

CRANFIELD UNIVERSITY

CHIARA RICCIO

IMPROVED DEPOSITION MODELLING FOR HEAT EXCHANGERS
IN PULVERISED FUEL COMBUSTORS

SCHOOL OF WATER, ENERGY AND ENVIRONMENT

PhD

Academic Year: 2018 - 2019

Supervisor: Prof. Nigel J. Simms

Associate Supervisor: Prof. John E. Oakey

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ABSTRACT

Co-firing biomass with coal is a promising and cost effective solution to reduce CO₂ emissions derived from the use of fossil fuels in existing power generation systems. However, deposition on heat exchangers (i.e. fouling and slagging) represents a major problem in power plants as it reduces boiler thermal efficiency, causes fireside corrosion and compromises the life of components until forced shutdown. The high complexity and multidisciplinary nature of this problem, which varies with boilers, fuel composition and combustion conditions, has made its prediction a major challenge.

In this thesis, Computational Fluid Dynamics (i.e. CFD) software, Ansys Fluent[®], was used and its features were enhanced with three User Defined Functions (i.e. UDFs) which were modified to predict deposit accumulation, deposit shape and surface temperature. The Eulerian-Lagrangian model was enabled to describe the gas flow field around tubes and the solid ash particle trajectories respectively. Unsteady simulations were run and the combined effect of deposit growth and surface temperature on the deposition flux calculations was included.

Experiments of co-firing Daw Mill coal-12 wt.% Miscanthus were carried out in a 100 kW_{th} pilot-scale pulverised fuel (PF) combustor at Cranfield. The flue gas temperature and composition were recorded and fly ash samples were analysed to fit the Rosin Rammler ash particle size distribution model. Moreover, deposits were collected on cooled ceramic probes to measure the deposition flux and the chemical composition.

The CFD model was applied to predict deposition on the cooled ceramic probes and the experimental results were used to set boundary conditions and to validate the model. The main challenges met in this work have been highlighted and possible solutions suggested. The model included several deposition mechanisms for ash particles and vapours and took into account the stickiness of the surface and the ash particles. Deposition has been studied for varying probe configurations and surface temperatures and the comparison between the experimental and modelling results was promising. Alkali vapour condensation enhanced the formation of deposit onto clean surfaces at lower temperatures. However, inertial impaction was the main deposition mechanism for bigger ash particles.

Keywords: Co-firing coal and biomass, fouling, particle deposition, vapour condensation, Computational Fluid Dynamics, unsteady simulations.

To my dad

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LIST OF NOMENCLATURE

Latin alphabet

A	Area	m^2
C	Concentration	kg/m^3
C_p	Specific Heat	$\text{J}/(\text{kg K})$
d	Diameter	m
D	Diffusion coefficient	m^2/s
E	Energy	J
E	Composite Young's modulus	Pa
f	Coefficient	-
F	Force	N
f	Frequency of vortex shedding	s^{-1}
g	Gravitational acceleration	m/s^2
h	Heat transfer coefficient	$\text{W/m}^2 \text{K}$
I	Inertial impaction rate	$\text{kg/m}^2 \text{s}$
k	Thermal conductivity	W/m K
m	Mass	kg
m	Deposition flux	$\text{kg}/(\text{m}^2 \text{s})$
n	Spread diameter	-
P	Probability	-
P	Pressure	Pa
$\dot{Q}$	Heat flux	W/m^2
R	Resistance	$\text{m}^2 \text{K/W}$
t	Time	s
T	Time period	s
t	Deposit thickness	m
u	Velocity	m/s
w	Perpendicular gas velocity component	m/s
Δt	Time step size	s
Δx	Cell size	m

Greek alphabet

α	Absorptivity	-
β	Mass transfer coefficient	m/s
γ	Impaction angle	rad
δ	Distance between particle and surface	m
ε	Emissivity	-
η	Efficiency	-
θ	Angle normal to each face	rad
Θ	Angular position	rad/degree
λ	Molecular mean free path length	m
μ	Dynamic viscosity	Pa·s
ρ	Density	kg/m ³
ρ	Reflectivity	-
ς	Surface tension	N/m
τ	Transmittance	-
τ	Characteristic time	s
ν	Poisson's ratio of material	-
ν	Phase	-
φ	Angle	degree
ϕ	Porosity	-
Ψ	Correction factor	-

Dimensionless numbers

C	Courant number
Kn	Knudsen number
Re	Reynolds number
Sc	Schmidt number
Sh	Sherwood number
Stk	Stokes number
St	Strouhal number
We	Weber number
Pr	Prandtl number
Nu	Nusselt number

Subscripts

∞	Far away from the obstacle
A	Area
AVG	Average
c	Condensation
cond	Conductive
conv	Convective
cr	Critical
D	Drag
dep	Deposit
eff	Effective
f	Fluid
<i>f</i>	Fouling
g	Gas
imp	Impaction
kin	Kinetic
l	Liquid
LV	Liquid-vapour
m	Melting
p	Particle
rad	Radiative
ref	Reference
S	Saturation
s	Surface
stick	Sticking
t	Tube
T	Thermophoretic
tot	Total
w	Wall
x	X direction

Abbreviations

1D	One dimensional
2D	Two dimensional

3D	Three dimensional
ar	As received
ASTM	American Society for Testing and Materials
BE	Brownian/Eddy diffusion
BSI	International, British Standard Institute
CCP	Cereal co-products
CCSM	Computer-Controlled Scanning Electron Microscopy
CEN	European Committee for Standardisation
CFD	Computational Fluid Dynamics
CHF	Chemical fractionation
daf	Dry ash free
df	Dry fuel
DPM	Discrete Phase Model
DRW	Discrete Random Walk
DTA	Differential Thermal Analysis
Eco	Economiser
EDX	Energy Dispersive X-ray
FB	Fluidised bed
FBP	Fluidised bed primary air
FBS	Fluidised bed secondary air
FC	Fixed carbon
FD	Forced draft
FTIR	Fourier Transform Infra-red
HHV	Gross heating value
ID	Induced draft
ISO	International Organisation for Standardisation
LHV	Lower or net heating value
MB	Main burner
MSW	Municipal solid wastes
OD	Outside diameter
OECD	Organisation for Economic Cooperation and Development
PF	Pulverised fuel
RANS	Reynolds-Averaged Navier-Stokes

RH	Rehaeater
SEM	Scanning Electron Microscopy
SH	Superheater
SRF	Solid recovered fuels
TGA	Differential thermogravimetric analysis
TH	Thermophoresis
UDF	User Defined Function
VM	Volatile matter
XRD	X-ray powder diffraction

1 INTRODUCTION, AIM AND OBJECTIVES

1.1 Background: Global energy demand

In 2017, global energy demand, especially for electricity, increased by 2.1%, more than twice compared with the previous year and it is expected to increase more through 2050 as a consequence of the global economic growth (International Energy Agency, 2018; U.S. Energy Information Administration, 2018a). Most of it comes from non-OECD (i.e. non-Organisation for Economic Cooperation and Development) countries, where demand is driven by emerging economies (U.S. Energy Information Administration, 2014). Therefore new and more efficient power plants are necessary across the world over the coming decades to satisfy the growing energy requirements and meet the environmental regulations.

More than 70% of the global energy in 2017 was provided by traditional fossil fuels (oil, gas and coal), nuclear and renewables contributed for the rest (Figure 1-1). Natural gas and oil still supply the majority of energy while coal usage projections remain flat through 2050 and the EU has set target to increase the use of renewable energy sources by 2020-2050 (U.S. Energy Information Administration, 2018a). “The Global Energy and CO₂ Status Report, 2017” stated that natural gas experienced a growth of 3%, a third of which from China, and the buildings and industry sectors which contributed to 80% of the global demand increase. Natural gas is abundant, efficient and cleaner than coal or petroleum products, therefore it represents an attractive choice to produce power and cut CO₂ emissions. Moreover, oil usage, linked to the transport and petrochemical sectors, increased by 1.6%, more than double the average annual rate over the past decade. Finally, coal demand increased, mainly in Asia, about 1%, after declining over the previous two years (International Energy Agency, 2018). In Europe, the use of coal is about 20% lower than other OECD countries (US, Japan, Australia). In fact, the goal for some of the European countries (except for Poland and Germany) is to reduce the use of coal until complete retirement of its power stations. Promising results have been already obtained in 2017 and 2018; for example the UK was able to supply electricity for several days using only gas, wind, nuclear and biomass, without coal (Vaughan, 2018). In fact, renewables (wind, solar, hydropower, and biomass) showed the highest growth rate in 2017 and were able to meet a quarter of the world energy demand. In

particular, wind and solar generation accounts for 64% of the total electric generation growth until 2050, whereas hydropower and nuclear power consumption will be relatively flat until 2050 (Figure 1-1).

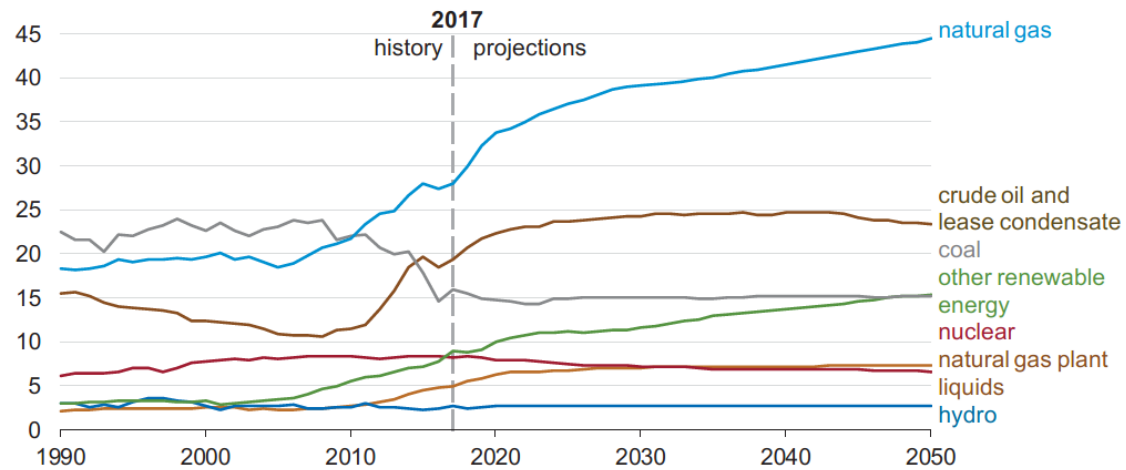


Figure 1-1: Energy production quadrillion British thermal units (U.S. Energy Information Administration, 2018a).

Traditional fossil fuels are the main reasons for greenhouse gas emissions, which cause global warming (e.g. Gogebakan *et al.*, 2009; Vassilev *et al.*, 2015). In this context, government policies and incentives have been established to increase and develop new technologies to encourage the generation of 20% of EU electricity from renewable resources by 2020 (15% in case of the UK) as required by the EU Renewable Energy Directive 2009/28/EC (European Parliament; European Council, 2009; Khodier *et al.*, 2012). This is in agreement with the current EU Research and Innovation Programme (i.e. HORIZON 2020) which has aims of reducing CO₂ emissions by 20%, increasing the share of renewable energies to 20% and finally increasing energy efficiency by 20% by 2020. A longer term goal considers a reduction in the CO₂ emissions by more than 70% below the current levels by 2050 (International Energy Agency, 2017).

However, carbon dioxide emissions increased by 1.4% in 2017, after being flat for the last three years (International Energy Agency, 2018). This was the result of global economic growth, lower fossil fuel prices and weak energy efficiency which improved only by 1.7% in 2017 compared with 2.3% on average in the last three years.

Currently, renewables are widely used in the electricity, heating/cooling and transport sectors and they are expected to play an increasingly role over the next century. Among them, biomass is an organic fuel, derived from plant matter and animals. The most common classification of biomass identifies the following types: woody plants, herbaceous plants/grasses, aquatic plants, manures and wastes. They are generally characterised by higher volatile matter content, lower heating values, less carbon, more oxygen, higher moisture content, usually lower density, wider size distribution and more volatile alkali content if compared with coal (Sahu *et al.*, 2014). The choice of biomass depends on the type of energy conversion process and the form in which the energy is required (Mckendry, 2002).

The main combustion systems used for solid fuels are: grate combustion, fluidised bed (FB) combustion and pulverised fuel (PF) combustion systems. They are different for the size of boilers, fuel quality, fuel pre-treatment, fuel-oxidizer ratio, gas flow and temperature conditions (Kleinhans *et al.*, 2018). Grate combustion uses a moving grate and air is supplied from below to burn the fuel which generally has high moisture and ash contents, variable particle sizes and does not require pre-treatments (straw, municipal solid wastes (MSW), wood). However, these systems have a limited scale and efficiency (15-30%). In fluidised beds, the fuel burns in a hot bed of small particles (e.g. quartz sand) fluidised with air and their intimate mixing guarantees a high heat transfer. They are characterised by lower and more uniform temperatures, bigger scale and are generally used for wood chips, solid recovered fuels (SRF) and coal with variable ash content. However, one of the main problems using these systems is the agglomeration of the bed caused by chemical reactions of inorganic vapours, salts or silicates that can lead to the plant shut down. Finally, in pulverised fuel boilers, preheated air or recirculated flue gas transports solid fuel particles, generally smaller than 200 μm , into the furnace. Temperatures are higher than fluidised bed, the combustion is generally completed before the flue gas reaches the convective areas of the boiler and efficiency up to 46% or even higher in supercritical systems (Yang, 2016; Kleinhans *et al.*, 2018).

Currently, pulverised fuel boilers represent the most common systems for power generation from coal. However, co-firing biomass with coal seems to be a promising

and flexible solution to reduce CO₂ emissions from coal fired power plants (Kurowski and Spliethoff, 2016; Yang *et al.*, 2016). Traditionally, the technology of co-firing biomass with coal in large pulverised coal-fired boilers is a more effective way of using biomass in terms of costs, system modifications and higher boiler efficiency if compared to firing 100% biomass in smaller boilers. However, the amount of available biomass is limited to fully replace fossil fuels and face the rising energy demands (Baxter, 2005; Roni *et al.*, 2017).

Co-firing 10-20% of biomass with coal has been widely used in the UK and Europe. In particular, the UK has been one of the countries with the largest technical potential in terms of available pulverised coal-fired boilers for biomass co-firing (Khodier *et al.*, 2012). This type of plants was initially designed only for coal combustion, therefore co-firing of coal and biomass, even with a percentage lower than 10%, required more studies. However, after reaching a peak of co-firing production in the UK, this rate started decreasing. In fact, in 2010-2011 some coal power stations were shut down or were fully converted to biomass and it was also encouraged the construction of smaller biomass boilers (Roni *et al.*, 2017).

Coal and biomass fired combustion systems present both outstanding challenges during their operations, such as deposition and corrosion on heat exchanger tubes. The inorganic matter present (in different forms and amounts) in both biomass and coal has an impact on gas emissions, vapours, fly ashes and deposits (Baxter, 2005). In fact, ash deposition is one of the most serious issues in pulverised fired power plants which can cause enhanced slagging and fouling, corrosion, limit the heat transfer between the hot combustion gas and the steam system used to generate power and lead to outages (Rushdi *et al.*, 2005; Kalembkiewicz and Chmielarz, 2012; Yang *et al.*, 2016).

Slagging is an ash related problem in high temperature areas of boilers (radiative) and fouling in the convective areas where the temperatures are lower. Their extent depends on the type of burner and the fuel (coal and biomass), however they represent serious problems as they can significantly affect the boiler thermal efficiency and also cause tube corrosion which results into higher maintenance costs and unexpected tube failures (Hussain *et al.*, 2013; Lu and Wang, 2015). These problems are expected to become

more important as increases in steam temperatures and pressures are used to improve energy conversion efficiencies (Nicol, 2013).

One of the main difficulties connected to the use of biomass to generate power, either when it is used by itself or with coal, is its variable elemental and mineral composition and particularly its variability in terms of volatile fraction, particle size, alkaline compounds, nitrogen and chlorine content which makes the extent of deposition difficult to predict (Pisa and Lazaroiu, 2012). Moreover, there are other limitations to extending co-firing technology such as: fuel supply, fuel storage, preparation and feeding (Baxter, 2005).

The multidisciplinary nature of this subject makes its study more complicated and, even though many experimental data and modelling have been carried out so far, the number of gaps in the field is still high. In fact, several studies have been conducted on a lab scale to predict deposit formation which seems to be different compared with industrial scale. Moreover, many indices and mechanistic models have been developed in the literature to predict deposition (Borio and Levasseur, 1984), but they are specific for certain boilers and fuels and cannot be generalised. In addition to that, they are not able to predict the most critical areas where fouling and slagging occur and the dynamic effect of deposit accumulation on heat transfer (Magda *et al.*, 2011).

Recent technological progress has made computational fluid dynamics (CFD) one of the best tools to study deposition onto heat exchangers as it enables calculation of both gas behaviour and particle trajectories, as well as the prediction of deposit location around tubes, deposition fluxes and heat transfer calculations. However, this modelling approach needs more studies to include the combination of different deposition mechanisms, and validation of the model with experimental data (Magda, 2012; Weber, Mancini, *et al.*, 2013).

There are many advantages of using a CFD approach, for example (Magda, 2012):

- Estimation of fouling and slagging in different combustion environment using different fuels.
- Correct prediction of areas where deposition occurs in order to help a better design of furnaces, burners, convective surfaces and soot or wall blowers.

- Predicting deposit growth can provide information in order to identify the optimal cycles for soot blowers such as the intensity and frequency of cleaning or to choose the best fuel and exclude the ones that may cause more deposition problems.

1.2 PhD Aim and Objectives

Aim:

The main aim of this PhD is to develop improved understanding and modelling of the compositions and fluxes of deposits forming on heat exchanger surfaces. This includes analysing the effects of gas composition, fly ash composition and ash particle size distribution and their impact on heat transfer.

Objectives:

- 1) To develop improved models including different deposition mechanisms to predict deposition on heat exchangers and the effect of the deposit on the surface temperature.
- 2) To investigate the heat exchanger deposits generated by the use of coal and biomass in pilot scale testing, including the study of the chemical composition of deposits, flue gas and fly ash properties.
- 3) To validate the CFD models with experimental results.
- 4) To improve the scientific understanding of deposit formation on heat exchangers including flue gas/ fly ash compositions and particle size distribution.

Scope of the study

This PhD project formed part of the Flex-E-Plant (Flexible and Efficient Power Plant) research programme that was started in 2013 in order to meet the new need of power generation industries. The main aspects considered in this programme were:

- Plant Efficiency - to reduce emissions and make decarbonisation economically feasible
- Plant Flexibility - varying power output to reflect demand
- Fuel Flexibility - firing and co-firing steam plant with biomass to reduce emissions create new challenges in plant engineering, monitoring and control and material performance

- Sustainability - to include the economic and environmental considerations linked to the decarbonisation technologies

All of these themes were considered in three work packages, each dealing with a specific scientific aspect of the power plants:

- plant operation and design
- combustion fuel and operability
- structural integrity and advanced materials

This PhD was part of the work package “combustion fuel and operability” and had the main focus of improving the understanding of deposition of fly ash and alkali vapours on superheaters and reheaters including a variety of mechanisms using both experimental and CFD approaches.

Some parts of this work have already been presented at conferences (posters and oral presentations) and submitted in papers as reported in Appendix H and Table 1-1.

