscor (surrogate to diesel oil). CFD simulations showed that methanol's high reactivity and flame speed shifted flame stabilization inward, lowered flame temperatures, and improved cooling effects.

Final engine tests compared bio-methanol and kerosene under constant power conditions, focusing on emissions. Methanol achieved up to 80% lower NO_x, 15% lower CO, and 10% lower CO₂ emissions, while bio-methanol reduced the lifecycle CO₂ footprint by 60%, highlighting significant environmental benefits. The observed performance improvements were mainly attributed to methanol's higher mass flow rate, which increased turbine throughput and power output at a given pressure ratio. Under constant power operation, this higher mass flow reduced overall fuel consumption, leading to lower direct CO₂ emissions. These results confirm methanol's strong potential for simultaneously improving efficiency and reducing emissions in aeroderivative gas turbines.

These findings highlight methanol's potential as a low-carbon alternative fuel. While most research has focused on liquid-phase methanol, this study explores the largely unexamined use of vapor-phase methanol in DLN systems, which could further reduce emissions through improved fuel-air mixing.

1.4 Methodology

The feasibility of methanol utilization in the analysed gas turbine was assessed using the methodology shown in Fig. 1.

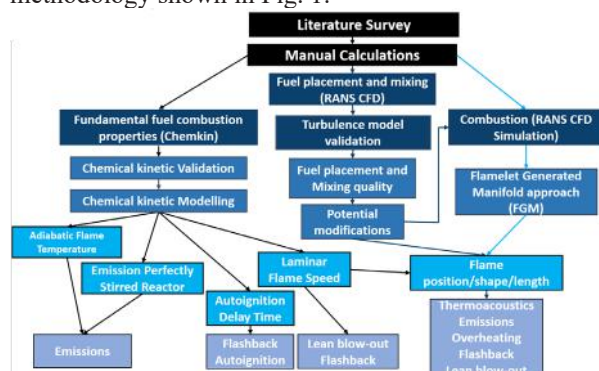


Fig. 1. Overview of the methodological framework employed to achieve the research objectives of the project.

The study began with a comprehensive literature review, summarized in the introduction, followed by a manual evaluation of the 'Dual Phase' firing concept, discussed in the next section. The analysis was structured into three key areas: chemical kinetics; mixing and fuel placement; and combustion modelling using CFD. The work focused on critical challenges associated with using a more reactive fuel like methanol, including emissions, autoignition behaviour, flashback risk, lean blowout limits, and burner overheating. Thermoacoustic effects were also considered, based on insights from previous methane/hydrogen blend studies.

2 Dual-Phase Firing Concept

The Dual-Phase firing concept builds on several key aspects. The Siemens Energy SGT5-2000E gas turbine is designed for dual-fuel operation on natural gas and diesel oil No. 2, using Siemens Energy Hybrid Burners, as shown in Fig. 2. The turbine features two silo combustors, each housing eight hybrid burners.

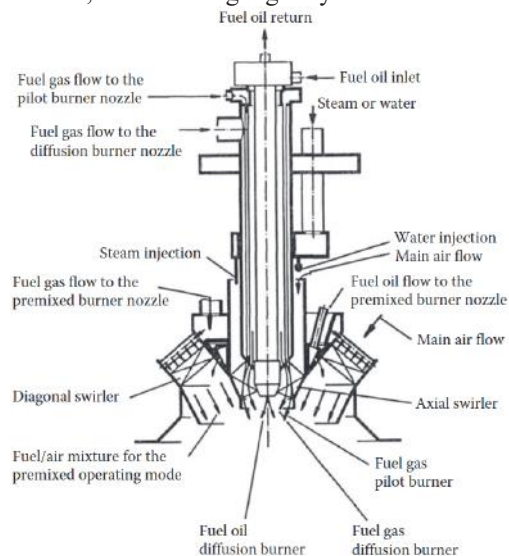


Fig. 2. Schematic of the Siemens Energy Hybrid Burner [11].

The dual-phase concept assumes that the turbine initially fires on liquid methanol to generate sufficient heat in the exhaust gases to enable methanol evaporation through a heat exchanger. Once enough heat is available, operation transitions to gaseous methanol, improving fuel-air mixing and reducing emissions. Switching to evaporated fuel simplifies mixing, as both air and fuel are in the same phase, and eliminates the evaporation time, increasing residence time in the mixing duct. A simplified schematic of the fuelling system is shown in Fig. 3. For this part of the study, basic estimations were made regarding the required modifications to the fuel oil injection system, along with calculations of their impact on the Sauter Mean Diameter (SMD) and evaporation rate during methanol firing.

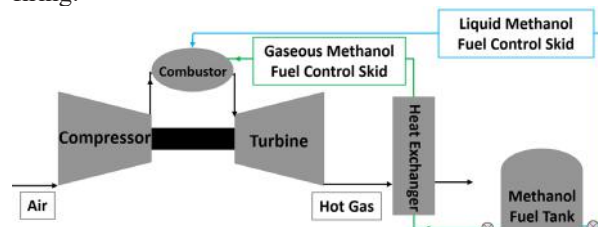


Fig. 3. Simplified scheme of the cycle arrangement for evaporated methanol firing.

2.1 Calculations of Sauter Mean Diameter

For the burner analysed in this study, Schetter et al. [12] reported a SMD of 25μm for diesel oil. To estimate the SMD for methanol, two empirical correlations were used, shown in Equations (1) and (2), as proposed by Lefebvre and McDonell [13] for liquid fuel injection in a jet-in-crossflow configuration.

$$SMD = 37 \left(\frac{\sigma \mu_L d_0}{\rho_A U_R^3 \rho_L} \right)^{0.25} \quad (1)$$

$$SMD = \frac{d_0}{0.267 \left(\frac{\rho_A U_R^2 d_0}{\sigma} \right)^{0.44} \left(\frac{\rho_L}{\rho_A} \right)^{0.3} \left(\frac{\mu_L}{\mu_A} \right)^{-0.16}} \quad (2)$$

Where: d_0 is orifice diameter, U_R is relative velocity of air to liquid, μ is dynamic viscosity, ρ is density. Subscripts L stands for liquid fuel, and subscript A stands for air. Methanol and diesel properties were sourced from [13,14] and [13,15], respectively.

Equation (2) provided results more consistent with the reference SMD reported by Schetter et al. [12] and was therefore used for further analysis. Using this correlation, it was found that methanol would produce droplets approximately three times smaller in SMD than diesel under the same geometric conditions. To maintain equivalent pressure loss and heat input, the methanol injection nozzle diameter would need to be increased by a factor of 1.5 compared to a standard diesel injector. Even with this adjustment, methanol's SMD remained 2.6 times smaller than diesel's without injector changes.

For further calculations, it was assumed following Lefebvre and McDonell [13] that both the heat transfer number and mass transfer number are equal. It was found that methanol's transfer number is roughly 2.5 times that of diesel, based on referenced properties. This indicates that methanol would evaporate more readily under turbine conditions, making evaporation less of a limiting step and allowing more time for fuel-air mixing. Improved mixing reduces rich zones, promoting uniform combustion and significantly lowering NO_x emissions.

However, further experimental research is essential, as spray dynamics are complex and secondary atomization, along with droplet size distribution beyond SMD, can heavily influence combustion behaviour.

2.2 Calculations of Required Heat for Evaporation

Another critical factor is assessing the heat required for fuel evaporation. According to Kliemke and Johnke [6], to prevent droplet formation in the fuel system, the burner fuel inlet temperature should be at least 15K above the evaporation point. For this analysis, a fuel supply pressure of 18 bar was assumed for the gaseous phase, requiring a methanol supply temperature of 452K.

Table 3. Heat Required for Evaporation of Ethanol and Methanol

Fuel	Heat required for evaporation [MW]	Heat required for superheating [MW]	Total heat required [MW]
Ethanol (467K)	18.5	0.7	19.2
Methanol (452K)	23.7	1.4	25.1

The heat required for ethanol evaporation was calculated using a heat balance approach and closely matched the reference modelling results by van Eil [16],

confirming the methodology's accuracy. Based on this verification, the same method was used to determine the heat requirements for methanol, with results summarized in Table 3. Analyses were based on pure methane as a baseline, adjusting ethanol and methanol mass flow rates to match the natural gas energy input on a LHV basis. The results suggest that implementing waste heat recovery could reduce methanol consumption by approximately 5–6%, improving overall fuel efficiency.

3 Chemical Kinetics

In this chemical kinetics study, key parameters including adiabatic flame temperature (AFT), laminar flame speed (LFS), and autoignition delay time (ADT) were evaluated under relevant operating conditions using Ansys Chemkin 2023R2. To maintain consistency with previous studies [3,16], the CRECK_2003_C1_C3_HT_NOX mechanism [17] was selected, as it showed good agreement with experimental data as reported by Harman-Thomas et al. [18].

3.1 Modelling Results

To investigate conditions representative of the analysed burner, chemical kinetics models were used to calculate the LFS, AFT, and ADT. Ethanol-related values were sourced from Abbott et al. [3] for ADT and Caputo [5] for AFT and LFS.

Fig. 4 shows the adiabatic flame temperature as a function of equivalence ratio for two cases: the premixed main burner (near an equivalence ratio of 0.5) and the diffusion flame region of the pilot burner (stoichiometric conditions). To match the mean base load flame temperature (1773K) reported by Prade et al. [11], methanol requires slightly leaner conditions (equivalence ratio 0.49) compared to methane (0.53), with a similar trend observed when compared to ethanol.

Under stoichiometric conditions, methanol combustion produces flame temperatures about 10K lower than methane and 18K lower than ethanol. This lower flame temperature suggests that methanol would generate reduced thermal NO_x emissions during diffusion flame operation.

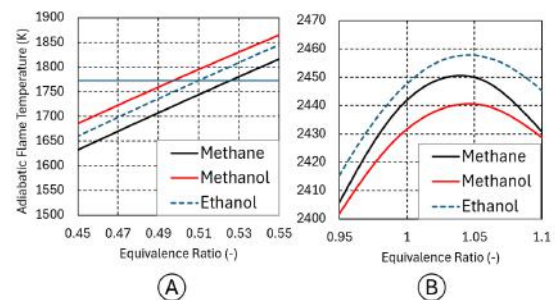


Fig. 4. Adiabatic flame temperature as a function of equivalence ratio for analysed gas turbine conditions. (A) lean conditions and (B) stoichiometric conditions. Ethanol data taken from Caputo [5].

The next parameter analysed is laminar flame speed (LFS), shown in Fig. 5 as a function of

equivalence ratio and in Fig. 6 as a function of AFT. Under lean conditions (equivalence ratios 0.4–0.8), methanol and ethanol exhibit similar LFS values, both significantly higher than methane. At an equivalence ratio of 0.5, methanol and ethanol show LFS values about 76% higher than methane, reducing lean blow-out risk but increasing flashback potential.

Under stoichiometric conditions, methanol's LFS is 43% higher than methane's and 12% higher than ethanol's. The largest difference occurs at an equivalence ratio of 1.25, where methanol's LFS is 166% higher than methane's and 74% higher than ethanol's, indicating a consistently higher flashback risk, especially under rich conditions.

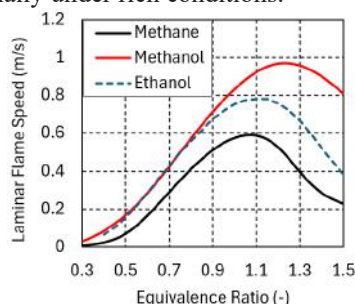


Fig. 5. Laminar flame speed as a function of equivalence ratio for analysed gas turbine conditions. Ethanol data taken from Caputo [5].

These results highlight the need for a well-designed mixing system in lean premixed turbines. For typical operating points equivalence ratios of 0.5 (main burner) and 1.0 (pilot) methanol's LFS is 142% and 44% higher than methane's, respectively. Although properly designed systems minimize the risk of local rich zones, such conditions could significantly increase flashback risk, particularly near the mixing duct exit, emphasizing the critical role of precise mixing design for stable combustion.