To achieve these aim and objectives, this study was divided into three main activities:

- 1) A CFD model was developed in Fluent[®] to predict deposit growth on superheaters and reheaters including a variety of deposition mechanisms. The model used an Eulerian-Lagrangian approach to describe the gas flow field around tubes and the solid ash particle trajectories respectively. User Defined Functions (i.e. UDFs) were developed to predict the deposition growth, deposit shape and temperature. The CFD deposition model was applied to predict deposition on air cooled ceramic probes in a pilot scale combustion rig at Cranfield University and a dynamic approach was used to include the effect of the deposit shape and temperature on the deposit growth.
- 2) Experiments were carried out in a 100 kW_{th} capacity downdraft pulverised fuel (PF) pilot scale combustor rig at Cranfield (Figure 1-2). A blend of Daw Mill coal-12 wt. % Miscanthus was fed at an average rate of 8 kg/hr and annular air cooled ceramic probes were used to study the deposition accretion. Thermocouples were used to check the temperature at different locations and on the probes whose temperatures were kept constant during the tests. Moreover, the gas composition was monitored with a Fourier Transform Infra-Red (FTIR) gas analyser. ESEM (Environmental Scanning Electron Microscope) and XRD (X-ray

Diffraction system) analyses were conducted for most of the ash samples. Finally, some fly ash samples were analysed with a Malvern Mastersizer 2000 to get ash particle size distributions.

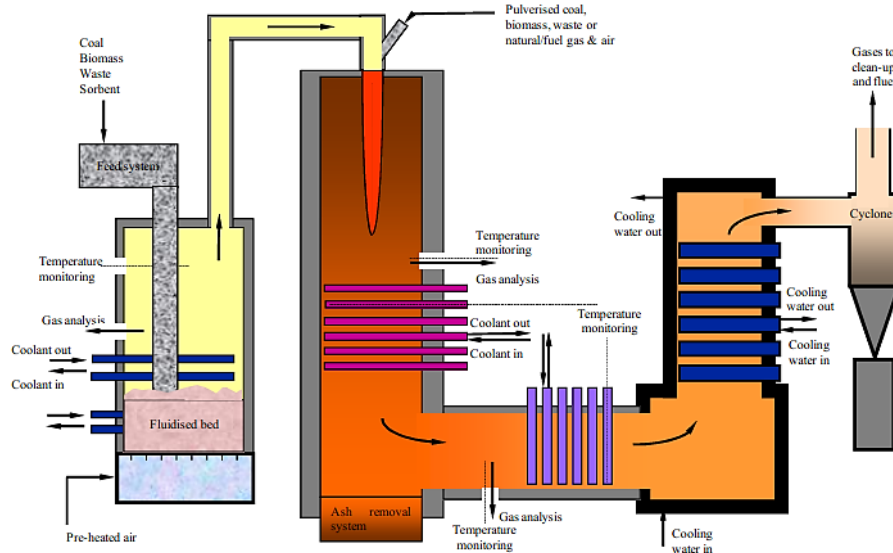


Figure 1-2: Schematic of the FB (left) and PF (right) combustors at Cranfield (Khodier, 2011).

- 3) Some of the experimental results (e.g. gas velocity and temperature, ash composition and ash particle size distribution etc.) were used as boundary conditions in the CFD model, some others (e.g. deposition flux) for its validation.

1.3 Thesis outline

This thesis is organised in nine chapters and eight appendices and it is structured as follows:

CHAPTER 2 presents a literature review of coal and biomass, co-firing, mineral matter transformation and main deposition mechanisms. It also includes an overview of different deposition models.

CHAPTER 3 shows the preliminary study necessary to develop the CFD model.

CHAPTER 4 presents preliminary qualitative CFD modelling results and discussions to predict the deposition growth, the deposit temperature and shape.

CHAPTER 5 shows the experimental set up and the main ash analysis techniques.

CHAPTER 6 presents the experimental results obtained using Daw Mill-12 wt.% Miscanthus in the combustion rig at Cranfield University.

CHAPTER 7 includes the model validation using the experimental results obtained in Cranfield's combustion rig.

CHAPTER 8 includes the general discussion about the results obtained, limitations of the work and possible improvements.

CHAPTER 9 concludes the thesis and suggests possible future work and applications.

1.4 List of presentations

The presentations delivered during the PhD are summarised in Table 1-1.

Table 1-1: List of presentations.

Event/Publication	Type of presentation
Flex E Plant consortium meetings—every six months	Oral presentation
Progress Reviews—Cranfield	Oral presentation
Research programme—Cranfield, May 2016	Oral presentation
Meetings at Doosan Babcock (Flex E Plant industrial partner) Glasgow, April & June 2017	Oral presentation
Meeting with Paul Kilgallon (Industrial Supervisor) Cranfield, February 2016, November 2017 & May 2018	Oral presentation
Conference—Heat Exchanger Fouling and Cleaning XII Madrid, June 2017	-Poster presentation -Paper in Appendix H
FeRN (Female Research Network)—Cranfield, June 2017	Poster presentation
Conference – 12 th ECCRIA The European Conference on Fuel and Energy Research and its Applications Cardiff, September 2018	Oral presentation
Deposition prediction in a pilot scale pulverized fuel-fired combustor	Paper published by the journal Fuel

2 LITERATURE REVIEW

2.1 Introduction

Traditionally, coal has been widely used to produce power but biomass and wastes are now playing an increasing role to reduce CO₂ emissions and produce energy in a sustainable way. This enables a responsible use of the available resources while providing energy constantly and in the respect of the environmental regulations (Wright, 2011).

However, relying on traditional fossil fuels represents a valid solution when renewables are not able to meet larger energy demands. As a consequence, fossil-fired plants have to operate at high efficiency, deal with the environmental emissions, face rapid energy demand with fast load cycling, be flexible and accept a variety of fuels (varying H/C ratios, different coals and biomass). In particular, these plants often work at very severe operating conditions (i.e. high temperatures) to push their efficiencies and these cause the degradation of materials in components and add to the need for maintenance. Therefore, further studies need to be carried out to guarantee a reliable and efficient use of renewable and traditional fuels.

An important aspect of power generation, especially in solid fuel-fired systems, is the choice of the fuel. In fact, its composition will affect the conversion process, the generation system (e.g. pulverised, fluidised, grate), the scale of the system (in the range of 500-800 MWe for coal fired boiler and less than 30 MWe for biomass), system efficiency (typically 35-47% for coal and up to 25% for waste fired systems), gas cleaning requirements and emissions, ash and other waste disposal as well as the economic viability (Simms, 2011b).

One of the main problems in using biomass is its large variability in terms of elemental and mineral composition which makes it difficult to predict the emissions of gas, vapours, fly ash and deposit formation. From this derives the need for improved modelling able to predict the ash behaviour in different combustion environments, to reduce the impact on the boiler performance and to avoid unexpected failures (Yang *et al.*, 2016).

Deposition on heat exchanger is a complex phenomenon that involves many mechanisms and species. Numerous models have been developed at different levels of difficulty to predict fouling and slagging (Kleinhans *et al.*, 2018). However, the current knowledge is not sufficient in terms of material properties and fuel behaviour (especially for biomass) and more studies need to be carried out to fill the gaps in the existing knowledge.

This chapter includes a literature review that covers coal and biomass properties; mineral matter transformations; an overview of ash deposition related problems; and the main deposition models and mechanisms.

2.2 Fuel characterisation overview

The choice of a fuel for a certain type of process (combustion, gasification, pyrolysis or anaerobic digestion) depends on its characterisation. Several standards were developed to characterise specific fuels (e.g. coal, biomass and waste) by different organisations (e.g. ASTM International, British Standard Institute (BSI), European Committee for Standardisation (CEN), International Organisation for Standardisation (ISO)) (Simms, 2011b).

Before describing in detail coal and biomass, the main fuel properties were reported below; they can be calculated in terms of weight % on different bases: as received fuels (ar), dry fuels (no water content (df)) and dry ash free fuels (no ash, no water content (daf)) (Simms, 2011b).

Chemical analysis (Simms, 2011b; BSI, 2019):

- Proximate analysis:

Moisture content is the amount of water in the fuel. It can change during sampling, storage and analysis.

Ash content indicates the residue left after the fuel combustion.

Volatile matter (VM) is the part of the fuel (excluding moisture) that is vaporised in the absence of air by heating at 950°C for 7 minutes. The main components are hydrocarbons, sulphur and chlorine components.

Fixed carbon (FC) is the mass remaining after the volatiles are released and it is generally calculated as a difference knowing all the previous values (on an as-

received basis). This value is different from the fuel carbon content as a large part of that ends up in the volatile matter. This parameter is useful to get indication about coke formation. The VM and FC contents suggest if the fuel is likely to be ignited to start the thermal process.

- Ultimate analysis indicates the content of carbon (C), hydrogen (H), oxygen (O), nitrogen (N), sulphur (S) and chlorine (Cl).
- Ash analysis is generally expressed as % by weight of the elements in the dry ash in terms on their highest oxides. However, these oxides are not representative of the actual chemical composition of the ash which is more complex, therefore care is needed in the data interpretation (Stringer, 1995).
- Minor and trace metal analysis is obtained using techniques such as (emission spectroscopy, flame photometry etc.) (Raask, 1985).
- Biochemical composition: e.g. cellulose, hemi-cellulose, lignin, fats, protein, pectin, starch, extractives, C5 and C6 sugars, total non-structural matter, carbohydrates, etc. (Koppejan and Van Loo, 2007).

Physical analyses (Simms, 2011b):

- Bulk density expressed in kg/m^3 .
- Grindability is an important parameter expressed with the Hardgrove index (BSI, 1981). It is quite significative for coals used in pulverised fuel fired power station.
- Abrasion is important for fuels that contain compounds of different hardness and are able to damage components in the power plant systems (quartz and pyrites in coal). The abrasion test consists in putting the fuel in a rotating mill (1500 revolutions per minute) to measure the mass loss of the four steel blades of known mass after 8 minutes of operation (Foster *et al.*, 2004).
- Particle size distribution is done to ensure the right fuel preparation before combustion. In fact, oversized fuel particles do not burn completely and this can also affect the boiler efficiency and increase the carbon content in ash residues. Particle sizes can be measured with standardised sieving, photometry and optical techniques.

Others:

- Energy content or calorific value is a measure of the energy released during the combustion of a certain amount of fuel (MJ/kg). This property is generally evaluated with a calorific bomb and specific standard methods. It can be expressed in terms of higher or gross heating values (HHVs) and lower or net heating values (LHVs), the difference between them is the heat of evaporation of the water formed from the hydrogen in the fuel and the moisture content in the fuel, included in the HHV and excluded in the LHV (ECN, 2019).

The HHVs can be calculated with the fuel elemental composition and one of the expressions available is the Milne formula in Equation (2-1) (Simms, 2011b; ECN, 2019):

$$\text{HHV}_{\text{milne}} = 0.341 \text{ C} + 1.322 \text{ H} - 0.12 \text{ O} - 0.12 \text{ N} + 0.0686 \text{ S} - 0.0153 \text{ ash} \quad (2-1)$$

Where C, H, etc. are the mass and the ash fractions in wt. % of dry material and HHV is the heating value in MJ/kg.

- Ash fusion is carried out to detect the behaviour of ashes under high temperatures as they become hard glassy slag. During these tests the fuel ash, in the form of cones, pyramid or cubes, is observed through windows in high temperature furnaces. Different ash fusion temperatures have been identified: Initial deformation temperature (the corner of the mould starts becoming rounded); softening temperature (the top of the mould becomes spherical); hemisphere temperature (the entire mould assumes a spherical shape); fluid temperature (the molten ash collapses) (Raask, 1985).
- Coal petrology is a technique that uses polished cross section of coal to determine the reflectance of three phases (liptinite, vitrinite and inertinite) within the coal structures (Speight, 2005).

2.3 Coal and biomass fuels

2.3.1 Coal

“Coal is the family name for a variety of solid organic fuels and refers to a whole range of combustible sedimentary rock materials spanning continuous quality scale” (International Energy Agency (IEA) Statistics, 2010). The main categories of coal are:

- Peat—typical in an early stage of coalification.
- Lignite (brown coal)—with high moisture content.
- Sub-bituminous coal.
- Bituminous coal—dense, usually black coal with a banded structure.
- Anthracite—glossy, hard, black coal with a high carbon content and low in volatile matter.

Coalification is the geo-chemical process that transforms vegetable matter into coal. The typical path of coalification, according to the local geographical and chemical actions, is shown in Figure 2-1.

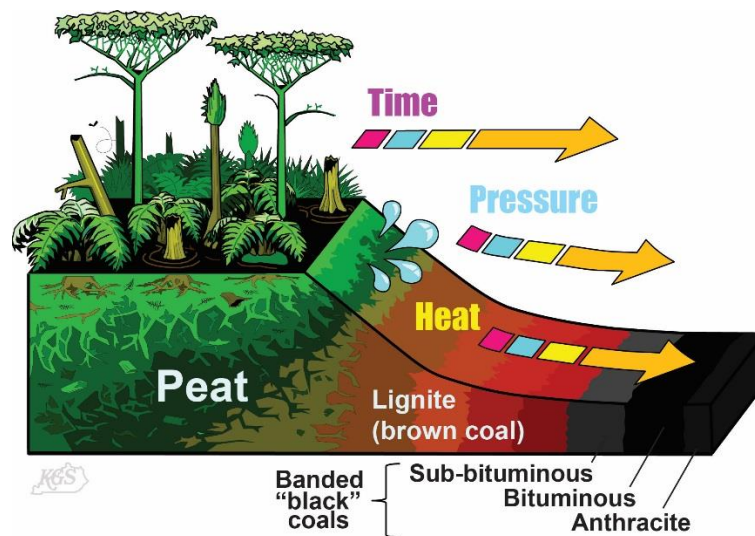


Figure 2-1: Schematic of coalification process (uky.edu, 2018).

Based on the gross calorific values, coal can be classified as hard (> 5700 kcal/kg) and brown (< 5700 kcal/kg), in both cases it contains organic and inorganic material. Coal formation begins with accumulation of vegetables (mosses, leaves, twigs, bark and other parts of trees) which, after microbiological transformation, turns into *peat* layers. This swamp may be covered by inorganic matter (sand and mud) that increases the

weight of sediments and under diagenic (i.e. biological) and tectonic (i.e. pressure and temperature) actions the peat loses some water and gas becoming a soft brown coal called *lignite* (still with a high moisture content). More gases and water are driven off by an increase in pressure and temperature leading to *bituminous* coal formation. Sustained higher temperatures and pressures cause bituminous coal to become a hard and black coal called *anthracite* (Magda, 2012).

Pressure and temperature are the main aspects that influence coal characteristics and its moisture and volatile contents generally decrease with time. Moreover the content of hydrogen and oxygen decreases moving towards anthracite coals, while the carbon and energy content increases. Therefore, lignite and sub-bituminous coals are considered low ranked coals and bituminous and anthracite higher ranked coals. The Van Krevelen diagram can help explaining the different characteristics of fuels; in fact it shows the H:C and O:C ratios and their effect on the calorific value of solid fuels (Figure 2-2). It also includes biomass and peat and how the transformation into coal affects their composition and thermal properties. The energy content is higher in carbon-carbon bonds than in carbon-oxygen and carbon-hydrogen bonds, therefore fuels with higher amount of oxygen and hydrogen have lower energy contents (Van Krevelen, 1950; Mckendry, 2002).

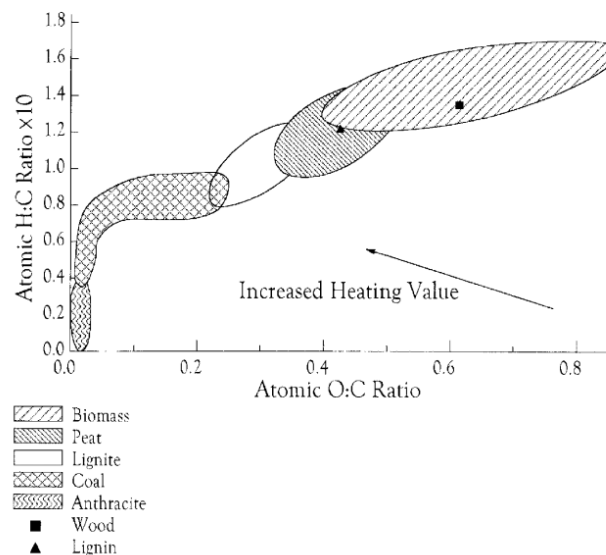


Figure 2-2: Van Krevelen diagram for various solid fuels (Mckendry, 2002).

Significant differences can be found in the composition of coals according to the location and local geology. Coal contains carbonaceous material and inorganic mineral matter (3-30 wt.%) (Stringer, 1995). The main inorganic matters include alkali and alkaline earth metal cations (Na^+ , K^+ , Mg^{2+} , Ca^{2+}), iron, calcium, magnesium and chloride minerals mainly in the form of salts of carboxylic acids which end up in the fuel and/or crystalline deposits from groundwater (Kleinhans *et al.*, 2018).

Minerals can be as small inclusion organically bounded within coal or excluded as free particles and independent from carbonaceous matrix or other minerals. The main minerals are: clay, sulphides, sulphates, carbonates, chloride, silicates, halogenides, oxides, phosphates, which go into ash in their initial form or as minerals with a new composition after transformations (water loss, melting, release of CO_2 , fragmentation, vapourisation, chemical reaction). However, standard ash analyses are not able to give a realistic description of fuel mineral matter composition (Stringer, 1995; Simms, 2011b). Moreover, trace elements (As, Ba, F, Mg, Ni, Ti etc.), which are present in coal with content below 1000 ppm, can be detected in fly ash, bottom ash, deposit and gases. Major elements and, in particular, minor and trace elements can cause operational problems such as fouling and corrosion. For example, S and Cl contents play an important role in the formation of fouling and slagging as well as corrosion of tubes (Benson and Sondreal, 1999).

2.3.2 Biomass

Biomass are organic materials such as plants, trees, algae and crops, which are considered renewable sources of energy as they are produced during photosynthesis using sunlight, water and CO_2 . The solar energy accumulated in its chemical bonds is released during biomass combustion with water and CO_2 which are then reused during the photosynthesis to produce the organic fuel. This closed circle, with a neutral conversion of CO_2 , makes biomass renewable fuels since they do not contribute to the greenhouse effect. In contrast, fossil fuels cannot be considered renewable because they release CO_2 in short term compared with the long time necessary for their formation (as explained in 2.3.1) (Baxter, 2005; U.S. Energy Information Administration, 2018b).

The main types of biomass are (Mckendry, 2002):

- Energy crops: woods (e.g. coppice, willow, poplar, cottonwood); grasses (e.g. Miscanthus, grass).
- Agricultural and waste materials: straw (wheat, barley, rice); forest residues.
- Processing residues from: olives, almond, nuts, sawdust, wood off-cuts.
- Seaweeds (natural and cultivated).
- Animal waste and sewage sludge.

Biomass composition is highly dependent on the origin and formation conditions as these can determine the enrichment or depletion of some elements. However, the main factors that influence biomass and biomass ash composition are (Baxter, 2005; Vassilev *et al.*, 2015):

- 1) Biomass resource (type of biomass, plant species or part of plants, growing processes and conditions, age of plants, fertilizer and pesticide used, harvesting time, collection technique, contamination, transport, storage, processing etc.).
- 2) Biomass fuel preparation (drying, cutting-grinding, densification and torrefaction).
- 3) Combustion technology and operating conditions, ash collection and cleaning equipment.

Biomass can be in forms of pellets, such as cereal co-products (CCP) or wood by-products. This increases their energy content and makes them easier to handle, transport, and store. In fact, an important characteristic of biomass is the bulk density; in particular the density of the processed product has an impact on the fuel storage and on its behaviour during the thermo-chemical-biological processing (Vassilev *et al.*, 2015).