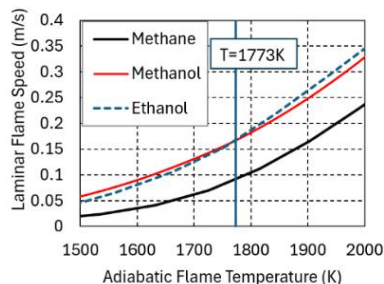


Fig. 6. Laminar flame speed as a function of adiabatic flame temperature for analysed gas turbine conditions. Ethanol data taken from Caputo [5].

Fig. 6 shows the relationship between laminar flame speed and adiabatic flame temperature for a homogeneous mixture. Under lean conditions at 1773K, the LFS for methanol is about 74% higher than that for methane, which leads to a higher flashback risk. At this temperature, methanol and ethanol exhibit similar laminar flame speeds of around 0.17m/s. In the low-temperature range, ethanol's flame speed is slightly lower than methanol's, but between 1800K and 2000 K, ethanol surpasses methanol. Overall, the results indicate a higher flashback risk with methanol and ethanol

compared to methane, while reducing the likelihood of lean blow-off.

Fig. 7 shows autoignition delay times for pure methanol, ethanol, and methane at lean conditions (equivalence ratio 0.5) Fig. 7 (A) and stoichiometric conditions Fig. 7 (B). Three vertical lines indicate key operational temperatures: flame temperature (1773K), compressor discharge temperature (608K, from Table 2), and burner corner recirculation zone temperature (1023K). The 1023K value is based on Eroglu et al. [19], who highlight that shorter ignition delays can trigger periodic flashes within the mixing zone, potentially progressing into steady flashback. In these areas, flame stabilization relies heavily on external recirculation, where hot gases interact with the fuel–air mixture. Local slower flow rate in the downstream direction within the mixing zone caused by flow disturbances or boundary layers can significantly influence emissions, thermoacoustic stability, and component durability.

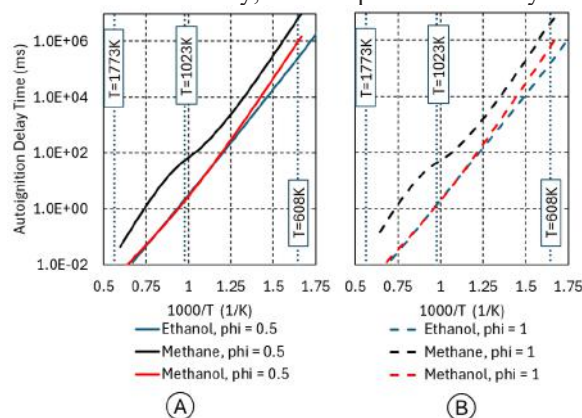


Fig. 7. Autoignition time delay as a function of 1000 divided by adiabatic flame temperature for (A) lean combustion (equivalence ratio equal 0.5), and (B) stoichiometric combustion at analysed gas turbine conditions. Ethanol data taken from Abbott et al. [3].

Under lean conditions (equivalence ratio 0.5), it can be observed that at 1023K, methanol and ethanol ignite about 28 times faster than methane. At 608K, methanol's ignition delay is seven times shorter than methane's but four times longer than ethanol's. At 1023K under stoichiometric conditions, methanol and ethanol exhibit ignition delays approximately 34 times shorter than methane. At 608K, methanol ignites about six times faster than methane but is still four times slower than ethanol. Given that ignition delays at 608K are on the order of hundreds of seconds, and residence times in industrial combustors are typically 10–20ms [20], autoignition in the mixing zone is unlikely under turbine conditions. These trends indicate that while ignition delay varies with temperature, it is not strongly influenced by equivalence ratio.

NO_x emissions were evaluated using a Perfectly Stirred Reactor (PSR) model in Chemkin with a 15ms residence time. As shown in Fig. 8, at a flame temperature of 1773K, methanol produces about 80% less NO_x than ethanol and around 10% less than methane. These results suggest methanol can slightly reduce NO_x emissions compared to methane and significantly outperform ethanol, making it a more favourable option for low NO_x combustion.

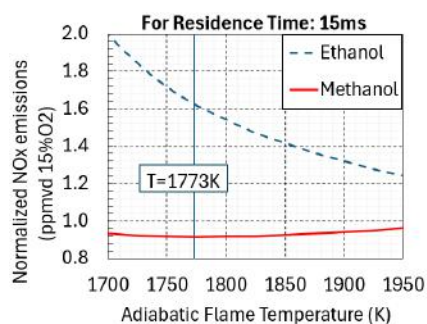


Fig. 8. Normalized NO_x emissions for methanol and ethanol in a PSR (15ms residence time), referenced to methane.

However, this analysis has several limitations. The PSR model assumes adiabatic conditions, while real combustors experience heat losses that significantly affect NO_x formation. Capturing these effects would require detailed combustor data, including cooling air distribution and heat transfer characteristics. A more realistic approach would involve a reactor network model, but this also depends on comprehensive system information. More significant limitation is the imperfect mixing in practical "premixed" burners. Since NO_x emissions are highly sensitive to mixing quality, as noted by Leonard and Stegmaier [21], actual emissions are likely significantly higher than those predicted by the idealized PSR model which only provides comparative indication of how difficult it will be to design a low NO_x burner for different fuels.

4 CFD Study

ANSYS Fluent 24R1 was used for this part of the analysis with double precision. Fig. 9 shows the computational domain, with red dashed lines marking mass flow inlets and a blue dashed line indicating the pressure outlet.

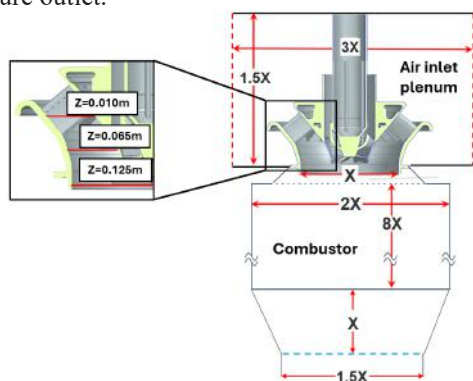


Fig. 9. Computational domain used in CFD simulation of mixing and combustion.