Biomass can be characterised according to the content of cellulose, hemicellulose, lignin and a small amount of other extractives in proportions that vary with the type of plant (Khodier, 2011). Cellulose is a glucose polymer, generally the largest fraction of biomass by weight (40–50%); hemicellulose is a mixture of polysaccharides, composed almost entirely of five-carbon monosaccharides, its portion represents 20–40% of the material by weight; lignin is a group of amorphous, high molecular-weight, chemically related compounds. The proportions between cellulose and lignin is one of the factors that determine if a plant is suitable for biochemical conversion processes, being the cellulose more biodegradable than lignin. Moreover, this ratio determines if a biomass

is suitable to be processed as energy crops. However, with the recent need for renewable fuels, biomass performances need to be compared with traditional fossil fuels and new standard analytical methods (initially developed for fossil fuels) have been developed also for biomass characterisation (e.g. ASTM International, 2010; BSI, 2010; CEN, 2010; ISO, 2010) (CEN, 2010).

Biomass generally has variable and higher moisture contents and lower ash content than coal (with some exceptions such as palm kernels, olive residue, nut wastes etc.) (Simms, 2011b). Moreover, biomass and biomass ash have a low content of trace elements. When compared to traditional fossil fuels, biomass has less C, fixed C, and S but more H and O. These trends can also be detected from peat to anthracite in Figure 2-2 and which implies higher energy content. On the other side, increased amount of H means more light hydrocarbons, higher volatility and lower ignition point which makes biomass very reactive at a lower combustion temperature (Vassilev *et al.*, 2015; Nunes *et al.*, 2016).

The content of other elements (N, S, Cl, P and metallic elements) can be variable according to the environment and the type of biomass, as well as the storage conditions, the harvesting, the growing etc. Biomass has a higher content of halogen and non-metals (i.e. B, Br, Cl, H, I, O, P) and alkaline and alkaline earth elements (i.e. Na, K, Mg, Ca, Rb, Sr). Generally, biomass that grows faster (e.g. energy crops) tends to have higher Cl, K and Na contents. In fact, the alkali metals in biomass can be easily released during combustion, react with the silica present in the ash and produce a sticky, mobile liquid phase with lower pH and ash fusion temperature which can block the airways until outages of the plant. Even if the biomass silica content is initially low, its concentration can be increased because of the soil contamination. In addition, some trace elements (Ag, Br, Cd, Co, Cr, Cu, Hg, Mn, Ni, Pb, Se, Ti, Zn, etc.) and solid ash particle residues obtained during the combustion can lead to inhalation risk and other problems such as emissions, deposition (fouling/slagging) and corrosion which can strongly restrict the boiler thermal efficiency (Vassilev *et al.*, 2015).

Some typical minerals and phases in biomass and biomass ash are: Ca-K-Mn silicates, Ca-Al-Mn oxides, K-Na-Ca chlorides and K-Ca-Mg-Na carbonates, sulphates and phosphates which have not been found in coal and coal ash. This could be due to an

enrichment of Ca, Cl, K, Mg, Mn, Na and P in biomass and biomass ash compared to coal and coal ash. On the other hand, Al-Fe-Si and Ti minerals are typical of coal and coal ash and they have not been found in biomass and biomass ash (Vassilev *et al.*, 2013; Vassilev *et al.*, 2015) .

Biomass can be used as fuels, however, their high variability in terms of composition compared to coal indicate the need for more investigations before switching coal power station to 100% biomass or co-firing. However, the tendency is to use biomass with high growth rate, ease of management and harvesting, less moisture content and low ash, alkali and trace component contents which can deeply affect the conversion processes. The main differences between coal and biomass are summarised in Table 2-1 (Vassilev *et al.*, 2015).

Table 2-1: Mean and range values for common characteristics of coal, biomass, coal ash and biomass ash wt. % on air-dried basis (extracted from Vassilev *et al.*, 2015).

Characteristic	Coal	Biomass	Coal ash		Biomass ash
Proximate analysis			Ash analysis		
VM	30.8 (12.2-44.5)	64.4 (30.4-79.7)	SiO ₂	54.06 (32.04-68.35)	29.14 (0.02-94.48)
FC	43.9 (17.9-70.4)	16.0 (6.5-35.3)	CaO	6.57 (0.43-27.78)	25.99 (0.97-83.46)
Moisture	5.5 (0.4-20.2)	14.7 (2.5-62.9)	K ₂ O	1.60 (0.29-4.15)	19.40 (2.19-63.90)
Ash	19.8 (5.0-48.9)	4.9 (0.1-34.3)	P ₂ O ₅	0.50 (0.10-1.70)	5.92 (0.54-40.94)
Sum	100.0	100.0	Al ₂ O ₃	23.18 (11.32-35.23)	4.49 (0.10-15.12)
Ultimate analysis			MgO	1.83 (0.31-3.98)	5.60 (0.19-16.21)
C (daf)	78.2 (62.9-86.9)	51.1 (42.2-60.5)	Fe ₂ O ₃	6.85 (0.79-16.44)	3.41 (0.22-36.27)
O (daf)	13.6 (4.4-29.9)	41.4 (20.8-49.0)	SO ₃	3.54 (0.27-14.42)	3.27 (0.01-14.74)
H (daf)	5.2 (3.5-6.3)	6.2 (3.2-10.2)	Na ₂ O	0.82 (0.09-2.90)	2.54 (0.09-29.82)
N (daf)	1.3 (0.5-2.9)	1.1 (0.1-12.2)	TiO ₂	1.05 (0.62-1.61)	0.24 (0.01-2.02)
S (daf)	1.7 (0.2-9.8)	0.20 (0.01-1.69)	Sum	100.0	100.0
Sum	Sum	Sum	Ash fusion test		
	100.0	100.0	DT (°C)	1251 (1105-1525)	1103 (670-1565)
			HT (°C)	1388 (1200-1575)	1319 (975-1665)
			FT (°C)	1411 (1205-1585)	1354 (1000-1700)
Other characteristics	Coal	Biomass	Coal ash		Biomass ash
Bulk density (kg/m ³)	1250 (1100-1300)	563 (250-954)	800 (400-1100)		194 (80-430)
HHV (MJ/kg ¹)	25.0 (16.0-34.0)	18.0 (14.0-22.0)			
Initial ignition by DTA-TGA (°C)	256 (190-322)	167 (144-190)			
Peak combustion by DTA-TGA (°C)	508 (415-600)	339 (324-351)			
pH of leachate	5.9 (2.2-7.5)	5.6 (5.1-6.8)	10.0 (6.2-12.5)		10.3 (8.1-12.9)
DWR	2.1 (0.2-8.4)	3.8 (0.3-15.1)	1.6 (0.2-7.2)		27.0 (3.9-45.1)

Abbreviations: A, ash yield; daf, dry ash-free basis; db, dry basis; DT, deformation temperature; DTA, differential-thermal analysis; DWR, dry water-soluble residue; FC, fixed carbon; FT, fluid temperature; HHV, higher heating value; HT, hemispherical temperature; M, moisture; TGA, thermo-gravimetric analysis; VM, volatile matter.

2.4 Co-firing biomass with coal

Renewable fuels have been strongly promoted in the last years by government policies and regulations; the European Union has set targets for a 20% reduction in CO₂ emissions by 2020 and a 70% reduction by 2050 (International Energy Agency, 2017). In this scenario, co-firing biomass and waste with coal represents one route to using such fuels in higher efficiency systems, initially designed for individual fuels. Increasing levels of biomass and wastes will be used for power generation as a consequence of global warming and of the limited availability of fossil fuels. In particular, biomass represents a valid form of energy if replanted immediately (Baxter, 2005; Munir, 2010; Hussain *et al.*, 2013).

The main limitations in using co-firing systems are (Khodier *et al.*, 2012; Pisa and Lazaroiu, 2012):

- 1) Fuel costs/availability/transport/handling/storage systems.
- 2) Different fuel preparation systems and milling process.
- 3) Combustion systems (use existing burners designed for coal or create new and separate ones, collection and cleaning equipment, down rating the boiler to use lower final steam temperatures, appropriate gas cleaning systems).
- 4) Slagging/fouling/corrosion: fuel differences can lead to unexpected deposits resulting in reduced heat transfer, increased cleaning, corrosion damage that can shorten life components.

As a consequence, further studies are necessary to better understand the behaviour of single fuels and co-firing to develop predictive models in order to control the combusting environment, find the right fuel match and identify possible chemical additives.

One of the advantages of co-firing coal with biomass is that the high volatile matter content in biomass implies faster devolatilisation, low ignition temperature, higher production of combustible gas and inorganic vapours, improved combustion with a more stable flame but these factors also make the combustion more difficult to control and create the need for a bigger reaction volume with a design able to achieve complete combustion (Jurado *et al.*, 2014; Nunes *et al.*, 2016). The lower biomass C content

reduces CO₂ emissions (Baxter, 2005). However, for biomass as well as for coal, incomplete combustion leads to unburnt C pollutants such as CO, methane, polycyclic aromatic hydrocarbons, dioxins, furans, tar, soot, and other hydrocarbons (Mckendry, 2002).

In addition, biomass ash content is much lower compared with coal which means less ash related problems. However, harvesting biomass can introduce contaminants and these can lead to operational problems. For example, the releasable alkali is higher in biomass and this is one of the main reasons for corrosion on heat exchangers and vapour condensation which can enhance the deposit accretion. For instance, biomass with higher content of Ca shows more slagging, fouling and corrosion problems and the high K, Si and Al content in straw and grasses leads to very low melting temperatures (lower than 950 °C). This combined with high chlorine contents have straw to be a problematic fuel. On the other hand, wood biomass is less troublesome, in fact their high content of calcium gives higher melting temperature. The main differences among some coal and biomass types are reported in Table 2-2 (Kleinhans *et al.*, 2018).

Among the herbaceous biomass, Miscanthus is one of the most used energy crops, especially in the UK for its rainfall and it has also been used for more than 10 years in Europe (Roni *et al.*, 2017). It grows quickly and can give a high dry matter yield. It also has a low inherent mineral content and a good energy yield which makes Miscanthus very similar to wood species (Mckendry, 2002).

Table 2-2: Typical ranges for ash content , ash fusion temperature and major ash forming elements for different fuel types (extracted from Kleinhans *et al.*, 2018).

Fuel type	LHV MJ/kg	Ash content wt. %	Ash fluid temperature °C	Major ash forming elements – and minerals sorted by type
Bituminous coal	25-30	3-25	1200-1500	Si, Al, Fe - quartz, kaolinite, illite, pyrite
Lignites	18-27	5-40	1100-1450	Si, Al, Ca, Mg, Fe, S - quartz, carbonates, gypsum
Herbaceous biomass	14-17	4-12	950-1300	Si, K, Ca and rel. high Cl content - silicic acids
Woody biomass	15-19	0.5-7	1150-1500	Ca, K, Si, Mg-oxalates
Manures and sludges	9-14	15-50	1000-1300	Ca, P, Si, Na, S (can vary strongly)
MSW/SRF	12-16	5-45	900-1300	Various compositions often rich in Cl and heavy metals

Abbreviations: Municipal solid waste (MSW), solid recovered fuels (SRF) also called residue-derived fuels (RDF).

Moreover, biomass (woody biomass) has a lower N content which means lower NO_x and ammonia emissions. Possible solutions to reduce the NO_x emissions are: low N fuels, staged combustion and injections of NH₃ or urea and blends of coal and biomass to produce NO and destroy ammonia and hydrocarbon radicals in the furnace (Simms, 2011b).

2.5 Mineral matter and its transformation

The inorganic matter in coal and biomass can be divided in four main groups (Tomeczek and Palugniok, 2002; Rushdi *et al.*, 2005; Magda, 2012; Gudka *et al.*, 2015; Kleinhans *et al.*, 2018) (Figure 2-3):

- *Dissolved salts*: deriving from contact of coal with sea water or dissolved salts from the liquid phase inside biomass (K⁺, Na⁺, Ca²⁺, Cl⁻, HPO₄²⁻, H₂PO₄⁻, SO₄²⁻, Si(OH)₃O⁻).
- *Organically bound ash forming compounds*: Inorganic elements in the organic compounds (K⁺, Na⁺, Ca²⁺, Mg²⁺, Fe³⁺, Al³⁺ and covalently bonded non-metals S, P, Cl).
- *Inherent minerals*: (Na, K, Ca, Si, Mg) bonded to the fuel matrix, they do not separate before combustion. The content of the inherent minerals represents 2 ± 4 wt. % (usually less than 10 wt. %) in the organic particles which mainly form small ash particles (0.01-0.1 µm). Intimately mixed with the organic fuel, they

can reach temperature higher than the extraneous mineral particles and more severe conditions of combustion (until melting). In fact, they transform within the char particles and are gradually released during the char fragmentation causing mostly slagging in the radiant section of the furnace.

- *Extraneous minerals particles:* (oxides, SiO_2 , Al_2O_3 , CaO , MgO , Na_2O , K_2O , and impurities from the soil for biomass) contain over 80-90 wt. % of the total mineral matter, they are separated from the organic matter as a result of the prior milling. The amount of excluded mineral grains increases with the finesse of the grinding since more extraneous minerals are liberated. Usually their size is in the range of $4 \pm 7 \mu\text{m}$ up to $40 \pm 70 \mu\text{m}$ (finer than organic particles of the size up to $100 \mu\text{m}$). After combustion, they form large ash particles ($10\text{-}90 \mu\text{m}$) that do not reach temperature high enough to melt and mainly cause fouling.

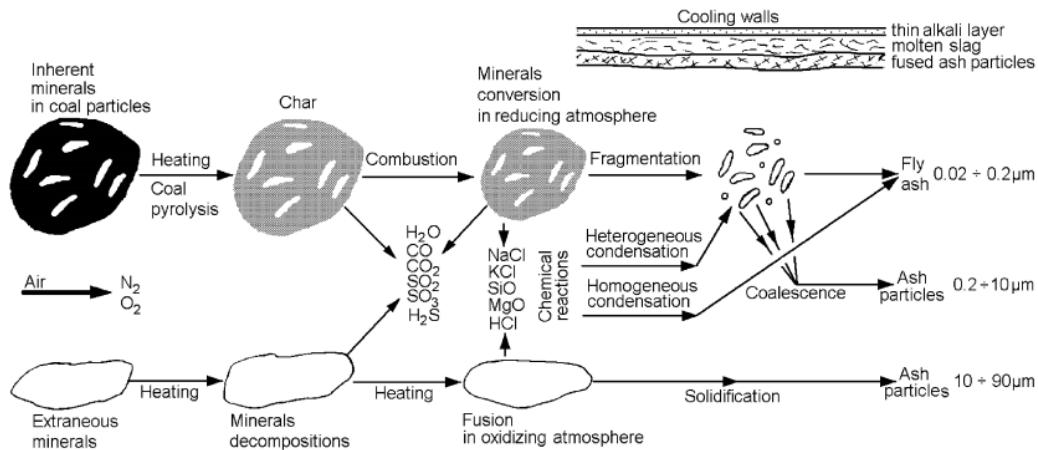


Figure 2-3: Mineral matter transformation mechanism (Tomeczek and Palugniok, 2002).

The formation of fly ash is a complex phenomenon that depends on different mechanisms (coalescence of the included minerals, fragmentation of the char particle, fragmentation of the excluded mineral particles, vaporisation of the inorganic matter, shedding of the surface ash for inherent and excluded mineral grains, sintering, abrasion, chemical reaction, collision, homogeneous and heterogeneous condensation, coagulation and nucleation) as shown in Figure 2-3 (Tomeczek and Palugniok, 2002; Kleinhans *et al.*, 2018).

With increasing temperatures, fuel particles become soft and swollen because of internal gas bubbles and, once devolatilised, they burn as char particles. After devolatilisation,

particles are more porous and the char fragmentation can produce ash particles of different diameters (1-10 μm). Fine ash particles are generated by chars with higher porosities, smaller wall thicknesses and spherical shapes. In contrast, bigger ash particles derive mainly from char particles with porosity $< 40\%$ and thicker walls with angular shapes (Magda, 2012).

Among the products of mineral decomposition there are solid particles and gases that give homogeneous chemical reactions and, as a consequence, heterogeneous or homogeneous vapour condensation. Fly ash of size $0.02 \pm 0.2 \mu\text{m}$ mainly come from homogeneous condensation and the fragmentation of inherent minerals. Moreover, at high temperatures (1300 up to 2300°C), coalescence of the fine molten fragments of mineral matter takes place and it produces ash particles of medium size $0.2 \pm 10 \mu\text{m}$ and a different composition because of the interaction between different inorganic materials. Moreover, sintering and shedding represent two additional ways of producing ash particles. Sintering of solid ash particles takes place at low combustion temperatures and shedding occurs as a consequence of fuel devolatilisation, when the gas can diffuse from particles and create char particles. Moreover, after initial heating, drying, devolatilisation and combustion, the char particles start exothermic heterogeneous oxidation (Tomeczek and Palugniok, 2002).

The behaviour of excluded mineral grains is very different if compared with the included ones. In fact, they are at lower temperatures and they are not exposed to a reducing environment due to char combustion characteristic of inherent minerals. Moreover, they tend to evolve independently from each other with low probability of interaction. The most important way of ash formation for excluded minerals is fragmentation. This process is due to thermal shocks inside particles because of the quick heating rates and escape of gas from the particle with final disintegration in smaller grains. There is still a current lack of knowledge about excluded minerals transformation; however, the largest ash particles ($10 \pm 90 \mu\text{m}$) derive from extraneous minerals transformation. Even if the ash chemistry does not really depend on the intensity of the fragmentation of excluded mineral, it will have an influence on the ash size distribution and therefore on slagging and fouling. Simultaneously with the

physical fragmentation, some chemical reactions (decomposition, oxidation, reduction) take place (Kleinhans *et al.*, 2018).

The amount of inorganic vapours (that include compounds of elements such as Na, K, Ca, Mg, P, S, Cl) released is difficult to determine as it depends on the fuel, the temperature and the residence time. Dissolved salts and elements that are organically bonded can vaporise during the combustion and release inorganic vapours in the gas phase. These vapours can then re-condense in the form of small particles also called aerosol or sub-micron ash particles (0.05 μm) which represents only about 1% of the total mass of the ash. However, the formation mechanisms of small ash particles is still not fully understood (Baxter, 1993).

Bituminous coal has generally got the lowest amount of vaporizable components. High-rank coals contain about 5-10 wt.% of non-mineral inorganics, low rank coals like lignite and brown coal contain about 10-40 wt.% of the total inorganic amount. For biomass, it depends on the type, in fact herbaceous biomass (straw) has higher content 15-69 wt. % and wood from 12 up to 56 wt. % (Figure 2-4).

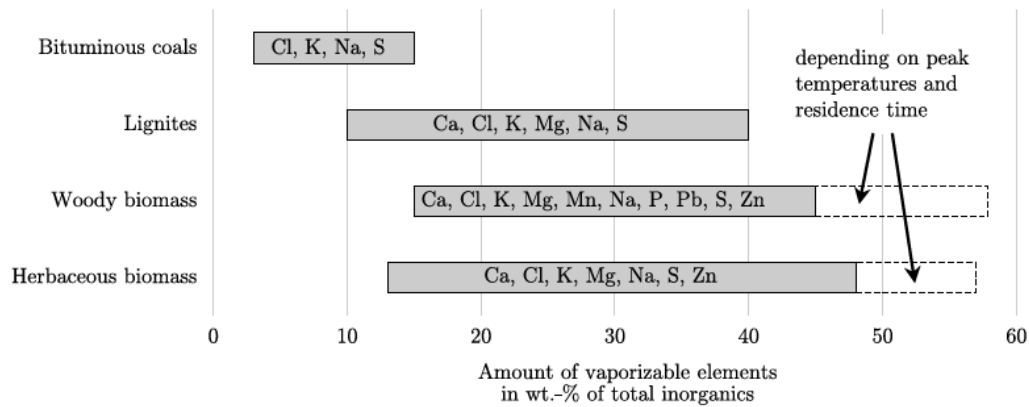


Figure 2-4: Estimate on the amount of elements that can vaporise during combustion of coal and biomass (Kleinhans *et al.*, 2018).