Based on prior chemical kinetics analysis, achieving a burner temperature of 1773 K with methane requires an equivalence ratio of approximately 0.53, corresponding to 17.7 kg/s of air and 0.54 kg/s of methane per burner. The boundary conditions applied were: a mass flow inlet at the injection nozzles and at the air inlet (red dashed line at the plenum inlet), and a pressure outlet at the exhaust (blue dashed line). All remaining domain surfaces were treated as adiabatic walls. For methanol, maintaining the same heat input

results in an equivalence ratio of about 0.49 and a fuel flow of 1.36kg/s. Following Prade et al. [11], 10% of the fuel was allocated to the pilot burner, and 90% to the main burner.

For spatial discretization, a second-order upwind scheme was used, with velocity–pressure coupling handled using the segregated flow algorithm SIMPLEC. For wall treatment scalable wall function has been utilized. Scalable wall functions maintain consistent performance across different grid refinements, preventing the deterioration observed with standard wall functions when $y^+ < 11$ (non-dimensional distance from wall). For coarser grids, the behaviour of standard wall functions remains unchanged.

Default values were used for the turbulent Prandtl number (0.85) and turbulent Schmidt number (0.7) in the mixing and energy equations, as these are considered appropriate for hydrocarbon fuels like methane and methanol, according to Swaminathan and Bray [22]. Used approach for closure of turbulence-chemistry interaction has been used finite-rate flamelet source.

Polyhedral cells were used for spatial discretization, combining hexahedral accuracy with tetrahedral ease. They improve mesh quality, enhance stability, reduce numerical diffusion, capture gradients more accurately, and are less sensitive to mesh stretching, making them ideal for complex flows. Validation of the most suitable turbulence model for jet-in-crossflow physics that is utilized for mixing has been presented by Harman-Thomas et al. [18]. Based on that it was found that Realizable k- ϵ is more suitable turbulence model for this application.

4.1 Grid Sensitivity Study

For the mesh sensitivity study, mixing and combustion were treated separately. The grid sensitivity cases used methane as the reference fuel. Mesh refinement for the mixing study followed the pattern shown in Fig. 10, while the refinement pattern for combustion is presented in Fig. 14.

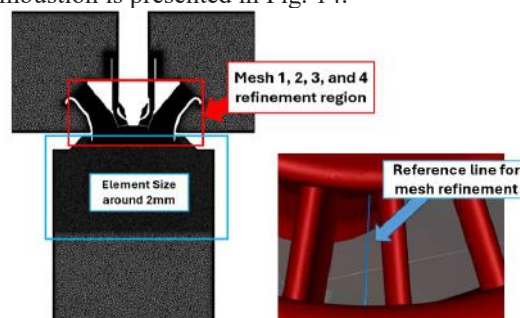


Fig. 10. On the left : mesh refinement for mixing CFD sensitivity study, on the right: location of the reference line between two trailing edges of swirling vanes.

All meshes were generated with a minimum orthogonal quality of about 0.10 (average 0.97) and a maximum skewness of about 0.90 (average 0.03) for both studies. The number of elements for the mixing meshes were 16.0, 19.9, 24.0, and 36.0 million for Meshes 1, 2, 3, and 4, respectively. For validation, velocity profiles in all directions, as well as temperature and the local fuel mass fraction normalized by the

maximum value from the coarsest grid, were inspected along the reference line shown in Fig. 10, located between the trailing edges of the two swirler vanes.

Regarding the results of the mesh refinement study, velocity profiles in three directions are not shown here, as all lines exhibited the same magnitude and trend. The main differences were observed in the fuel mass fraction, where Meshes 3 and 4 showed similar behaviour, with element sizes in the mixing duct ranging from 0.5 to 1.5 mm, as illustrated in Fig. 11. These results indicate that the mesh is sufficiently fine to capture proper mixing. To further validate the mesh sensitivity study, an additional analysis of “unmixedness” defined in Equations (4) and (5), was carried out. The corresponding results are presented in Fig. 12, with planes locations shown in Fig. 9.

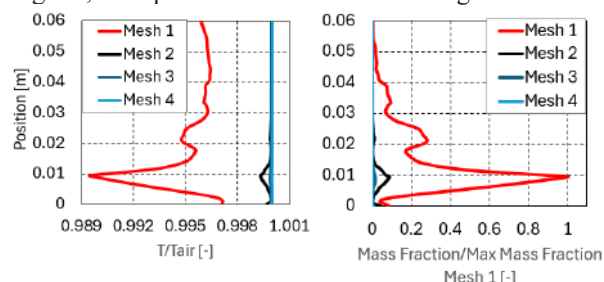


Fig. 11. Normalized mass fraction of fuel and temperature across reference line for different meshes in reference methane case.

Meshes 3 and 4 exhibit the same characteristics for this parameter across the analysed planes, while Mesh 2 also shows similar trends and values. Based on these observations, Mesh 3 was selected for the mixing quality analysis.

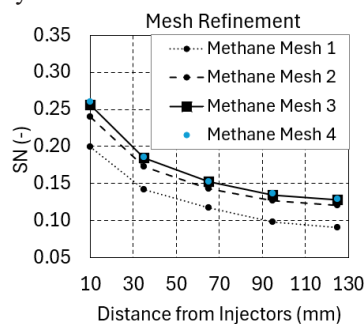


Fig. 12. Normalized unmixedness parameter for different meshes in reference methane case.

For the final verification of the numerical methods, Fig. 13 presents the y^+ values along the burner walls. The values range from near 0 up to 300, with the main region of interest around 120-150, indicating a proper numerical approach for applying the scalable wall function with the grid settings used in Mesh 3.

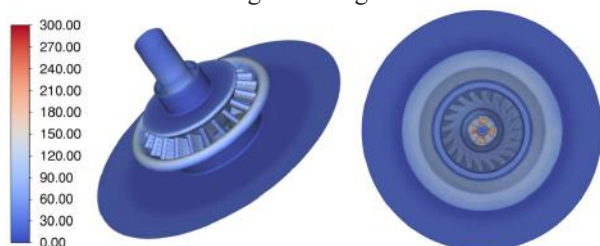


Fig. 13. Final mesh (Mesh 3) y^+ contour on burner walls.