2.6 Ash deposit formation

Solid ash particles and inorganic vapours transported in the combustion gases can impact the surface of heat exchangers and form deposit. Deposition is one of the most serious problems for technical and economical function in pulverised coal and biomass fired power plants. Some examples of ash related issues are slagging in the higher

temperature radiant section, and fouling in the lower temperature convective pass (Figure 2-5) and an example of deposition on superheater tubes is reported in Figure 2-6. Slag deposits are mainly liquid phases of silicate and they may contain FeO and FeS. The presence of Na, Mg, Ca, K, and Fe determine the liquid behaviour of slag deposits as they can interact with silicates and reduce the initial melting point. Fouling deposits are generally less liquid than slags and are a combination of silicates and sulphates that bind the particles together. Deposits involved in the high-temperature fouling tend to be layered. The inner part is powdery, made of particles deposited on an initial sticky layer of condensed vapour. As a consequence of the deposit insulation, the outer layer is at a higher temperature and in a liquid state which makes it act as a collector of particles. When using coals with a high content of Calcium, low temperature deposits have been found to be made of sulphate and calcium. In these lower temperature conditions, the silicates do not have the same bonding effect and they are mainly unreacted (Valero and Cortes, 1996; Yan *et al.*, 2001; Weber *et al.*, 2013; Yongtie *et al.*, 2017; Zheng *et al.*, 2017).

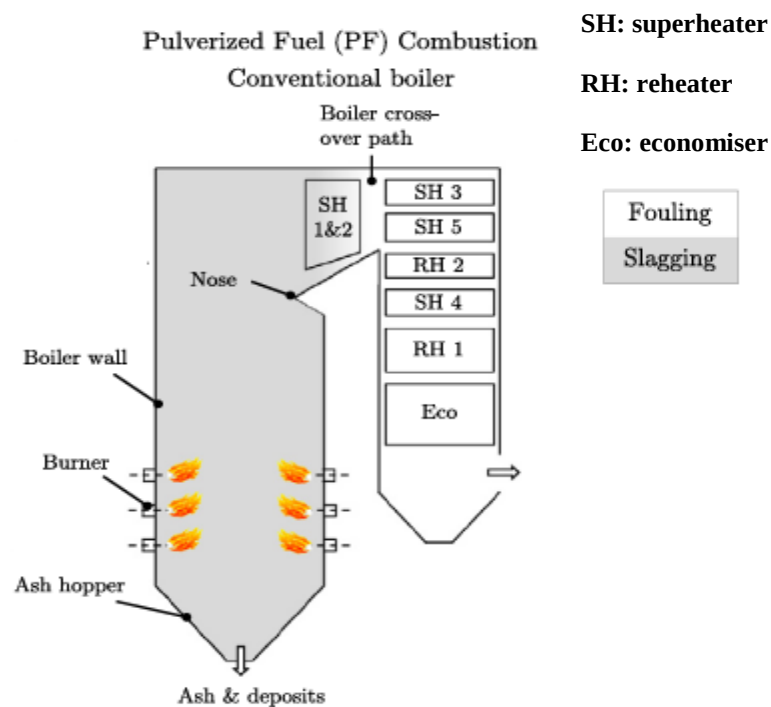


Figure 2-5: Fouling and slagging location in a conventional pulverised fuel (PF) combustion boiler (extracted from Kleinhans *et al.*, 2018).

Ash deposit problems are often interconnected. In fact, slagging reduces waterwall heat transfer and alters the temperature distribution in the boiler with the consequence of changing the ash deposition in the convective areas. Moreover, fouling on tubes can reduce the cross-sectional area for the flow gas which increases the flue gas fan workloads and the local gas velocities causing fly ash erosion (Borio and Levasseur, 1984). However, the main focus of this thesis is fouling formation and modelling on superheaters and reheaters.



Figure 2-6: Ash slagging (left) (Mengenai, 2014); deposit fins on superheater tubes (right) (Tomeczek et al., 2004).

The main factors that influence the deposition growth are: particle size, mineral distribution inside particles, mineral-coal or mineral-mineral association, chemical composition, fly ash density, impacted surface, combustion chamber design, geometry of tubes bundle and thermal and gas-dynamical conditions close to the heating surfaces (Tomeczek *et al.*, 2004). Particle size and density determine the ash particle path and the probability of impacting the heat exchanger surfaces. Chemical composition and temperature give information about the particle viscosity and its “stickiness” which is the property of a particle to deposit on the surface because of its low viscosity while, if the particle has a high viscosity, it is more likely to rebound off the wall. Moreover, the condition of the deposition surface is quite important as a sticky surface tends to

increase particle deposition independently from the particle viscosity and size (Zhou *et al.*, 2007; Schulze *et al.*, 2011; Garba *et al.*, 2013).

The viscosity and surface tension are the main properties that affect the particle stickiness for silicate rich ashes. For herbaceous biomass and wood, richer in alkali salt, the liquid melt fraction is more appropriate to describe their behaviour. Moreover, the particle kinetic energy and the angle of impact are two additional parameters necessary to describe the stickiness. In fact if all kinetic energy is dissipated during the impact, the particle will remain on the surface (Yang *et al.*, 2018).

Fouling and slagging represent a serious concern in coal and biomass combustion systems and they can cause (Rushdi *et al.*, 2005; Waclawiak and Kalisz, 2012; Nunes *et al.*, 2016):

- Insulation and deterioration of heat transfers, thus reduction of boiler thermal efficiency until outages.
- Narrowing of the flue gas path, increasing the flue gas path pressure drop.
- Blocking of the ash discharge.
- Damage to the steam generator.
- Erosion and corrosion leading to unscheduled outages.
- High maintenance costs.

Modelling deposition on heat exchangers is a complex phenomenon, in fact while the physics behind particle impaction are fairly well understood, it is still difficult to predict exactly what fraction of impacting particles will stick (Magda *et al.*, 2011).

For this purpose three different efficiencies can be defined as follows (Weber, *et al.*, 2013; Beckmann *et al.*, 2016) (Equations (2-2), (2-3), (2-4)):

- 1) Impaction efficiency is the ratio of the number or mass of particles that impact the tube surface to the number or mass of particles released during combustion (or injected at the inlet).

$$\eta_{imp} = \frac{\text{Mass of particulate impacting wall}}{\text{Total mass of particulate injected}} \quad (2-2)$$

- 2) The sticking efficiency measures the tendency of particles to stick when they hit the surface.

$$\eta_{stick} = \frac{\text{Mass of particulate depositing on wall}}{\text{Mass of particulate impacting wall}} \quad (2-3)$$

- 3) The depositing efficiency shows the amount of particulate mass that deposits on the surface.

$$\eta_{dep} = \frac{\text{Mass of particulate depositing on wall}}{\text{Total mass of particulate injected}} \quad (2-4)$$

Based on these definitions, the depositing efficiency is equal to the product between the impaction and sticking efficiency (Equation (2-5)).

$$\eta_{dep} = \eta_{imp} * \eta_{stick} \quad (2-5)$$

2.7 Deposition mechanisms

The main mechanisms that can cause ash deposition or mass transport to a surface are illustrated below (Atkinson, 1991; Tomeczek and Palugniok, 2004; Mueller *et al.*, 2005; Zhou *et al.*, 2007; Tomeczek and Waclawiak, 2009):

2.7.1 Inertial impaction (particle diameter $d_p > 10 \mu\text{m}$)

Inertial impaction is considered the main ash deposition mechanism when particles have enough momentum to overcome the drag force of the flow gas, penetrate the flow field around the obstruction (boundary layer and stagnation zone) and impact as reported in Figure 2-7. The inertial deposition rate I is function of the time (t) and angular position (Θ) as in Equation (2-6) (Simms, 2011a).

$$I(t, \Theta) = u_f C_{ash,1} \eta_1 f_{stick} s \quad (2-6)$$

Where u_f is the gas velocity [m/s], $C_{ash,1}$ is the mass concentration of large fly ash [kg/m^3], η_1 is the impaction efficiency as defined by (Wessel and Righi, 1988) (Equation (2-7)), f_{stick} is the total sticking coefficient and s is the surface area [m^2] at the angle section $\Delta\Theta$.

$$\eta_1 = \frac{2\Delta y_0}{d_t \Delta\Theta} \quad (2-7)$$

Where Δy_0 is the distance between the starting position of two adjacent particle streamlines, $\Delta\Theta$ is the angle between impact locations of those streamlines on the cylinder and d_t is the tube diameter [m].

After reaching the tube, some particles tend to stick to its surface and begin (or sustain further) deposit growth. This stickiness tendency depends on the particle properties at the moment of impact as well as those of the impacted surface (i.e. previously accumulated layer, roughness of metal surface, surface tension, particle mass and speed of gas, angle of impact and viscosity) (Magda, 2012).

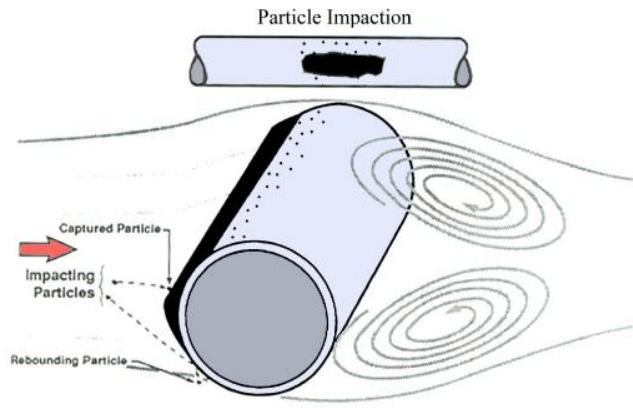


Figure 2-7: Inertial impaction mechanism on a cylinder in cross flow (Baxter, 1993).

Impaction efficiency is function of Stokes number, a dimensionless number characterising the behavior of particles suspended in a fluid flow. It is defined as the ratio of the characteristic time of a particle (or droplet) τ_p to a characteristic time of the flow or of an obstacle τ_g (Equations (2-8) to (2-10)) (Kær *et al.*, 2006; Kleinhans *et al.*, 2018).

$$\tau_p = \frac{\rho_p d_p^2}{18\mu_g} \quad (2-8)$$

$$\tau_g = \frac{d_t}{2u_\infty} \quad (2-9)$$

$$Stk = \frac{\tau_p}{\tau_g} = \frac{\rho_p d_p^2 u_\infty}{9\mu_g d_t} \quad (2-10)$$

Where τ_p [s] is the relaxation time of the particle (the time that a particle, at an initial velocity as free stream, needs to reach equilibrium velocity due to drag (friction)), u_∞ [m/s] is the fluid velocity of the flow far away from the obstacle, d_t [m] is the characteristic dimension of the obstacle (typically its outer diameter), ρ_p and d_p , are the particle density [kg/m³] and diameter [m] respectively, μ_g the dynamic gas viscosity [Pa·s].

A particle with a low Stokes number follows fluid streamlines, while a particle with a large Stokes number is dominated by its inertia and continues along its initial trajectory (Wessel and Righi, 1988). With small particles, inertia is too small to overcome the drag force and cross the streamlines of the gas between the rows where the velocity increases. The Stokes number can describe the drag force in a low Reynolds number regime where the drag force is a linear function of the Reynolds number. This relationship is not valid at high Reynolds number, therefore a correction factor Ψ is included for particles that do not obey Stokes' law and can be computed for a given Reynolds number (Re_p) based on particle diameter and free stream velocity to define the effective Stokes number (Stk_{eff}) as in Equations (2-11) to (2-13) (Kleinhans *et al.*, 2018).

$$\Psi(Re_p) = \frac{3(Re_p^{\frac{1}{3}}\sqrt{0.158} - \tan^{-1}(Re_p^{\frac{1}{3}}\sqrt{0.158}))}{Re_p 0.158^{3/2}} \quad (2-11)$$

$$Re_p = \frac{\rho_p d_p u_\infty}{\mu_g} \quad (2-12)$$

$$Stk_{eff} = \frac{\tau_p}{\tau_g} = \frac{\rho_p d_p^2 u_\infty}{9\mu_g d_t} \Psi \quad (2-13)$$

A typical expression of the impaction efficiency as a function of Stokes (Kær *et al.*, 2006) is in Equation (2-14) and its value is higher for bigger particles than smaller if the same number of both particles is injected.

$$\eta_{imp} = \left[1 + b(Stk_{eff} - a)^{-1} - c(Stk_{eff} - a)^{-2} + d(Stk_{eff} - a)^{-3} \right]^{-1} \quad (2-14)$$

For $Stk_{eff} > 0.14$, $a = 0.125$, $b = 1.25$, $c = 1.4 \cdot 10^{-2}$, $d = 0.508 \cdot 10^{-4}$.

Using a computational approach, the impaction efficiency on the front face of the cylinder can be calculated as the ratio between the number of particles impacting on the cylinder front face and the number of particles in the projected area of the cylinder further upstream by (2-15) (Weber *et al.*, 2013; Kleinhans *et al.*, 2018):

$$\eta_{front} = \left(\frac{n_{p,imp}}{n_{p,\infty}} \right) \quad (2-15)$$

However, if the particle position is described by the coordinates of its centre and it is treated as a point (zero particle diameter), it is necessary to modify the impaction efficiency considering that in reality the particle possesses a finite diameter and it hits the surface being away from it by a distance equal to the particle radius (Weber *et al.*, 2013) (2-16).

$$\eta_{front} = \left(\frac{n_{p,imp}}{n_{p,\infty}} \right)_{cfdcomputed} + \frac{d_p}{d_t} \quad (2-16)$$

This additional term is called interception parameter and can make the impaction efficiency greater than 1.

2.7.2 Eddy impaction ($d_p < 10 \mu\text{m}$)

Eddy impaction involves fine ash particles that tend to follow the flue gas streamlines and be blown by turbulent eddies (vortex) onto the surface where they can eventually deposit. Since turbulent eddies are difficult to be described, this mechanism is less understood and it is related mainly to empirical coefficients (Haugen and Kragset, 2010; Khodier, 2011).

An expression was proposed to calculate the particle sizes that impact the rear side of the heat exchangers (Equation (2-17)) (Simms, 2011a).

$$d_p \leq \dot{m}^{0.5} \left[\left(\frac{\rho_g u'_g}{\mu_g} \right) \left(\frac{\rho_p}{\rho_g} + 1 \right) \right]^{-0.5} \quad (2-17)$$

Where d_p is the particle diameter [m], $\bar{m}$ is the macroscale of the turbulence and can be equal to the cylinder diameter [m], ρ_g is the gas density [kg/m³], u'_g is the root mean square velocity of the gas in the wake of the tube [m/s], μ_g is the gas viscosity [Pa·s] and ρ_p is the particle density [kg/m³].

2.7.3 Thermophoresis ($d_p < 1 \mu\text{m}$)

This mechanism involves very small particles and it is due to the presence of thermal gradients as in Figure 2-8. Because of this force, ash particles move against the gradient of temperature towards the cooler heat exchanger surfaces. The deposit generated by thermophoresis is generally more distributed around steam/water tubes than inertial impaction (which occurs only on the tube upstream side) and is less sticky than condensation deposit. However, when the deposit builds up, its surface temperature increases and the temperature difference between the gas and the deposit surface decreases reducing the thermophoresis (Atkinson, 1991; Leppänen *et al.*, 2014; Kleinhans *et al.*, 2015).

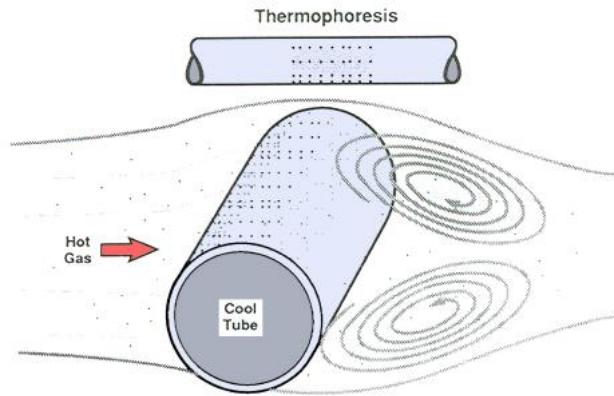


Figure 2-8: Thermophoresis mechanism on a cylinder in cross flow (Baxter, 1993).

The thermophoretic force F_T can be expressed as (Baxter, 1993):

$$F_T = 6\pi\mu_g d_p f(Kn) \nabla T_g \quad (2-18)$$

Where $Kn = \frac{2\lambda}{d_p}$ is the Knudsen number, a dimensionless number defined as the ratio of the molecular mean free path length to a representative physical length scale (particle radius); $f(Kn)$ is an expression function of the particle diameter, Knudsen number, and

several material properties; ∇T_g = temperature gradient in the gas phase at the particle position.

Thermophoresis is a temperature driven mechanism and its small contribution in fouling and slagging is still not clear because of the complexity of the correlations and deposit structure. However, the thermophoretic effect has been included in many CFD studies mainly using the Talbot model (Talbot, 1980) and it was found out that thermophoresis can slightly increase the impaction efficiency and its contribution is more significant at early stages as it is affected by the increase of surface temperature (Yang *et al.*, 2017). However, there is still a lack of CFD studies to explain and validate what has been observed experimentally (Kleinhans *et al.*, 2018).

2.7.4 Brownian diffusion ($d_p < 1 \mu\text{m}$)

This deposition mechanism is caused by the motion (diffusion) of small particles, which can reach the tube surface randomly through molecular diffusion (Hewett and Sellier, 2015).

2.7.5 Vapour Condensation

During combustion, alkali compounds (Na, K, P, Cl, S) are released in the combustion gas in the form of vapour, liquid and/or solid particles (Atkinson, 1991). Condensation of vapours from the hot gas phase on the cool surface of tubes occurs if the vapour partial pressure, at the relatively cold temperature of a tube, exceeds the vapour saturation pressure (Kohl *et al.*, 1975) (Figure 2-9). The vapour pressure of alkali compounds depends on their concentration in the gas phase, thus condensation of alkali salts is governed not only by the temperature gradient but also by the mass fraction of the salts in the fuel and gas phase reactions (Atkinson, 1991; Magda, 2012).

Condensation can occur on particles or deposit surfaces (heterogeneously) or homogeneously in the gas phase creating small particles (Baxter, 1993). This phenomenon is more relevant when biomass or fuels with large amount of inorganic materials (particularly alkali salts) are used and it is very significant especially on clean surfaces as it creates a uniform initial sticky layer which promotes particle deposition. In fact, alkali vapour condensation starts the fouling processes on cold surfaces of heat exchangers, in particular when biomass is used alone or in co-firing with coal

(Kleinhans *et al.*, 2018). When coal is used on its own, vapour condensation may be less significant and slower than the inertial impaction. (Figure 2-10).

The deposit outer surface temperature increases with its thickness, and at a certain temperature, higher than the saturation temperature of the condensable species, the condensation process slows down (Zhou *et al.*, 2007).

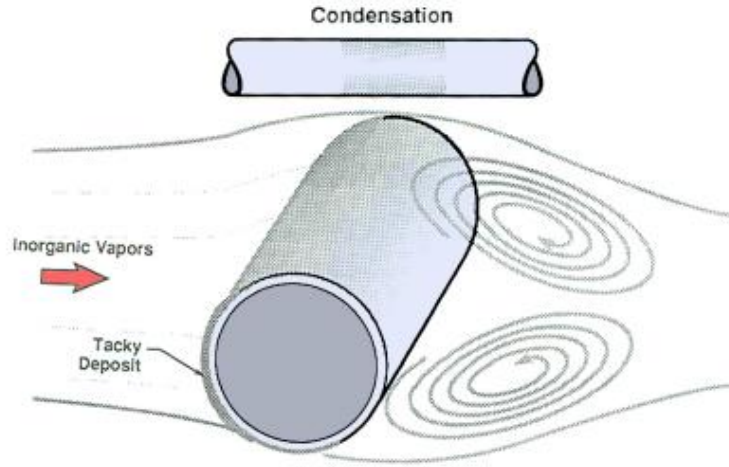


Figure 2-9: Vapour condensation on a cylinder in cross flow (Baxter, 1993).

The probability of particles to remain on the surface is defined as (Tomeczek and Waławiak, 2009):

$$P_{stick} = Sm_{c,i} \quad (2-19)$$

Where S is a constant (generally equal to $62 \text{ [kg/(m}^2\text{s)]}^{-1}$ estimated on the basis of final deposit on single industrial vertical superheater tube after nine months with dimensions opposite the deposition flux (Tomeczek and Waławiak, 2009).

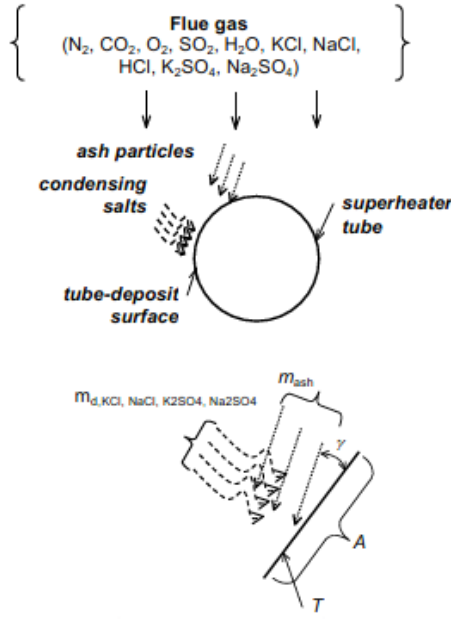


Figure 2-10: A schematic view of deposition with the condensation phenomenon (Waclawiak and Kalisz, 2011).

The flux of condensable species diffusing per unit surface area towards the outer surface of the tube can be calculated by Equation (2-20) (Tomeczek *et al.*, 2004):

$$m_{c,i} = \beta_i \frac{P_i - P_{si}}{P} \rho_g \quad (2-20)$$

Where the mass transfer coefficient β_i [m/s] of the i th component is (Tomeczek *et al.*, 2004):

$$\beta_i = \frac{Sh D_i}{d_t} \quad (2-21)$$

With D_i the diffusion coefficient of the i th component through the flue gases [m²/s], Sh is the dimensionless Sherwood number used in mass-transfer operation. It represents the ratio of the convective mass transfer to the rate of diffusive mass transport. It can be defined as function of Reynolds (Re) and Schmidt (Sc) numbers (Bird *et al.*, 2002) and different formulations exist according to the flow characteristics and Reynolds number (Equation (2-22)).

$$Sh = f(Re, Sc) \quad (2-22)$$

The vapour pressure P_i [Pa] is taken from the gas stream before the boundary layer of the tube and the main condensing species are: KCl, NaCl, Na_2SO_4 , K_2SO_4 . The saturation pressure P_s [Pa] is calculated according to the Antoine Equation (2-23) (Tomeczek *et al.*, 2004) and P is the gas pressure [Pa]:

$$\frac{P_{s,i}}{P_n} = \exp\left(A_i - \frac{B_i}{T + C_i}\right) \quad (2-23)$$

A , B and C are given constants in Table 2-3, $P_n = 10^5$ Pa and T is the tube temperature.

Table 2-3: Constants A_i , B_i , C_i used to calculate the saturation partial pressure of alkali compounds (Simms, 2011a).

Component	A	B	C	T [K]
Na_2SO_4	15.03	37452.4	0	1150-1800
K_2SO_4	18.08	39449.6	0	1150-1800
KCl	11.01	17132	-122.70	1094-1680
NaCl	11.68	19315	-82.60	1138-1738

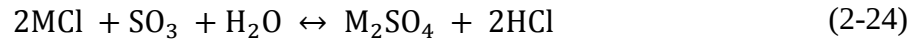
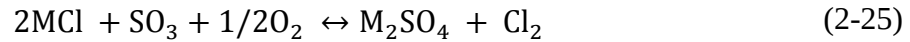
Some species (K_2SO_4) condense at high temperature (950-1200 °C) on fly ash particles in the superheater region or within boundary layers of heat exchangers. Alkali chlorides (KCl) instead are already supersaturated at lower temperatures, therefore they will condense on the tube. An important property is the vapour dew point of a compound below which condensation of the vapour leads to sub-micron particle formation in the boundary layer of the tube, enhancing the deposit build up. At surface temperatures higher than the dew point, chemical reactions can occur between the inorganic vapour(s) and solid ash particles or deposit. These reactions can change the melting temperature or create a sticky surface which increases the deposition accumulation (Kleinhans *et al.*, 2018). However, there is still a lack of knowledge about alkali species content during devolatilisation, char combustion and their concentration in the gas stream (Atkinson, 1991).

2.7.6 Heterogeneous chemical reactions

Chemical reactions between previous solid deposits or ash particles and the gas phases can change the sintering and melting temperature of deposits, determine whether a

particle sticks or not and affect the number of particles captured during inertial impaction processes. The most important chemical reactions are sulphation, oxidation, alkali absorption (e.g. silica absorbs alkali material to form silicates (SiO_3^{-2}) which melt at lower temperatures than silica) (Couch, 1994; Tomeczek and Waclawiak, 2009; Kleinhans *et al.*, 2018).

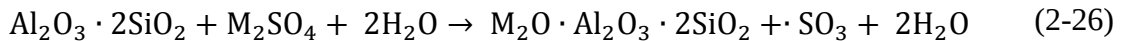
Moreover, the interaction of Fe, Na, Ca, Al and Si can lead to the formation of low temperature eutectics. Reactions from alkali absorption are slower than sulphation, these reactions can occur in the deposits layer and between solid and gaseous compounds (Equations (2-24) to (2-25)) (Kleinhans *et al.*, 2018).



Where M can be Na or K and both reactions could occur also with SO_2 rather than SO_3 ; however, sulphation is faster with SO_3 than SO_2 .

Biomass and coal combustion both produce H_2O which can react with chlorine and produce HCl. This acid, in certain conditions of temperatures, interacts with the tube metal and causes corrosion.

Alkali absorption mainly happens in the presence of aluminosilicates (kaolinite) able to absorb alkali sulphates or alkali chlorides (Equations (2-26) and (2-27)) (Kleinhans *et al.*, 2018).



This process forms low-melting point silicates and it is slower than sulphation but, above the alkali metal chloride or sulphate dew point temperature, when condensation cannot occur, it becomes faster in particular in the presence of molten aluminosilicates. Moreover, sodium silicate formation is quite high when NaOH reacts instead of NaCl. However, all chemical reactions are function of temperature that varies significantly inside the deposit layers and studies of chemical transformation of inorganic matter are still rare and unclear (Kleinhans *et al.*, 2018).

2.7.7 Others

There are also some other mechanisms such as electrostatic forces and photophoresis which are less responsible for deposit formation. However, impaction and thermophoresis are the main mechanisms for transporting particulate material to a surface. Equation (2-28) summarises the main deposition mechanisms and how they contribute to the deposition flux (Zhou *et al.*, 2007).

$$\frac{dm(t, \Theta)}{dt} = C(t, \Theta) + TH(t, \Theta) + BE(t, \Theta) + I(t, \Theta) - S(t, \Theta) - S_f(t, \Theta) \quad (2-28)$$

Where $m(t, \Theta)$ is the deposit weight, $C(t, \Theta)$, $TH(t, \Theta)$, $BE(t, \Theta)$ and $I(t, \Theta)$ are the condensation, thermophoresis, Brownian/Eddy diffusion and impaction rates respectively as a function of time t and angle around the tube Θ . $S(t, \Theta)$ is the shedding rate due to drop detachment and $S_f(t, \Theta)$ is the mass accumulation rate in a control domain caused by melt film movement (Zhou *et al.*, 2007). However, in this thesis the last two contributions are neglected.

When the probe is clean, only vapours and fine sticky particles contribute to the formation of an initial deposit layer. Once the initial deposit is formed, inertial impaction continues the ash deposit build up and chemical reactions complete the process accumulating more deposit.

The deposit surface temperature increases with the thickness of the deposit making it a more efficient collector. As the deposit thickness and the surface temperature increase, the outer part of the deposit melts down, may form drops at the bottom of the probe, which eventually detach when the surface tension cannot support their weight. Finally, at stable local conditions, a steady state can be reached and the deposition of new material is balanced by the loss due to the shedding (Zhou *et al.*, 2007).

The contribution of different deposition mechanisms have been studied in a short period of time and Figure 2-11 shows that both thermophoresis and condensation decrease quickly because of the decrease of the temperature gradient between the flue gas and the deposit surface (Zhou *et al.*, 2007). In this paper, KCl condensation was studied and its contribution to deposition was much higher than thermophoresis. Moreover, it was demonstrated that the Brownian and Eddy diffusion contribution to deposit growth were

negligible. In the first stage, when the probe surface was cool and clean, KCl condensation represented the main deposition mechanism. Once the layer was formed, the particle impactions on the front and the rear sides of the probe were dominant, however deposition rate on the upstream side by the inertial impaction was much larger than that by the intermediate sized particles and vortex interaction deposition on the downstream side of the probe.

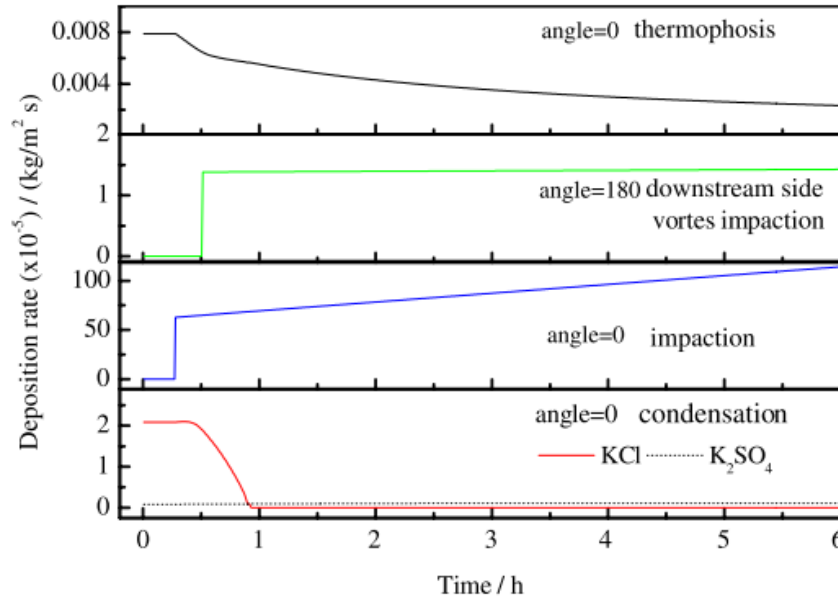


Figure 2-11: Contributions to the deposit growth by different deposit formation mechanisms (Zhou *et al.*, 2007).

2.8 Deposition modelling

Ash deposition models can be schematised into three main levels: empirical indices, mechanistic models and computational fluid dynamics (CFD) models (Zhou *et al.*, 2007; Yongtie *et al.*, 2017)

Some researchers have predicted deposition with empirical indices based on coal and ash composition (Alkali index (kg alkali/GJ), base to acid ratio, base percentage (%)) (Borio and Levasseur, 1984; Couch, 1994; Stam *et al.*, 2009; Gudka *et al.*, 2015) These indices provide information about potential fouling or slagging using the fuel characteristics determined by CCSEM (Computer-Controlled Scanning Electron Microscopy) and CHF (Chemical Fractionation) (Laumb *et al.*, 2008). However, these

indices are less accurate when applied to other fuels or operating conditions and most of them use the fuel and/or bulk ash properties that can give misleading results.

Mechanistic models, which strongly simplify the calculations on the combustion process and the fluid dynamics, have been used to predict ash deposit behaviour and define the tendency of ash deposition (Rushdi *et al.*, 2005; Zhou *et al.*, 2007). These 1D models cannot describe properly the gas and particles flow close to the heat transfer tubes and the recirculation zones downstream from the tubes (Tomeczek *et al.*, 2004). Moreover, they cannot represent properly the real superheaters behaviour since the deposition between tubes after some months of usage does not have a 1D character (Tomeczek and Waclawiak, 2009). However, they represent a good starting point to develop more sophisticated and comprehensive mathematical models of ash deposition and its impact on heat transfer in boilers.

An example is the deposition flux calculation suggested in Equation (2-29) (Tomeczek *et al.*, 2004):

$$m = P_1 P_2 C_{p,s} w \quad (2-29)$$

With: m deposition flux [$\text{kg}/(\text{m}^2 \text{ s})$], P_1 the probability that a particle will hit the heat transfer surface according to Equation (2-30), P_2 the probability of the solid particle to stick to the surface (function of the vapour condensation or particle viscosity), $C_{p,s}$ the concentration of particles in the gas stream [kg/m^3] and w the gas velocity component perpendicular to local point of heat transfer surface [m/s] (Tomeczek *et al.*, 2004).

$$P_1 = \frac{A_{duct} - A_{free}}{A_{duct}} \quad (2-30)$$

Where A_{duct} is the duct cross-section area [m^2] and A_{free} [m^2] is the cross section of the free path for flue gases.

Detailed combustion information and fluid dynamics predictions can be obtained by the CFD approach (2D or 3D). In this case, sub models of combustion mechanisms, ash transportation, particle deposition and accurate description of boundary conditions must be included. Fluent[®] is one of the CFD software used, it can describe the gas flow and particle behaviours, predict the deposit accumulation and the heat and mass transfer.

Moreover, it allows a dynamic study of the increase of surface temperature and deposit thickness and their effects on the deposit accretion (García Pérez *et al.*, 2014).

However, even applying simplifications and using advanced computers, CFD calculations can be computationally expensive, in particular when a transient approach is used (García Pérez, 2016). This technique has been used in this thesis to study the flow gas, ash particle trajectories and deposition growth and an overview of the recent literature is reported below.

2.8.1 Ash particle trajectories

Particle trajectories can be described in Fluent[®] with the Discrete Phase Model (DPM) which uses the Euler-Lagrange approach to track the particle trajectory. The Eulerian model describes the continuous phase and the Lagrangian model is used to describe particle trajectories (Guha, 2008).

Fluent[®] predicts the trajectory of a discrete phase particle by integrating the force balance on the particle in a Lagrangian reference frame. In the force balance, the particle inertia is balanced with the forces acting on the particle and can be written for the x direction in Cartesian coordinates as in Equation (2-31) (Fluent, 2001):

$$\frac{du_p}{dt} = F_D(u_g - u_p) + \frac{g_x(\rho_p - \rho_g)}{\rho_p} + F_x \quad (2-31)$$

Where $F_D(u_g - u_p)$ is the drag force per unit particle mass:

$$F_D = \frac{18\mu_g}{\rho_p d_p^2} \frac{C_D Re}{24} \quad (2-32)$$

The drag force is always opposite to the relative particle velocity and it represents the resistance that a particle meets because of the presence of the gas (continuous phase). Where u_g is the fluid phase velocity [m/s], u_p is the particle velocity [m/s], μ_g is the molecular viscosity of the fluid [Pa·s], ρ_g is the fluid density [kg/m³], ρ_p is the density of the particle [kg/m³] and d_p is the particle diameter [m].

Re is the relative Reynolds number, defined as (Fluent, 2001):

$$Re = \frac{\rho_f d_p |u_p - u_g|}{\mu_g} \quad (2-33)$$

The drag coefficient is (Fluent, 2001):

$$C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \quad (2-34)$$

Where the constants a_1 , a_2 , a_3 are functions of Reynolds and are applicable to smooth spherical particles.

For non-spherical particles the relation becomes (Fluent, 2001):

$$C_D = \frac{24}{Re} (1 + b_1 Re^{b_2}) + \frac{b_3 Re}{b_4 + Re} \quad (2-35)$$

Where the coefficients b_1 - b_4 are related to the shape factor (Appendix A, section A.3).

In Fluent[®], the force of gravity on the particle g_x can be included, as the default value of gravitational acceleration is zero. The additional force terms F_x are: Thermophoretic Force, Brownian Force and Saffman's Lift Force.

Small particle trajectories can be calculated in Fluent[®] enabling the *stochastic methods (random walk)* to include the effect of instantaneous turbulent velocity fluctuations on the particle trajectories (Tomeczek and Waclawiak, 2009; Waclawiak and Kalisz, 2012; Lee *et al.*, 2014) as shown in Figure 2-12. Without considering the turbulent effect, particles with diameter less than 10 μm do not hit the tube surface and the impacting mass flux equals 0 for all tubes. Moreover, tubes in convective superheaters are located close to each other with fine regular distances (pitch). Previous results have shown that this layout leads to a rebound effect of particles between the tube spaces (Figure 2-13).

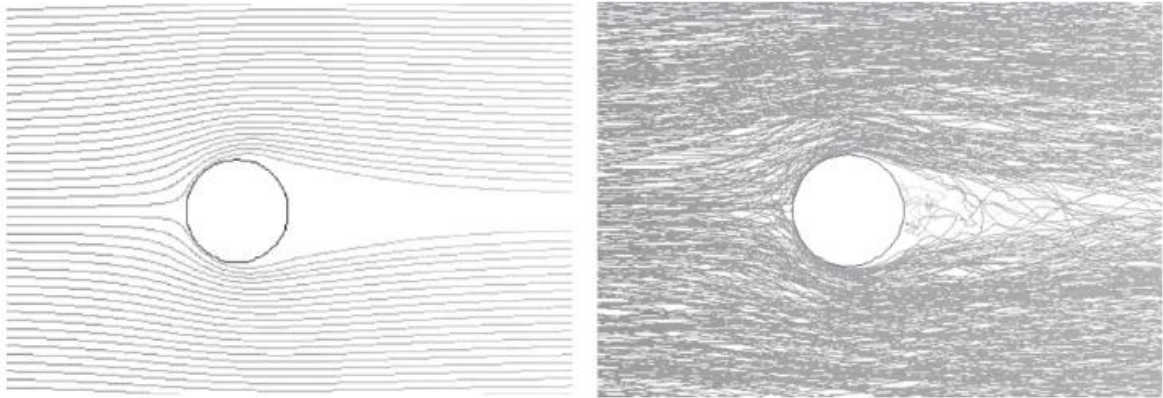


Figure 2-12: Example of trajectories for 10 μm particles, 9 m/s with (right) and without (left) “Stochastic Tracking” option (Wacławiak and Kalisz, 2012).

Inertial impaction is the process by which the majority of the particles are transported to the deposition surface due to their sufficient inertia to transverse the gas stream lines and impact the surface. This process is the most important for particles larger than 10 μm and the highest impaction rates occur at the cylinder stagnation point and decrease with angular positioning along the surface (Noll and Pilat, 1970).

Particle trajectories have been studied with different particle diameters, shape factor and normal and tangent restitution coefficient (Lee *et al.*, 2014; Wacławiak and Kalisz, 2014). The main results show that the inertia of particles larger than about 10 μm is sufficient for their trajectories to deviate from the gas streamlines in regions of strong streamlines curvature (around superheater tubes). Therefore they hit and rebound off from the tube surfaces. Smaller particles instead do not have enough inertia to overcome the drag force and cross the streamlines of the gas.

In Figure 2-13, particle trajectories of different diameters have been reported for three in line tubes. In this particular case, the rebounding effect is increased because of the influence of the neighboring rows. This effect was studied also by Wacławiak and Kalisz, 2012, 2014.