The meshes used in the combustion sensitivity study contained 28.8, 21.9, 33.6, and 40.3 million elements for Meshes 1, 2, 3, and 4, respectively. The difference in element count between Meshes 1 and 2 is mainly due to different refinement region approaches, although both are characterized by the same element size within the refinement region, as shown in Fig. 15.

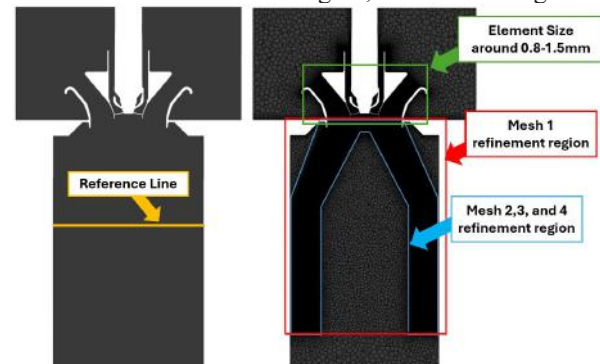


Fig. 14. Mesh refinement for combustion CFD sensitivity study.

A coarser mesh near the axis shows trends consistent with denser meshes, although small differences in the flame front are observed. The mesh size in the mixing duct was kept the same for all meshes and set slightly larger than in the grid used for the fuel mixing quality study, but close to the reference values between Meshes 2 and 3 from the non-reactive flow mesh-independence study. This choice reduced computational cost while maintaining results comparable to the non-reactive mixing study.

To quantify the combustion simulations, two parameters were analysed along the reference line shown in Fig. 14: the progress variable and normalized temperature defined as the local temperature divided by the mean flame temperature. The results of this mesh sensitivity study are presented in Fig. 15. All meshes yielded comparable values with only slight shifts in flame position. Following best practices where the flame region elements are finer than those in the mixing duct and given the similarity of results, the finest mesh (Mesh 4) was selected for the combustion study, as it also reproduced the flame location trends observed with denser meshes.

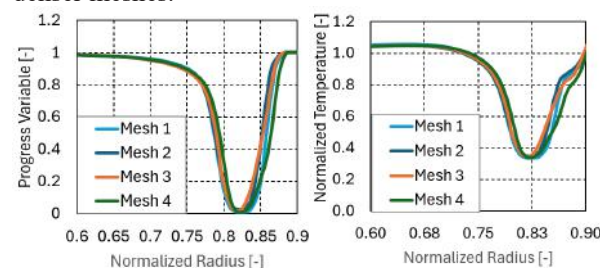


Fig. 15. Progress variable and normalized temperature across left side of reference line for different meshes in reference methane case.

4.2 Fuel-Air Mixing Quality Study – Non-Reactive Flow

The computational domain used for the CFD mixing analysis is shown in Fig. 9, along with the

previously described solver settings. Mixing quality was evaluated across five measurement planes, three of which are marked in Fig. 9. Mixing contours represent the normalized equivalence ratio, defined as the local equivalence ratio divided by the global equivalence ratio applied at the boundary conditions.

Both modified and unmodified geometries were analysed. Modifications have been applied to the main fuel injectors. For the modified cases, two approaches were used: a uniform increase and a non-uniform increase in the gaseous fuel nozzle diameter. In the non-uniform approach, the nozzle nearest the outer annulus remained unchanged, while each nozzle moving inward was increased by a factor of K , as shown in Fig. 16. The pilot injection tube's inner-to-outer radius ratio is about 0.7, with dimensions in the tens of millimetres. Increasing the pilot nozzle diameter presents engineering challenges and structural risks, making such modifications impractical. Addressing these limitations would require a full pilot system redesign, which is beyond the scope of this study. This is why the pilot burner remained unchanged.

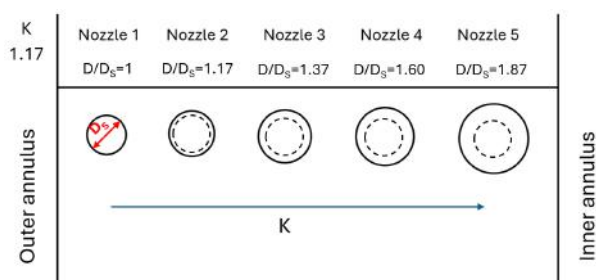


Fig. 16. Sketch of injection vane for non-uniform increase in nozzle diameter (where D_s is the standard injector diameter and D is the modified injector diameter).

However, this approach may introduce thermoacoustic instability risks, as noted by Witzel [23], due to changes in the radial fuel distribution. Since no detailed stability margin is available for this burner type, a full feasibility assessment would require thermoacoustic modelling. For this study, it is assumed that the modifications do not significantly impact burner stability or lead to combustion-driven instabilities.

Fig. 17 and 18 show a cross-sectional view of the domain and the mixing duct outlet contour of the normalized equivalence ratio. In Fig. 17, methanol without nozzle modifications achieves nearly perfect mixing. However, with uniform nozzle enlargement presented in Fig. 18, rich zones form near the walls, resembling the unmodified methane case. Notably, rich regions near the outer annulus mixing duct outlet (highlighted with red circles) could pose a major risk when operating with more reactive fuel.

In contrast, the non-uniform nozzle diameter increase shifts fuel distribution closer to the burner axis, reducing the flashback risk in rich zones a concern previously highlighted in Fig. 5 for low-velocity regions, especially with methanol's higher flame speed.

Another observation from Fig. 18 is that in non-reactive flow, both methane (unmodified) and methanol with uniform nozzle increases ($D/D_s=1.44$) cases show higher equivalence ratios in the corner recirculation zones, potentially leading to increased NO_x emissions.

In the non-uniform configuration ($K=1.17$), lower equivalence ratios are seen in these zones, which could raise CO emissions. Additional heat losses to the burner structure and cooling effects, not captured in the model, may further increase CO levels. However, higher temperatures in the post-flame zone may promote more complete combustion after the gases leave the recirculation areas.