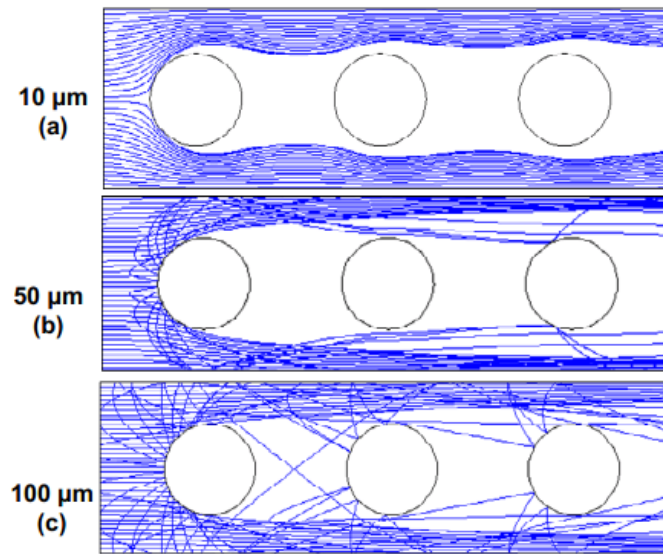


Figure 2-13: Trajectories of particles with diameters of (a) 10 μm ; (b) 50 μm ; (c) 100 μm and a velocity of 7 m/s (Lee et al., 2014).

2.8.2 Ash particle sticking behaviour

The deposition flux, defined as a mass of deposit formed per unit of surface area and time, is function of the particle concentration in the gaseous phase and the possibility of hitting the surface. Ash particles in combustion systems can be in the form of liquid droplets with Newtonian fluid flow behavior, solid elastic particles or something in between with a partially molten structure. Because of the complexity of the process, it is possible to assume that the main components of the gas are (Tomeczek *et al.*, 2004):

- particles heated in the combustion chamber above the melting temperature T_m with low viscosity (below 9 Pa s). They can stick on the cold heat transfer surfaces and trap other particles.
- solid particles of temperature lower than T_m . The only possibility for these particles to deposit when they hit the surface is the presence of a sticky layer of condensed vapours on the tube surface or on the surface of particles that deposited earlier. However, non-sticky particles cause erosion when they collide with non-sticky particles on the surface as they can remove some of these particles from the deposit (Walsh *et al.*, 1990).
- Vapour condensation on the heat exchanger surfaces.

Generally, particles tend to deposit in the flow stagnation, recirculation, the vortex separation and reattachment regions (Hosseini *et al.* , 2017).

The main parameters that determine the particle deposition are listed below (Kleinhans *et al.*, 2018):

- Particle properties (melt fraction, viscosity, surface tension, energy).
- Particle kinetic energy and its deformation after impaction.
- Particle size, shape and surface roughness.
- Angle of impaction.
- Substrate/surface roughness and geometry.
- Substrate properties (melt fraction, viscosity, surface tension, energy).
- Force between particles and surface (e.g. adhesion or van der Waals forces).

A particle (molten/semi-molten or solid) may impact on a clean or sticky surface (substrate) with an angle ϕ and kinetic energy $E_{p,kin} = 1/2m_p u_p^2$, function of the particle mass and velocity. If during the collision the particle dissipates its kinetic energy it will stick, if its kinetic energy is higher than the energy dissipated during the collision, it will rebound (Thornton and Ning, 1998). Deformations, friction between surface and particle, adhesion or vibrations are the main reasons for energy dissipation (Figure 2-14).

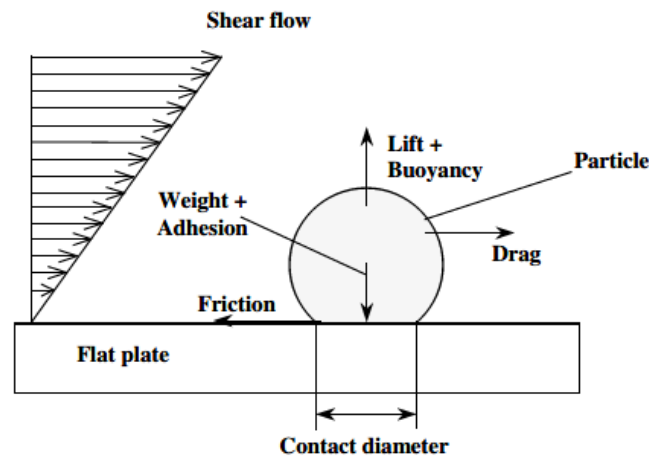


Figure 2-14: The force balance for a particle resting on a flat surface and subjected to a shear flow (Abd-Elhady and Malayeri, 2013).

The collision can be elastic or inelastic: ideally, an elastic collision occurs if the kinetic energy of the two interacting bodies is the same before and after hitting without converting in other forms of energy. In a real scenario, an inelastic collision occurs when kinetic energy is converted in other forms with and without plastic deformation (Kleinhans *et al.*, 2018). However, a plastic deformation would be more suitable to describe the behaviour of particles with low viscosity at high temperatures when they impact a cold surface (but this is out of the scope of this thesis).

When a particle hits a surface, an interface is formed which depends on particle and surface properties. The contact diameter between particle and surface, also called spread diameter, depends on particle viscosity, surface tension/energy and roughness. The contact angle between surface and particle is big for ash particles which mean less adhesiveness, low wettability due to high surface tension and low free surface energy. The main forces acting on a particle are (Figure 2-14): drag, friction and shear forces created by the flow in the boundary layer (acting parallel to the substrate/surface) and lift, buoyancy, gravity and adhesion forces (thermophoresis, surface forces due to adhesion, van der Waal forces) which are perpendicular. Moreover the thermal shock from the hot flue gas to the cool surface of the tube represents another reason for particles to stick (Abd-Elhady and Malayeri, 2013; Kleinhans *et al.*, 2018).

Several models have been developed to study the sticking probability P_{stick} of a particle impacting on a surface and they have been summarised in the following sections.

2.8.2.1 Bonded deposit models

2.8.2.1.1 Critical melt fraction/softening temperature

This approach considers the softening temperature ($T_{softening}$) of coal or biomass ash particles (Beckmann *et al.*, 2016).

$$P_{stick} = \begin{cases} 0 & \text{if } T_p < (T_{softening}) \\ 1 & \text{if } T_p \geq (T_{softening}) \end{cases} \quad (2-36)$$

If the particle temperature (T_p) is higher than the softening temperature, the particle sticks, otherwise it rebounds (Equations (2-36)). One possible approach to evaluate the softening temperature is based on the particle composition or on melting curves of the

mineral matter. These curves are realised using differential thermal/thermogravimetric analysis (DTA/TGA) or, for simple systems, thermodynamic calculations.

A typical example of melting curve is reported in Figure 2-15 where the melt fraction is a function of the temperature. It is possible to identify different temperatures on the curve: the first melting temperature T_0 , the inflection temperature T_c , the complete melting temperature T_{100} . Generally, a temperature equal to ten/fifteen percent melt fraction can be considered the sticky temperature (Mueller *et al.*, 2005; Zhou *et al.*, 2007).

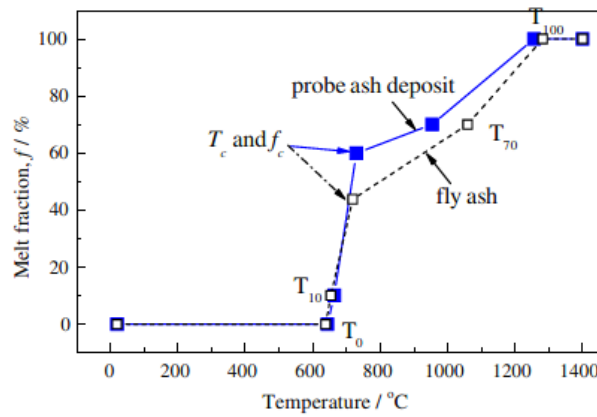


Figure 2-15: Typical melting curve for ash deposit and fly ash in a straw fired grate boiler (Zhou *et al.*, 2007).

This model has been widely used for predictions of ash and vapour deposition in biomass fired boiler and several values of melt fractions have been suggested to predict the particle behaviour. Another way of approaching this model is based on the definition of the sticking probability as a function of the particle melt fraction f_p (Kær *et al.*, 2004, 2006; Akbar *et al.*, 2016) as is Equations (2-37).

$$\begin{aligned}
 P_{stick} &= 0 \text{ if } f_p = 0 - 0.15 \\
 &1 \text{ if } f_p = 0.15 - 0.7 \\
 &0 \text{ if } f_p = 0.7 - 1
 \end{aligned}
 \tag{2-37}$$

Thermodynamic calculations can be carried out to define the behaviour of ash particle at a certain temperature and detect its melt fraction. However, it is important to notice that

more complex systems may melt at a temperature different from the single components. Mueller found that deposits will build up for surface temperatures at which the melt fraction is between 0.15 and 0.70 but, above this value, an equilibrium between deposition and flowing off will be established (Mueller *et al.*, 2005). However, these numbers might change according to the operating conditions and the fuel used. Moreover, it was noticed that this model works better for small particles ($d_p < 75 \mu\text{m}$), while for bigger particles an energy criterion (explained later) is more appropriate (Kleinhans *et al.*, 2018).

2.8.2.1.2 Critical viscosity model

This model has been widely used in the literature and it was first suggested to predict deposition of discrete particles while using bituminous coal (Walsh *et al.*, 1990). According to this model, the particle sticking probability depends on the particle viscosity (μ_p) and a reference viscosity (μ_{ref}), generally determined from experiments (Richards *et al.*, 1993; Lee and Lockwood, 1999; Costen *et al.*, 2000; Kær *et al.*, 2004, 2006; Wieland *et al.*, 2012). The particle viscosity can be calculated considering its chemical composition and temperature and many empirical correlations were developed (Senior and Srinivasachar, 1995; Lee and Lockwood, 1999; Vargas, Frandsen and Johansen, 2001; Wieland *et al.*, 2012). At lower viscosity, particles are softer and the probability to stick is higher than at higher value of viscosity (Equations (2-38)):

$$P_{stick}(T, X) = \begin{cases} \frac{\mu_{ref}}{\mu} & \text{if } \mu_p > \mu_{ref} \\ 1 & \text{if } \mu_p \leq \mu_{ref} \end{cases} \quad (2-38)$$

Some correlations have been suggested for various temperature ranges to define the sticking probability of ash particles containing more than 5 wt.% iron (as Fe_2O_3) (Tomeczek *et al.*, 2004). Moreover, many values of reference viscosity (μ_{ref}) have been proposed (from 1 Pa s to 10^9 Pa s), but they depend strongly on the type of fuel, the chemistry and melting behaviour (Walsh *et al.*, 1990; Weber *et al.*, 2013; Beckmann *et al.*, 2016). However, a wrong evaluation of these parameters may over or under predict the actual viscosity.

A variation of this model is based on the particle critical viscosity (Costen *et al.*, 2000; Modlinski, 2014) and it states that if the particle viscosity is lower than the critical viscosity, the particle will stick otherwise it will rebound (Equations (2-39)).

This model was also reformulated using the temperature of critical viscosity, function of the mineral matter composition. When the particles exceed the critical viscosity temperature, the particle sticks on the surface. Since this temperature range is very large, a lot of studies and experiments have been carried out in order to improve the understanding and find reasonable values and mathematical correlations for the reference viscosities (e.g. Schulze *et al.*, 2010; Schulze *et al.*, 2011). The viscosity based approach has been widely applied for biomass ashes that show higher melting point compared to coal ashes, however experimental investigations are necessary to provide more data.

$$P_{stick}(T, X) = \begin{cases} 0 & \text{if } \mu_p > \mu_{cr} \\ 1 & \text{if } \mu_p \leq \mu_{cr} \end{cases} \quad (2-39)$$

With $\mu_{ref} \neq \mu_{cr}$

A correlation between the critical viscosity and the particle kinetic energy was first proposed by Richter ($\mu_{ref} = 0.01 \mu_{cr}$) (Richter, 2002) and used in other works (Schulze *et al.*, 2003; Modlinski, 2014).

Increasing the particle kinetic energy, particles need a lower viscosity and therefore a higher temperature to stick. In fact, smaller particles show higher sticking probability at a certain temperature and chemical composition (El-Batsh, 2001; Kleinhans *et al.*, 2018). However, this correlation is the result of experimental investigations with soda-lime glass particles whose behaviour is similar to coal fly ash.

$$\log_{10}(\mu_{cr}) = -0.9699 \log_{10} \left(\frac{E_{p,kin}}{E_{p,kin0}} \right) + 5.5962 \quad (2-40)$$

With $E_{p,kin}$ ash particle kinetic energy and $E_{p,kin0}$ kinetic energy of the smallest particle assumed to be $E_{p,kin0} = 4.35e^{-11}$ J (Srinivasachar *et al.*, 1990).

A limitation of these models is the current lack of correlations between ash properties and temperature. Moreover, many works have used bulk ash chemistry rather than the individual chemical composition of fly ash particles, which can lead to wrong conclusions (Kleinhans *et al.*, 2018).

2.8.2.2 Powdery deposit

This model was applied to predict solid ash particle deposition on a smooth surface. Three main forces are taken into account to assess if a particle will be captured or not: the normal elastic rebound force $F_{s,n}$, van der Waals adhesion force $F_{v,w}$ and normal component of gravity F_G as shown in Figure 2-16.

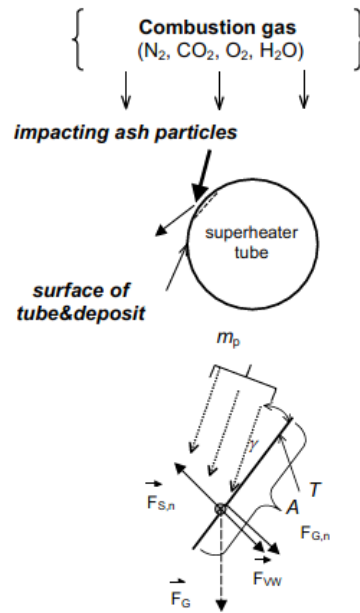


Figure 2-16: A schematic view of the powdery deposition (Wacławiak and Kalisz, 2011).

The fouling probability P_f can be calculated as follows (Wacławiak and Kalisz, 2011):

$$P_f = 0 \text{ if } F_{s,n} > (F_{v,w} \pm F_{G,n})$$

$$1 \text{ if } F_{s,n} \leq (F_{v,w} \pm F_{G,n})$$
(2-41)

With:

$$F_{s,n} = K d_p^2 w_p^{1.2}$$
(2-42)

Where K is a constant depending on particle and deposition surface elasticity, w_p is the perpendicular component of impaction velocity [m/s].

In previous works, several values of K have been used but a correlation between K and the particle diameter was also suggested (Wacławiak, 2010):

$$K(d_p) = G \left(\frac{d_p}{d_{ref}} \right)^n \quad (2-43)$$

Where G is a constant ($G = 1$), d_{ref} is a reference diameter ($d_{ref} = 20 \mu\text{m}$) and n is an exponent which should be assumed ($n = 2$) and then verified in order to improve the model predictions. In fact, the major difficulty in solving this model is the determination of the constant values (Wacławiak, 2010).

The van der Waals force is:

$$F_{v,w} = \frac{B d_p}{6 \delta^2} \quad (2-44)$$

Where B is a molecular interaction constant ($B = 1 \cdot 10^{-17} [\text{Kg s}^{-2} \text{m}^2]$) and δ is a distance between the particle and the deposition surface ($\delta = 0.5 d_p [\text{m}]$) (Wacławiak and Kalisz, 2011, 2012).

Finally, the gravity force is given by (Wacławiak, 2010):

$$F_G = \frac{1}{6} \pi d_p^3 \rho_p g \quad (2-45)$$

Where g is the gravitational acceleration [m/s^2] and it is taken into account because it can enhance (or not) the deposition according to the flue gas direction.

These equations were taken from a Russian book (Zanieczyszczonych, 1992) where it is explained that in a zone of contact between particles and the surface some microscopic deformations take place and the result is a reaction called rebounding force. This model was applied in less severe conditions of temperature (flue gas temperature = 500-550°C; surface temperature = 440°C) (Wacławiak and Kalisz, 2012) and, by some other authors (Lee *et al.*, 2014), to describe the ash deposition in heavy fuel oil steam generator.

However, this approach does not include the vapour condensation and is more suitable for clean surface and dry solid particles.

For temperatures below the melting points of the particulate (dry conditions) the van der Waals is the dominant sticking force. However, during combustion, alkali vapours are released and, at temperature lower than their dew point, they can condense modifying the sticking process. As a consequence, this effect can increase the sticking of the surface and the particle according to the so called liquid bridge formation (El-Batsh, 2001).

2.8.2.3 Energy conservation models

In this section, deposition modelling is based on energy conservation of a particle at the moment of the impact. This model has been used to predict deposition for solid particles or liquid droplets impacting a smooth surface (Kleinhans *et al.*, 2018). The energy balance has been used to derive the particle critical velocity (Equation (2-46)) (Kleinhans *et al.*, 2018).

$$E_{kin,i} + E_{surf,i} = E_{def} + E_{ad} + E_{surf,r} + E_{kin,r} \quad (2-46)$$

With: $E_{kin,i}$ particle kinetic energy, $E_{surf,i}$ particle surface energy, E_{def} work of viscous dissipation (deformation), E_{ad} work of adhesion with the index i for initial conditions of impacting particle and r rebounding particles. If $E_{kin,r} = 0$, particles stick. Some other forms of energy (van der Waals, elastic wave propagation, rotational energy of particle, potential energy) are neglected in this equation. If the particle has more kinetic energy than the energy dissipated in the collision the particle bounces off the surface, but if the collision can dissipate all of the particle kinetic energy, the particle will stick. Therefore, a value of velocity, called critical or capture velocity u_{cr} can be defined according to Equations (2-47) to (2-52) (El-Batsh, 2001).

$$u_{cr} = \left[\frac{2E}{d_p} \right]^{\frac{10}{7}} \quad (2-47)$$

$$E = 0.51 \left[\frac{5\pi^2(k_1 + k_2)}{4\rho_p^{3/4}} \right]^{2/5} \quad (2-48)$$

$$k_1 = \frac{1 - v_s^2}{\pi E_s} \quad (2-49)$$

$$k_2 = \frac{1 - v_p^2}{\pi E_p} \quad (2-50)$$

$$E_s = E_p = 3 * 10^{20} \exp(-0.02365 T_{AVG}) \quad (2-51)$$

$$T_{AVG} = \frac{T_s + T_g}{2} \quad (2-52)$$

Where: E is the composite Young's modulus [Pa], v Poisson's ratio of material [-], with s referring to the surface and p to the particle proprieties and T_{AVG} is the average temperature [K] between the gas and the surface.

The equations above can be used to calculate the critical velocity u_{cr} and establish the stickiness criteria based on a comparison between the critical particle absolute velocity and the particle absolute velocity or its normal component (Weber *et al.*, 2013; Yang *et al.*, 2016) (Equations (2-53)).

$$P_{stick} = 0 \text{ if } |u_p| > |u_{p,cr}| \quad (2-53)$$

$$1 \text{ if } |u_p| \leq |u_{p,cr}|$$

If the particle velocity is smaller than the capture velocity, the particle sticks, otherwise it rebounds and continues the trajectory until it leaves the domain or impacts the surface at another place (Losurdo, 2009; Weber *et al.*, 2013).

A similar approach was used in another work where a numerical model was developed to predict fouling formation by particles impacting a solid surface. The material properties of both particle and surface were taken into account as they affect the energy losses and the surface energies that will determine the sticking or rebound of the particle (Bouris and Bergeles, 1996).