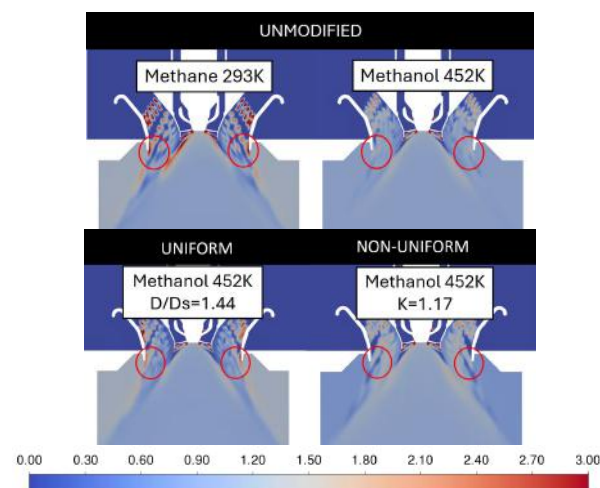


Fig. 17. Computation domain cross section contour for unmodified methane and unmodified/modified methanol fired burner of normalized equivalence ratio.

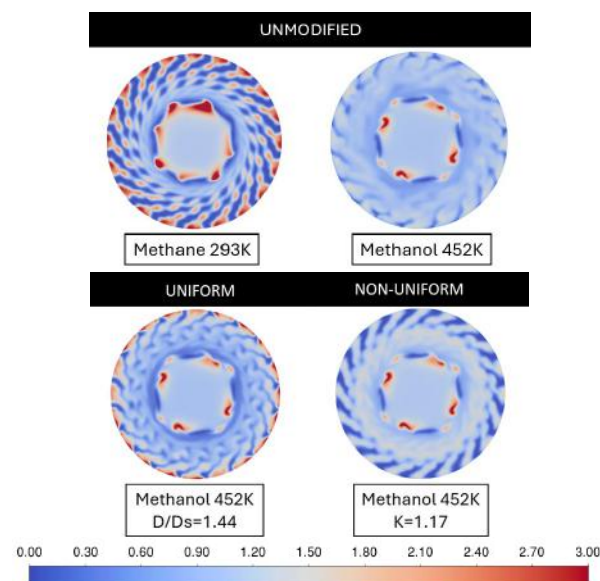


Fig. 18. Mixing duct outlet plane ($z=0.125\text{m}$) contour for unmodified methane and unmodified/modified methanol fired burner of normalized equivalence ratio.

At the mixing duct outlet contour plane shown in Fig. 18, regions closer to stoichiometric conditions, especially near the outer annulus, are more pronounced in the methanol cases. This broader distribution could increase flashback risk during transients, suggesting a need to revise power transition strategies. In all methanol cases, the pilot region's fuel distribution remains unchanged, as the pilot geometry was not modified.

Another key observation is that in methanol cases, the entire mixing duct outlet radius is filled with fuel due to the increased mass flow, indicating improved mixing

compared to the reference methane case. To quantify this, the "unmixedness" parameter defined by Hornsby and Norster [24] was applied, providing a more objective assessment of mixing quality.

$$S = \sqrt{\frac{\sum (C_i^2 M_i)}{\sum M_i} - \left(\frac{\sum C_i M_i}{\sum M_i} \right)^2} \quad (3)$$

Where: C_i is the mass fraction of fuel at cell i , and M_i is the mass flow through cell i . When $S=0$, air and fuel are perfectly mixed. Its value for fully unmixed air and fuel depends on the overall mass-based air–fuel ratio, making direct comparisons between different fuels or equivalence ratios difficult. To overcome this, Sun et al. [25] proposed a normalized unmixedness parameter, defined in Equation 5, where S_0 represents the value of S for completely unmixed air and fuel:

$$S_0 = \sqrt{\frac{1}{\left(\frac{A}{F} + 1\right)} - \left(\frac{1}{\frac{A}{F} + 1}\right)^2} \quad (4)$$

$$S_N = \frac{S}{S_0} \quad (5)$$

Here, A/F denotes the mass-based air–fuel ratio. With this normalization $S_N=1$ indicates fully unmixed conditions, and $S_N=0$ indicates perfect mixing independent of fuel type or mass flow. This enables direct comparison of mixing quality between methane and methanol. Fig. 19 shows the variation of this parameter across the measurement planes, whose locations are given in Fig. 9.

Both modifications show similar mixing behaviour to unmodified methane based on the unmixedness parameter. However, the non-uniform nozzle diameter increase with methanol provides slightly better mixing than the reference methane at 293K case, while the uniform increase with methanol results in slightly poorer mixing. Overall, both modifications exhibit poorer mixing quality compared to the unmodified geometry fuelled with methane at 452K. Increasing the D/D_s ratio or factor K reduces pressure loss across the injectors but also lowers mixing quality, potentially leading to higher NO_x emissions, as noted by Leonard and Stegmaier [21]. Still, the modified geometry fired with methanol exhibits lower mixing quality than the unmodified geometry fired with methane at 452K.

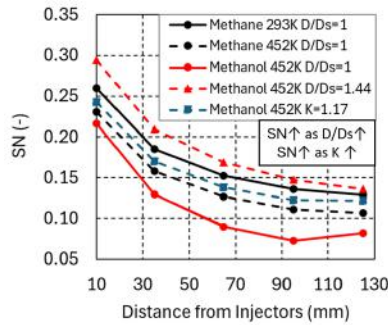


Fig. 19. Normalized unmixedness parameter for different fuels, conditions and injection nozzle modification.

An interesting observation at the mixing duct exit plane ($z=0.125$ m) is that, while unmodified methanol shows improved mixing at earlier plane, mixing quality deteriorates slightly at the mixing duct outlet. As shown

in Fig. 19, the use of the diffusion pilot increases the unmixedness of the mixture at the mixing duct exit, likely due to interactions between the main and pilot burner flows, which were not present in the earlier plane that considered only the main burner flow.

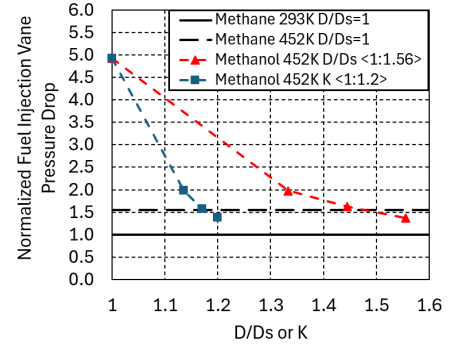


Fig. 20. Normalized fuel injection vane pressure drop for different fuels, conditions and injection nozzle modification.

Fig. 20 shows the normalized fuel injection vane pressure drop for various modifications relative to the reference methane case at 293K. Contour plots across the injection vane indicate that all modifications result in pressure losses similar to methane at the same methanol temperature (452K). However, methanol with $K=1.17$ and $D/D_s=1.44$ show slightly lower mixing quality compared to methane at 452K. Since the burner is compatible with heated fuel, and such elevated temperatures are achievable in other DLN systems (as discussed by Erickson et al. [26]), these configurations are included in the reactive flow simulations.

Overall, the results highlight the need to carefully balance mixing quality and pressure loss in methanol-based modifications, with both factors playing a critical role in emissions and combustion stability.

4.3 Combustion RANS Study

For this part of the study, the Flamelet Generated Manifold (FGM) model was selected to simulate the partially premixed burner using primary premixed flamelets. The FGM model was chosen due to its suitability for partially premixed combustion and its previous use in DLN modelling studies, such as by Wiranegara et al. [27]. The turbulent Prandtl and Schmidt numbers were set to 0.85 and 0.7, respectively, as standard values for hydrocarbon fuels. Additionally, the thermal NO_x emissions mechanism within the software has been applied. For this purpose, the NO transport equation was solved using the O-atom route of the Zeldovich mechanism (see the equations below). An equilibrium approach was adopted: the main combustion reactions are assumed to equilibrate first, and NO formation is then calculated from the resulting high-temperature equilibrium composition.



Prompt NO_x has not been investigated, since the main contribution in gas turbines is normally associated with thermal NO_x and this approach has been taken to

assess relative emissions for the different cases. However, due to the presence of rich spots observed in the mixing quality study, the contribution of Prompt NO_x , as well as the interaction of thermal NO_x through OH pathways, should ideally be considered in future studies to better account for emissions in colder and fuel-rich regions.

For turbulence–chemistry interaction, a temperature-based approach with algebraic variation using the β -PDF was applied. While this method may not provide highly accurate predictions of absolute emission values, it offers useful insight into temperature variations and their effects. Further research is therefore needed to reliably quantify emissions.

This approach was also employed to identify general trends in the formation of thermal NO_x , which remains the dominant pollutant produced by gas turbines. Additionally, heat losses must be taken into account, as they significantly affect emission rates. At the same time, incorporating heat loss influences FGM table generation, increasing its size and, consequently, the computational resources required for modelling.

The boundary conditions have been kept the same as in the previous simulations to provide the same heat input as the reference methane case to provide the mean flame temperature equal to 1773K. The combustor walls were modelled as adiabatic, which introduces limitations in accuracy, as noted by Poinso and Veynante [28]. In reality, heat losses would lower combustor temperatures, reduce NO_x emissions, and modify flame behaviour. Specifically, adiabatic walls promote flame attachment by eliminating temperature gradients, whereas non-adiabatic walls create gradients that hinder attachment and stable flame formation, with additional effects from vortex breakdown in the detachment region.

A realistic treatment of combustor wall temperature would require detailed information on cooling strategies, wall materials, and temperature distribution (factors that lie beyond the scope of this study). It is important to note that this work focuses on a numerical test case rather than a real combustor. The assumption of adiabatic walls was therefore chosen to ensure consistency across analysed cases and to facilitate comparison, as the modelled combustor is entirely theoretical and can be reasonably idealized with adiabatic boundaries.

Regarding the chemical-kinetic mechanism used in the CFD simulations, the laminar flame speed was verified using Ansys Chemkin 2023R2. For methane the GRI 3.0 [29] (325 reactions, 53 species) has been selected as it has been used in different studies like [27], and showed close agreement to detailed CRECK_2003_C1_C3_HT_NOX mechanism [17]. For methanol reduced chemical-kinetic mechanisms, three of them have been taken into account proposed by Pichler and Nilsson in [30] (55 reactions, 18 species), Liang et al. [31] (74 reactions, 19 species), and Tang et al. [32] (82 reactions, 25 species). Result of verification gas been presented in Fig. 21.

As it can be observed in terms of methane GRI 3.0 fit quite well to the values obtain in chemical kinetic study using CRECK_2003_C1_C3_HT_NOX.

However, under near-stoichiometric conditions, it underpredicts the laminar flame speed. For methanol the closest to the reference mechanism has been found to be skeletal chemical kinetic mechanism proposed by Liang. Due to these results this mechanism has been utilised in presented CFD study for methanol.

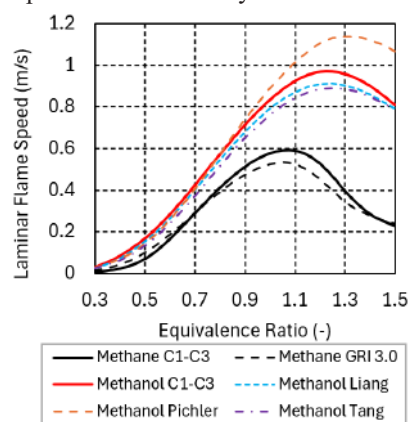


Fig. 21. Verification of reduced chemical kinetic mechanisms under turbine-representative conditions through comparison with detailed chemistry.

Based on these settings, Fig. 22 (left) shows normalized temperature contours and (right) the iso-surface of the progress variable ($c=0.8$) indicating flame surface for the analysed cases. The normalized temperature in Fig. 22 is defined as the local temperature divided by the mean flame temperature. Every methanol flame is overall shorter than the methane at 293K reference based on progress variable iso-surface.

As observed, the rich pockets in the corner recirculation zones (Fig. 18) for the reference methane case and the uniform nozzle increase for methanol result in high-temperature regions in Fig. 22, potentially increasing NO_x emissions and causing silo combustor overheating. A narrower flame cone angle is observed for the uniform nozzle increase case, due to higher flame speeds in rich zones noted in the earlier chemical kinetics study.