This model has been widely applied in particle technology studies where solid particles (not molten) impact on a clean surface (no sticking layer) (Thornton and Yin, 1991). It was used to predict deposition in different environments: from powder inhalers (Milenkovic *et al.*, 2013) to heat exchangers (Mueller *et al.*, 2005; Losurdo, 2009; Ai *et al.*, 2011; Weber *et al.*, 2013; Zha *et al.*, 2013; Losurdo and Bertrand, 2014) and turbine vanes (Barker *et al.*, 2011; Ai and Fletcher, 2016). However, the Young's modulus and the Poisson number values for ash particles are still unknown and many simplifications have been done (Bouris and Bergeles, 1996).

Another energy conservation based model used for slagging of ash droplets on heat exchangers has been developed by Yang *et al.*, 2018. The main steps that determine the sticking/rebounding process can be summarised as follows:

- 1) Ash droplets have a certain kinetic energy before impaction on a surface.
- 2) When ash droplets impact on the surface for inertial and viscous forces, their kinetic energy is transferred to the surface energy and can be dissipated.
- 3) When ash droplets are flattened on the surface, they do not have any kinetic energy but have maximum surface energy.
- 4) If ash droplets have enough energy to detach, the rebound takes place.

This model takes into account the ash chemistry, particle physical properties, deposit surface properties and furnace operation conditions (Yang *et al.*, 2018). The sticking criterion is based on the correlation between the excess energy ratio (E^*) and the sticking efficiency (E_{stick}) (Equations (2-54) and (2-55)).

$$E^* = \frac{1}{4}d_m^2(1 - \cos \theta) + \frac{2}{3d_m} - 0.00536d_m^{4.70}(1 - \cos \theta)^{0.591} - 1 \quad (2-54)$$

$$E_{stick} = \exp(aE^*) \text{ if } E^* > 0$$

$$1 \text{ if } E^* \leq 0 \quad (2-55)$$

Where $a = -9.21$, θ is the contact angle [degree] and d_m is the maximum spread ratio, also defined as the ratio between the maximum spread diameter and the original droplet size (d_p) (Equation (2-56)).

$$d_m = 1 + 0.259We^{0.317} \quad (2-56)$$

$$We = (\rho_p u_p^2 d_p) / \zeta_{LV} \quad (2-57)$$

With We , Weber number defined in Equation (2-57), ρ_p is the particle density [kg/m³], u_p is the normal component of the ash droplet impact velocity [m/s] and ζ , the liquid-vapour surface tension [N/m].

This model has demonstrated to give good predictions of fly ash deposition at high temperatures (slagging). However, one drawback is the need for material properties, difficult to be determined (e.g. contact angle, surface tension, etc.) for different fuels.

2.8.2.4 Summary

Overall, a comparison between the main models used in the literature and summarised in this section shows that the sticking efficiency is higher for small particles at high temperatures, which impact with a low velocity and small impaction angle (Fu *et al.*, 2017; Hosseini *et al.*, 2017). However, the impact angle meaning is still not fully understood because of a lack of experimental information. In fact, the main challenge of these models is the determination of material proprieties as function of temperature and composition, for such a wide range of ash particle compositions and structures.

Ash sticking models are mainly based on ideal conditions such as perfectly spherical particles or droplets impacting on a clean solid surface of well-known properties. In real boilers, the conditions are very different and complex. In fact, particles are generally irregular and this shape determines different impaction and deformation behaviour. Moreover, they have a variable chemical composition and, even if mullite and quartz have been reported to be the major components of fly ash, at high temperatures they can melt and behave differently. In fact, there is still a lack of studies of particle stickiness behaviour at high temperatures.

Moreover, in a real power plant, the surface of the tube is really clean and smooth only when it is started for the first time. On a clean tube, only particles in a sticky condition will deposit and when the deposit builds up its surface temperature increases, becomes sticky and able to collect more particles whether they are tacky or not. As a consequence, the effect of the surface roughness and stickiness should be taken into account as, once the deposit is formed on the surface (powdery, sintered or molten), the stickiness tendency changes with the surface properties (Kleinhans *et al.*, 2018).

The formation of an initial oxide layer on the tube surface is often neglected and it is where the condensation of alkali vapours starts from. However, it is quite complicated to capture all the mechanisms involved, such as the stickiness of the particle and the surface or the chemical reactions of alkali vapour and fly ash particles that can change the material properties. For example, when a particle impacts on the surface it creates a glue between the surface and the fly ash particle which is difficult to detect in experiments and even more in modelling predictions. At this purpose, a total sticking probability (P_{tot}) was defined to predict deposition as a function of the particle and surface stickiness (Kær *et al.*, 2006; Schulze *et al.*, 2011) (Equation (2-58)).

$$P_{tot} = P_s(1 - P_p) + P_p(1 - P_s) + P_sP_p \quad (2-58)$$

Where P_s is the surface stickiness probability and P_p is the particle stickiness probability.

For spherical particles it is possible to include the detachment model taking into account the effect of the fluid flow on the particle deposition. Rolling, sliding and lifting are the main mechanisms of detachment but rolling is dominant. Therefore, the detachment of particles from smooth surfaces is caused by the fluid dynamic in the viscous sublayer. If the external forces (drag and lift) exceed the sticking force, the particle will be detached (El-Batsh, 2001). However, this aspect is not investigated further.

Recent works have studied ash related problems with CFD models extended by User Defined Functions (i.e. UDFs). They were able to predict the behaviour of gas and particles and ash particle deposition in a small domain around the heat exchangers without including combustion or ash formation (Tomeczek and Wacławiak, 2009; García Pérez, 2016; Yang *et al.*, 2018).

The main UDFs used are (ANSYS FLUENT, 2009a):

- DEFINE_DPM_EROSION to calculate the deposition flux using the mass flow rate of ash particles, area of the face hit by particles and the impaction angle.
- DEFINE_DPM_BC to specify boundary conditions for particles. The function is executed every time a particle touches a boundary of the domain, except for symmetric or periodic boundaries. It is possible to define a separate DEFINE_DPM_BC UDF for each boundary.

- DEFINE_GRID_MOTION to calculate the growth of the deposit taking into account time, deposit density and deposition flux.
- DEFINE_PROFILE to calculate the increasing deposit surface temperature. This UDF can be used to study a generic variable at a boundary condition.

The deposition flux $m_{f,A}$ [kg/m² s] can be calculated as function of the sticking probability P_{stick} , or P_{tot} , the mass flow rate m_p [kg/s] of particulate matter striking the deposition surface A [m²] and the impaction angle γ [rad] according to Equation (2-59) (Waclawiak and Kalisz, 2012).

$$m_{f,A} = P_{stick} \frac{dm_p}{dA} \sin(\gamma) \quad (2-59)$$

CDF models are able to predict deposit formation and location, so soot-blower positions and soot blowing intervals can be optimised. This tool can also be used to identify the right location for the injection of additives.

In the literature, the real superheaters are simplified for computational reasons and an example of the tubes arrangements and mesh is reported in Figure 2-17 (Waclawiak and Kalisz, 2011).

$s_1/d_t = 1.5-2$ and $s_2/d_t = 1.5-3$ for convective superheaters;

$s_1/d_t = 5-10$ and $s_2/d_t = 1.5-1.1$ for radiant superheaters.

However, there are some works where wider configurations have been used (Yang *et al.*, 2016).

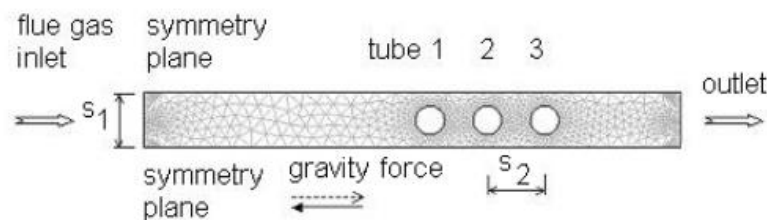


Figure 2-17: Mesh for modelled in-line superheater tube bank (Waclawiak and Kalisz, 2011).

Good results were obtained using CFD with the critical viscosity approach and reference viscosity model, however an appropriate choice of the reference viscosity

values is necessary since this varies with the fuel. In other studies, energy and momentum conservation criteria have been used but the main problem was to find the right value of Young's modulus and the Poisson number as a function of temperature and for different ash particle chemistry. Relatively good results were obtained applying the melt fraction model with a thermodynamic study of the melt fraction (Kleinhans *et al.*, 2018).

Figure 2-18 shows an example of how the shape of deposit and its thickness change according to the approach used. In fact, when the powdery deposit model is applied, the maximum thickness found was about 9 mm after 32 hours of operation; instead for bonded deposits the deposit height detected was almost 74 mm after 5 hours of operation. Moreover, independently of the model, deposit accretion occurs mainly on the upstream of the tube as confirmed in pilot and industrial scale boilers.

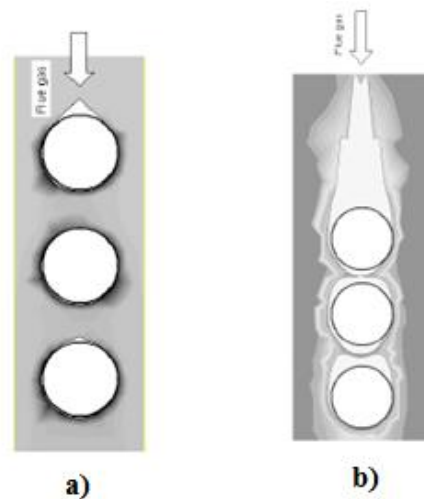


Figure 2-18: Shape of predicted deposits: a) powdery model on steam reheater tubes after 32 hours, b) bonded deposits formed by plastic ash particles on superheater tubes after 5 hours (Waclawiak and Kalisz, 2011).

Finally, additional studies are necessary to develop a more complete CFD model to predict ash formation in particular in coal and biomass co-firing. In fact, ash formation is quite well understood for coal but, biomass needs more research as there are still no suitable models for wood or herbaceous biomass (Kleinhans *et al.*, 2018). Moreover, future studies will be necessary to address the role of deposit structure and how to consider this in advanced CFD models.

2.8.3 Deposit shape

In some recent works, the deposit shape prediction has been modelled in Fluent[®] using DEFINE_GRID_MOTION UDF. Once the deposition flux $(m_{f,A})_i$ [kg/(m² s)] at each node i , has been predicted the deposit thickness t_i [m] can be calculated with the deposit density ρ_{dep} [kg/m³] and the exposure time [s].

The node can be displaced considering the deposition thickness at each node of the cylinder t_i and its direction, obtained with the angle θ normal to each face (García Pérez *et al.*, 2014; Fornasier, 2016).

This procedure allows changing and moving the grid vertices to simulate the deposition growth. During the calculation, one vertex drags two faces and according to this kind of movement, the best mesh is the triangular (unstructured). However, this grid does not guarantee high accuracy but it is the only one that is allowed by the “remeshing” option in Fluent[®].

One of the biggest and most frequent issues of using grid motion is that an overlap between neighbouring faces can occur and lead to an error called “negative volume” which does not allow the simulation to be completed (Figure 2-19).

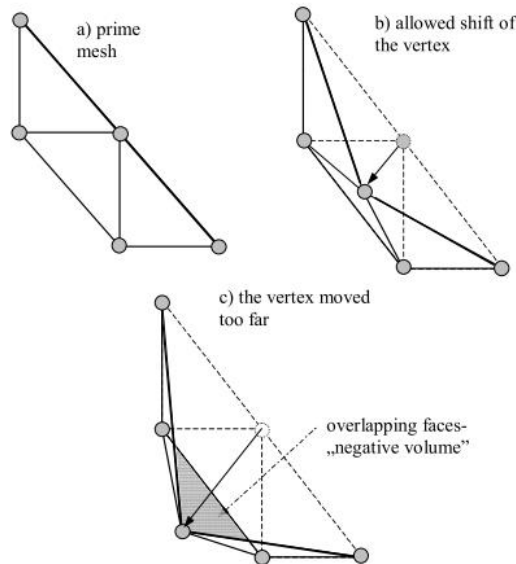


Figure 2-19: Schematic of negative volume generation (Waclawiak and Kalisz, 2011).

However, the deposit shape simulation is very important as the deposit build-up can modify the tube geometry, cause an increase in the gas velocity and have an impact on deposition mechanisms and flux (Bouris *et al.*, 2005; El Gharbi *et al.*, 2015).

2.8.4 Deposit temperature

During combustion in utility boilers, heat is transferred from hot flue gases to the steam inside the tubes by radiation, convection and conduction (Figure 2-20). In particular, heat is transferred from the hot flue gas (T_g) to the deposit surface (T_{dep}) by radiation and convection, by conduction through the deposit and the tube wall (T_{wall}) and finally to the coolant by convection (Zbogor *et al.*, 2005).

Deposit formation has an impact on each heat transfer mechanism, insulates the heat exchangers and reduces the heat transfer between the combustion gas and the water-steam cycle which strongly affects the boiler thermal efficiency (Richter *et al.*, 1984). In fact, deposit formation changes the flow dynamics around tubes and can determine an increase in the gas velocity (Furmański, 1995). Moreover, the formation of deposit layers on tubes influences the conductive and radiative heat transfer. The deposit properties are different from the clean tube surface and less thermal radiation is absorbed and emitted. In particular, the radiative properties of deposits (emissivity ϵ_{dep} , absorptivity α_{dep}) are influenced by the microstructure of deposits (Furmański, 1995). Since material radiative properties are function of the temperature, deposit formation influences the flue gases emissivity ϵ_g and transmittance τ_g as well as the deposit properties since the deposit temperature changes (Chen and Ramer, 1994). Moreover, deposits have a lower thermal conductivity ($0.2 < k_{dep} < 4$ W/m K) if compared to steel tubes (ferritic steel has higher thermal conductivity than austenitic steel) ($12 < k_{steel} < 57$ W/m K) and this reduces the conductive heat transfer through the deposit (Kleinhans *et al.*, 2018).

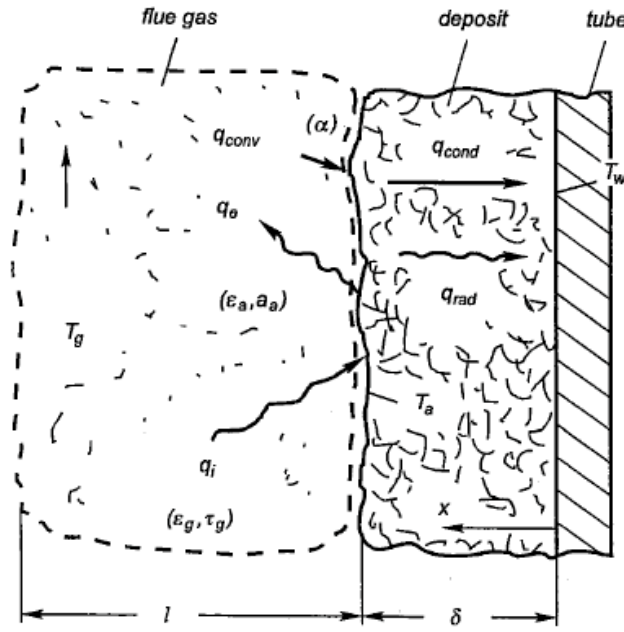


Figure 2-20: Interaction of gas radiation and convection with heat conduction and radiation in the ash deposit (Furmański, 1995).

The convective heat flux $\dot{Q}_{conv}$ [W/m²] is expressed by Equation (2-60) (Furmański, 1995):

$$\dot{Q}_{conv} = h_{conv}(T_g - T_{dep}) \quad (2-60)$$

With h_{conv} being the convective heat transfer coefficient [W/m² K], T_g and T_{dep} the gas and the outer deposit temperatures [K].

The heat flux exchanged by thermal radiation between the flue gases and the surface of the ash deposit is calculated as (Furmański, 1995):

$$\dot{Q}_{rad} = \dot{Q}_i - \dot{Q}_e \quad (2-61)$$

With: $\dot{Q}_i$ the incident radiation from the gas which takes into account the gas transmissivity τ_g (generally equal to zero) [W/m²], $\dot{Q}_e$ the emitted radiation from the deposit ($\tau + \rho + \alpha = 1$, with ρ being the reflectivity) (Furmański, 1995).

$$\dot{Q}_i = \epsilon_g(\sigma T_g^4) + \tau_g \dot{Q}_e \quad (2-62)$$

$$\dot{Q}_e = \varepsilon_{dep}(\sigma T_{dep}^4) + (1 - \alpha_{dep} - \tau_{dep})\dot{Q}_i \quad (2-63)$$

Assuming flame emissivity equal to unity (valid for large boilers) and neglecting the heat transfer through the wall and the steam (therefore assuming a constant wall temperature) it can be stated that the total external heat flux $\dot{Q}_{tot}$ [W/m²] is function of the convective and radiative contributions and is equal to the conductive heat flux through the deposit $\dot{Q}_{cond}$ according to Equation (2-66) (Kleinhans *et al.*, 2018).

$$\dot{Q}_{tot} = \dot{Q}_{conv} + \dot{Q}_{rad} = h_{conv}(T_g - T_{dep}) + \sigma\alpha_{dep}T_g^4 - \sigma\varepsilon_{dep}T_{dep}^4 \quad (2-64)$$

$$\dot{Q}_{cond} = \dot{Q}_{tot} \quad (2-65)$$

$$\dot{Q}_{cond} = \frac{T_{dep} - T_{wall}}{\frac{r_{dep}}{2\pi k_{dep}} \ln(\frac{r_{dep}}{r_{wall}})} = h_{conv}(T_g - T_{dep}) + \sigma\alpha_{dep}T_g^4 - \sigma\varepsilon_{dep}T_{dep}^4 \quad (2-66)$$

Where: T_{wall} is the tube wall temperature [K], k_{dep} the deposit thermal conductivity [W/m K], r_{dep} , and r_{wall} , the deposit and tube radius [m], σ is the Stephan-Boltzmann constant [W/m² K⁴], ε_{dep} the deposit emissivity, α_{dep} the absorption coefficient of the deposit layer, τ_{dep} the deposit transmissivity (equal to zero).

Heat transfer calculations have often simplified the cylindrical tube surface to a slab and the thermal resistance R is calculated as follows:

$$R = \frac{t_{dep}}{k_{dep}} \quad (2-67)$$

Where t_{dep} is the deposit thickness [m].

Moreover, the heat transferred by conduction and radiation through the deposit $\dot{Q}_a$ is in Equation (2-68) (Furmański, 1995).

$$\dot{Q}_a = \dot{Q}_{rad} + \dot{Q}_{cond} \quad (2-68)$$

The conductive component of heat flux [W/m²] is:

$$\dot{Q}_{cond} = -\frac{k_{dep}dT}{dx} \quad (2-69)$$

However, for high optical thickness ash layer, the radiative component of the heat flux can be expressed as:

$$\dot{Q}_{rad} = -\frac{k_r dT}{dx} \quad (2-70)$$

The effective thermal conductivity of the ash can be introduced (Furmański, 1995):

$$\dot{Q}_a = -(k_{dep} + k_r) \frac{dT}{dx} = k_{eff} \frac{dT}{dx} \quad (2-71)$$

Where k_{eff} is the effective deposit thermal conductivity [W/(m K)].

According to the deposition mechanisms, the deposit can be loose and dusty in case of gravity deposition, dense and compact for inertial impaction (with either sticky particles or deposit) or columnar structures (due to the shadow effect of existing deposit). As result of the insulating effect of deposition, the outer layer surface of the deposit increases in temperature and it can even approach the gas temperature. The higher temperature causes melting and interaction of the particles resulting in the formation of a liquid phase which has higher emissivity/absorptivity than sintered or powdery deposit and it can transfer the heat easily compared to thick sintered deposits. However, molten deposits are difficult to remove (Furmański, 1995).