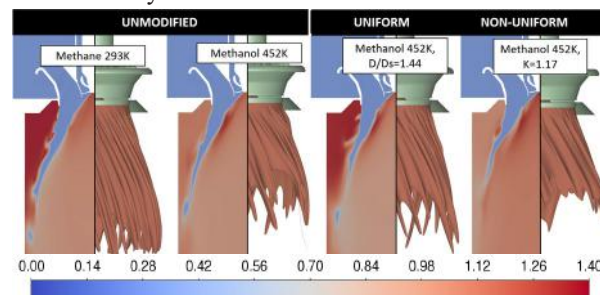


Fig. 22. On the left normalized temperature contour on the right iso-surface of progress variable ($c=0.8$) marking flame surface.

In the cases of methanol firing without modifications and with a non-uniform nozzle diameter increase ($K=1.17$), the flames are noticeably shorter compared to the other cases, though they exhibit a similar cone angle to the reference methane case. In the unmodified methanol-fired geometry, this is mainly due to near-perfect mixing, where mass diffusion has less influence on flame shape, closely resembling a perfectly premixed flame. This also leads to lower temperatures

in the recirculation and post-flame regions, contributing to reduced NO_x emissions.

In the non-uniform nozzle modification case, the shorter flame is due to a higher fuel concentration and slightly elevated equivalence ratio near the middle radius of the mixing plane (Fig. 18). While this increases post-flame temperatures, the rise is still much lower than the high temperatures observed in the recirculation zone of the reference methane case.

For emissions prediction, comparisons were made to a reference methane at 293K case by evaluating emissions at the outlet of the computational domain. The methanol-fired burner without modifications reduced NO_x emissions by 92% of the methane reference level, while CO emissions increased by 16%. A uniform increase in nozzle diameter led to a 22% rise in CO emissions and a 40% increase in NO_x emissions compared to the methane reference. In contrast, non-uniform nozzle enlargement reduced NO_x emissions by 86% of the reference level but increased CO emissions by 28% during methanol combustion.

The most effective configuration for reducing emissions and minimizing flashback risk linked to higher flame speeds near the outer wall is the unmodified methanol-fired geometry. It achieves the greatest NO_x reduction compared to the reference methane case but also shows a slight increase in CO emissions, likely due to the higher overall mass flow through the fuel passages. The 16% increase corresponds to about a 0.5 to 1ppm_{dry} increase in CO emissions. In the case of uniform nozzle diameter increase, both CO and NO_x emissions rise. This is attributed to higher fuel mass flow, poorer mixing quality, and a shorter, wider flame, resulting in larger high-temperature regions in the corner recirculation zones (as seen in Fig. 22). These results suggest that uniform nozzle enlargement may not be the best strategy for reducing emissions. With a non-uniform increase in nozzle diameter, a significant reduction in NO_x emissions is achieved, approaching the ideal mixing observed in the unmodified methanol-fired geometry. However, this configuration also results in the highest CO emissions, likely due to lower temperatures in the corner recirculation zones. This aspect will require further investigation, especially during part-load operations, when CO emissions might be higher.

Thermoacoustic behaviour is complex and typically analysed by solving linearized Navier–Stokes equations, where the mean flow is frozen and only acoustic perturbations are considered. These models, applied through 3D thermoacoustic codes or simplified 1D network models, provide valuable insights into system stability. According to Beita et al. [33], hydrogen enrichment promotes higher-frequency instabilities due to flame shortening, a trend expected with evaporated methanol. Since Killingholme’s gas turbines use large silo combustors with low-frequency modes, shorter flames could shift instabilities to higher frequencies, potentially improving stability, although combustion tuning would likely be needed when transitioning from natural gas to methanol.

5 Conclusions

The adoption of bio- and e-fuels is essential for achieving carbon neutrality by 2050. As the shift from fossil fuels to green alternatives accelerates, methanol stands out as a promising candidate. The results suggest that the dual-phase concept is a promising strategy for using methanol in power generation gas turbines. Methanol shows strong potential in SGT5-2000E turbines, particularly in evaporated form. Initial operation would require liquid methanol firing to provide evaporation heat, and simple estimates indicate that, with minor modifications for higher fuel mass flow, liquid methanol could reduce NO_x emissions compared to diesel due to its smaller droplet size and higher transfer number. However, experimental validation of spray behaviour is still needed. Using evaporated methanol could also reduce fuel consumption by 5–6% through waste heat recovery, offering additional benefits.

Additionally, focusing on its chemical structure increased flame speed, and associated with it increased risk of flashback become challenging. This required a careful modification of the system to accommodate the larger mass flow of the fuel. Uniform nozzle enlargement offered limited improvements in mixing and pressure loss reduction, and could increase NO_x emissions and flashback risk. This indicates that simply enlarging injection holes is insufficient for evaporated methanol firing. A better approach involves non-uniform nozzle modifications that direct fuel toward the burner axis, creating leaner mixtures near the walls, reducing flashback risk, improving mixing, and reducing pressure losses. Although this slightly enriches and raises temperatures on the burner axis, it effectively minimizes flashback in critical zones and helps control NO_x formation.

Combustion modelling showed that methanol produced shorter, thicker flames due to its higher flame speed, with the shortest flames achieved using non-uniform nozzle modifications. A richer central mixture combined with methanol’s high reactivity significantly reduced NO_x emissions and flashback risk, while minimizing hot spots in corner recirculation zones unlike the uniform nozzle and reference methane cases. Methanol firing can significantly lower NO_x emissions by enhancing the performance of the existing fuel injection system, improving both mixing and emissions characteristics. However, based on experimental results, a more precise evaluation of NO_x will be possible, allowing for higher accuracy when assessed using CFD simulations. This is recommended for further investigation. Overall, the results confirm methanol’s strong potential for retrofitting existing gas turbines at Killingholme Power Station, offering significant emissions improvements over the original SGT5-2000E setup.

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Use of methanol as a potential alternative fuel in a power generation gas turbine

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