The chemical composition is very important for the thermal conductivity, in fact dense deposits of Al_2O_3 and MgO showed to have lower thermal conductivity at higher temperature while SiO_2 thermal conductivity increases with temperature. Deposit porosity depends on grain size, temperature, physical state and chemical composition of the impacting particle and existing deposit. When temperatures are higher, salts start melting and the liquid fills the pores which reduces the deposit porosity. The deposit thermal conductivity should be calculated considering the contribution of each component's thermal conductivity since the gas can be retained in the deposit and its thermal conductivity influences the deposit thermal conductivity (Furmański, 1995).

In order to study the heat transfer through the deposit, it is necessary to know the thermal and physical properties of the deposit. First of all, the deposit thermal conductivity can be calculated as a function of its porosity and thermal conductivity of the gas and solid phase according to the following equations (2-72) to (2-74) (Robinson *et al.*, 2001; Magda, 2012):

$$k_{dep} = (1 - F)k_g + Fk_s \quad (2-72)$$

$$F = \frac{2^n}{2^n - 1} \left(1 - \frac{1}{(1 + \phi_{dep})^n} \right) \quad (2-73)$$

Where k_g and k_s are the gas and solid thermal conductivity respectively [W/m K] and F , the weighting factor between the gas and the solid, function of the deposit porosity ϕ_{dep} and an empirical parameter ($n= 6.5$).

Moreover, the deposit porosity ϕ_{dep} can be calculated considering the initial porosity $\phi_{dep,0}$ and the ratio between the melt v_l and solid deposit phase v_s .

$$\phi_{dep} = 1 - \left[(1 - \phi_{dep,0}) + \frac{v_l}{v_s} (1 - \phi_{dep,0}) \right] \quad (2-74)$$

The amount of liquid and solid in the deposit is calculated by using chemical equilibrium methods and then estimating the density of the liquid phase as a function of the chemistry (Yang *et al.*, 2017).

The effective thermal conductivity of the ash deposit increases with the ash density. Deposit growth is an unsteady process, the initial deposit porosity refers mainly to the first layer of alkali vapours condensed on the heat exchanger surfaces with high transparency and an initial porosity of ~ 0.6 and thermal conductivity of 0.08-0.1 W/m K (high resistance to heat flow). However, the local porosity tends to decrease when the deposit grows because of the formation of liquid able to fill the pores and impede the transport of hot gas radiation to the walls. Due to the high density, the deposit is non-transparent to thermal radiation and it is already totally opaque for a layer exceeding 0.7 mm, with a higher thermal conductivity (0.2-1.7 W/m K). It has been demonstrated that the increase in content of iron oxides leads to a higher density of the deposit which may

be the main reason for the increase of the effective thermal conductivity (Furmański, 1995).

Some expressions for gas and solid thermal conductivities have been suggested depending on the temperature (Magda, 2012), however, in other works the gas has been approximated to nitrogen ($k_g = 0.06$ W/(m K)) and the solid to silica at high temperature ($k_s = 4$ W/(m K)) (Richards *et al.*, 1993) and $k_s = 2.17$ W/(m K) for SiO₂ at 800 K (Tomeczek *et al.*, 2004).

In many works, the insulation due to deposit accretion was included to develop predictions of deposit surface temperature. Recent CFD studies have been carried out to study the heat transfer with a dynamic approach that can include the effect of an increasing temperature on deposition accretion. In some cases the tube wall temperature was assumed to be constant and iterative calculations were done to find the updated deposit temperature (Costen *et al.*, 2000). Therefore, the deposit temperature T_{dep} can be calculated as in Equation (2-75):

$$T_{dep} = \dot{Q}_{tot}R + T_{wall} \quad (2-75)$$

Formation of deposit has a deep influence on heat transfer in the boiler especially in the first stages of ash deposition. In fact, already after a few hours since beginning of the boiler operation, the deposit layer can reduce the heat transfer by almost a half due to a resistance that it offers to the heat flux. The ash layer quickly builds up and attains a thickness of cm in coal-fired boilers. The deposit can require regular air (or water blowing) or application of vibrations in order to maintain acceptable boiler performance. By using some additives in the fuel, such as MgO, the deposit can be removed easily from the tube surfaces; however additives cannot change the amount of ash deposits. Forecast of thermal and radiative properties of ash deposits is difficult due to the complex interaction of different factors such as conditions of the flue gases, heat transfer in the boiler, chemical reactions, phase and microstructure transformations in the ash deposit (Gudka *et al.*, 2015; Yang, 2016).

Two main CFD approaches have been identified in the literature to study the deposit surface:

- 1) Using DEFINE_PROFILE as a boundary condition on the tube surface where the temperature is calculated with Equation (2-75).

According to this criterion, the deposition flux calculated in DEFINE_DPM_EROSION can be used to calculate the deposition thickness. This value is applied in two UDFs: DEFINE_GRID_MOTION, which simulates the deposition shape, and DEFINE_PROFILE. However, this approach is not able to study the temperature gradient inside the deposit (Figure 2-21).

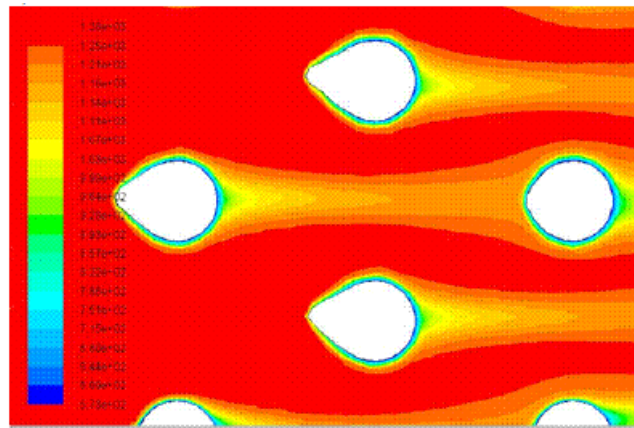


Figure 2-21: An example of temperature field, and deposit shape on air preheater tubes after three years at velocity 5 m/s (Waclawiak, 2016).

- 2) The second approach involves the use of two UDFs: DEFINE_DPM_EROSION and DEFINE_GRID_MOTION.

In this case, the tube surface is surrounded by a thin layer of deposit. The interface between the fluid and the solid (deposit) is called double coupled wall (wall and its shadow according to Fluent[®] terminology) as in Figure 2-22.

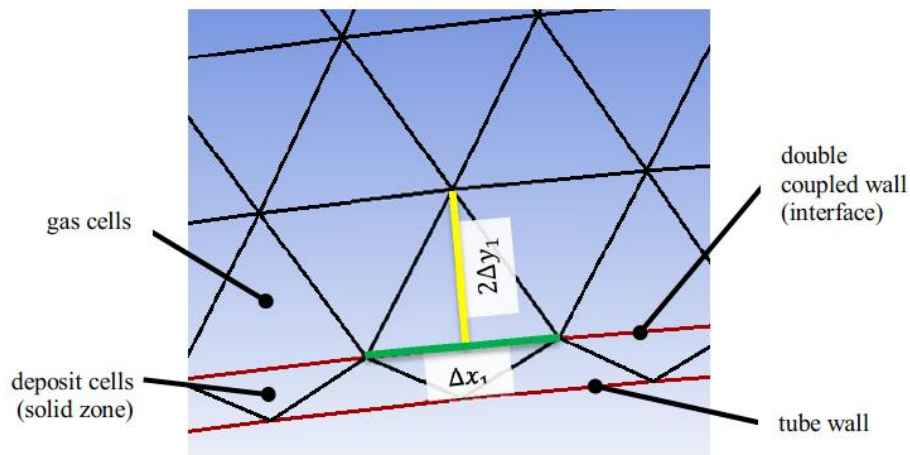


Figure 2-22: Representation of double coupled wall: detail of the first layers of cells in the near-wall regions of a tube (García Pérez et al., 2014).

The two UDFs are applied to the interface and Fluent[®] is able to calculate the surface temperature of the growing deposit knowing the gas and solid thermal properties. An example of the effect of the deposit growth on the temperature and on the gas velocity is in Figure 2-23.

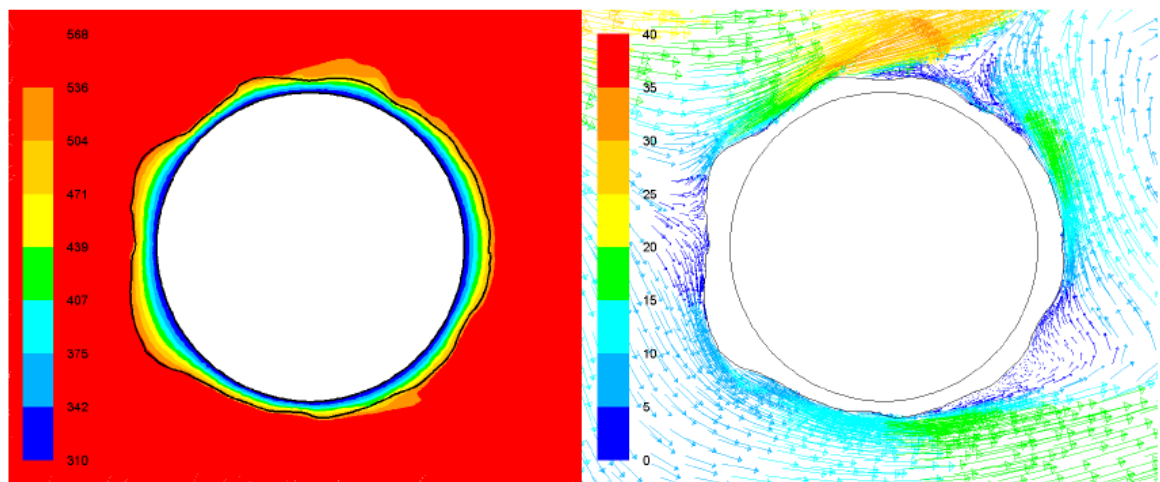


Figure 2-23: Modelled deposit shape and contours of temperature in the deposit and in the flow around it after 2 hours of growth [°C] (left). Velocity field at the same location at the same moment as in the image on the left (right) (García Pérez et al., 2014).

In this way it becomes possible to see the temperature gradient through the deposit from the colder layer, closer to the tube wall, to the outer layer in contact with the gas that, as a consequence of the insulation effect, exits at higher temperature compared to a clean

tube, affecting the thermal efficiency (García Pérez, 2016). However, even if this approach can give a more detailed description of the phenomenon, it is more difficult to realise because of the double coupled wall meshing and the need for a high resolution mesh.

2.9 Summary

The literature review in this chapter highlights the complexity of deposit formation on heat exchangers which depends on the fuels, combustion technology, operating conditions and it requires a multidisciplinary approach in order to be fully understood. Ash related issues have been studied for many years since the deposit build-up on tube walls can lead to corrosion, deteriorate the boiler thermal efficiency until unexpected outages.

In a context where the attention has moved towards alternative source of energy (e.g. biomass) used alone or with traditional fossil fuels to reduce CO₂ emissions and increase the boiler efficiency, more studies need to be carried out to predict the fuels behaviour in utility boilers and identify the best operating condition and cleaning solutions.

Previous studies developed 1D empirical and mechanistic models where deposition fluxes were calculated taking into account the bulk ash chemical composition which can bring to different results compared to SEM/EDX analyses of single particles.

The progress in computer technology has allowed the development of CFD techniques that can simulate the gas flow, ash particle trajectories and deposit prediction according to several sticking models. Moreover, using this approach, it is possible to study the dynamic effect of the deposition growth on flow behaviour and on surface temperatures. However, these models still rely on experimental data to provide chemical and physical characteristics of gases, ashes and deposits. In fact, further investigations need to be carried out to fill the existing gap about the behaviour of less known fuels, such as biomass, especially when they are co-fired and considering that ash and deposit characteristics can deeply differ from a pilot scale to an industrial scale plant.

3 CFD MODELLING METHODOLOGY

3.1 Introduction

Computational fluid dynamics (CFD) combines fluid mechanics with mathematics and computer science. This approach significantly reduces lead times and costs in design and production compared to experimental based techniques, and is also able to solve flow problems that the analytical approach cannot answer. However, the modelling assumptions (e.g. boundary conditions, material properties etc.) and the numerical errors in computations imply that there will be differences between the computed results and reality (Tu *et al.*, 2007c; Mahmood *et al.*, 2012).

CFD modelling has been recognised to be one of the best existing tools to study deposition on heat exchangers (Saber and Ashtiani, 2010; Chapela *et al.*, 2018). In this work, Fluent[®] was chosen as commercially available CFD software widely used in industry. Different versions were applied during the course of this PhD according to the availability (from Fluent[®] 16.2 to Fluent[®] 17.1) and they were extended by User Defined Functions (UDFs). These are functions (programmed by the user in C language) that can be linked with the solver to customise physical properties, boundary conditions, supply external model equations, etc. In particular, three UDFs (sections 3.7, 3.8, 3.9) were chosen as starting points from the Fluent[®] UDF manual (ANSYS FLUENT, 2009a), modified and compiled in Fluent[®] using Microsoft Visual Studio. Therefore, an initial reinforcement of fluid dynamics and coding knowledge was required before starting to develop new models.

In this chapter, the methodology applied to develop the model is explained. It has been used to carry out simulations with increasing levels of difficulty: starting from simple examples (one tube, data from the literature, single deposition mechanisms) to more complicated scenarios (combination of deposition mechanisms and higher number of tubes) until model validations with experimental results (Chapters 4 and 7 respectively). In fact, the understanding of deposition on heat exchangers obtained during the experiments was used to improve and validate the framework mathematical model previously built for deposit predictions. The model consists of two main interacting

phases: the gas flow which was studied with the Navier Stokes equations and the second discrete phase whose behaviour was simulated with the Discrete Phase Model (DPM).

The three main elements of a CFD model analysis are reported below and their link is shown in Figure 3-1:

- pre-processor
- solver
- post-processor

Some of them will be discussed in this chapter to illustrate how the deposition models have been developed.

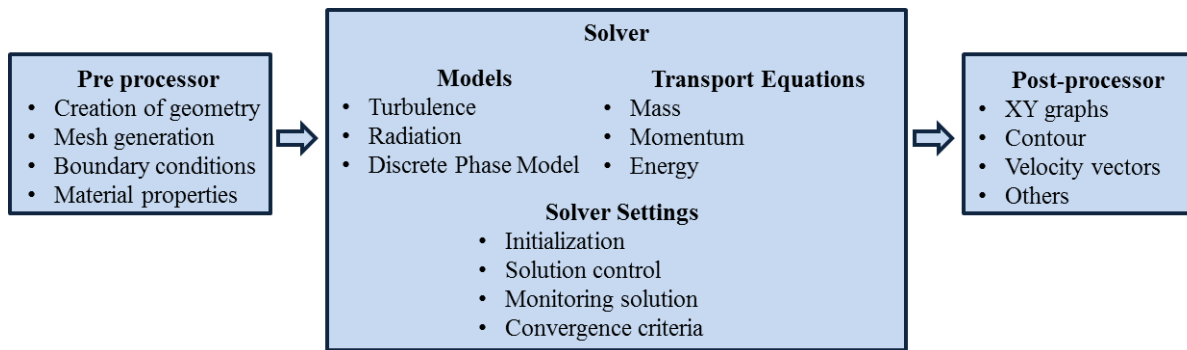


Figure 3-1: Main elements of a CFD analysis and their inter-connectivity (modified from (Tu *et al.*, 2007b)).

A detailed description of the main equations used by Fluent[®] for the gas flow and particles is given in Appendix A (Tu *et al.*, 2007a; ANSYS FLUENT 12.0 UDF Manual, 2009; Canonsburg, 2015).

3.2 Creation of the flow geometry

The first step in any CFD analysis is the creation of the flow geometry (i.e. the computational domain) representative of the physical domain (Tu *et al.*, 2007a). Deposition on heat exchangers is a typical example of external flow scenario around tubes (Hewett and Sellier, 2015). In this work, the geometry was simplified to a two-dimensional rectangular domain which contains the cylinder; the fluid enters at the left boundary and exits at the right boundary of the computational domain.

This type of problem requires that the length of the domain allows the formation and shedding of vortices typical of flow past a cylinder. Moreover, in this particular case, the top and bottom boundary effects may influence the flow passing around the cylinder. Therefore, the height of the domain should be fixed at a distance able to remove any boundary effects on the fluid flow surrounding the cylinder, but at the same time be manageable for CFD calculations (Tu *et al.*, 2007b).

Different tube arrangements have been used in the literature. These vary if the superheaters are convective or radiative (Tomeczek and Waclawiak, 2009; Waclawiak and Kalisz, 2012; Lee *et al.*, 2014) and some of them were applied at the beginning of this research project as part of the learning process (Weber *et al.*, 2013; Waclawiak and Kalisz, 2014) (Appendix F).

One of the first geometries investigated, with one tube (diameter $d_t = 38$ mm) in the middle of the domain, and its boundary conditions are given in Figure 3-2. Similar geometries were applied in previous works (Weber *et al.*, 2013; Yang *et al.*, 2016). In this particular case, for the top and bottom walls, the mirror symmetry of the geometry was used and *symmetry* was chosen as boundary condition since it also reduces computational effort (Bouhairie and Chu, 2007; Salim and Cheah, 2009). However, other non-symmetric geometries were developed later and, for these, *wall* was used as boundary condition for the top and bottom wall (zero fluid velocity at the wall). Once the CFD tools had been learnt and the model settled upon, the real configuration of Cranfield combustion rig (Chapter 4) was investigated and then particular cases were used for model validation (Chapter 7).

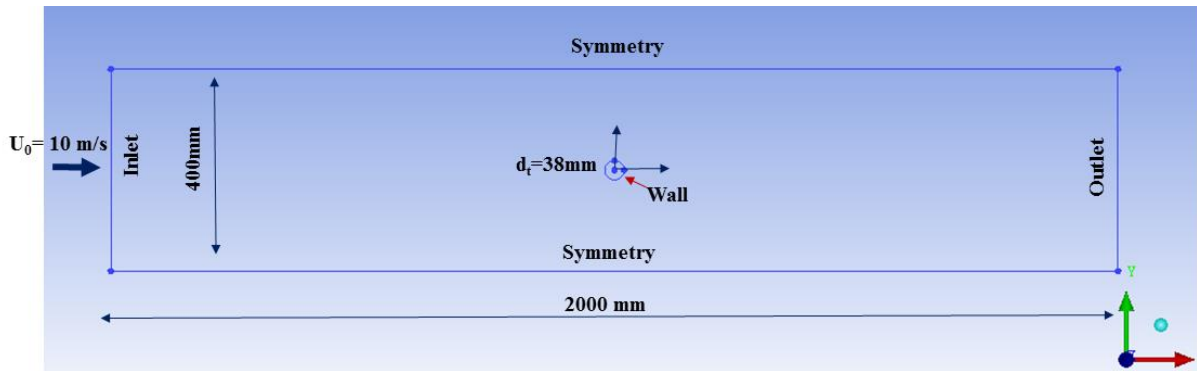


Figure 3-2: 2D geometry and boundary conditions for deposition study around one tube (tube diameter $d_t = 38$ mm) (modified from (Weber *et al.*, 2013)).

3.3 Mesh generation

The mesh generation represents one of the most important steps during the pre-process stage (Tu *et al.*, 2007b). The domain previously created was divided into a number of smaller, non-overlapping subdomains in order to solve the flow physics inside the geometry. The accuracy of a CFD solution depends on the number of cells in the mesh within the computational domain. However a compromise should be found between an accurate solution and computational costs (Dröge, 2007).

Firstly, a structured mesh (with quadrilateral cells) was generated using ICEM CFD 16.2, one of the available software for mesh quality (Yang, 2016). The regular connectivity of this type of grid allows a better convergence and a higher resolution but, at the same time, increases the computational costs. The structured mesh and its magnification around the cylinder are reported in Figure 3-3 and Figure 3-4 respectively.

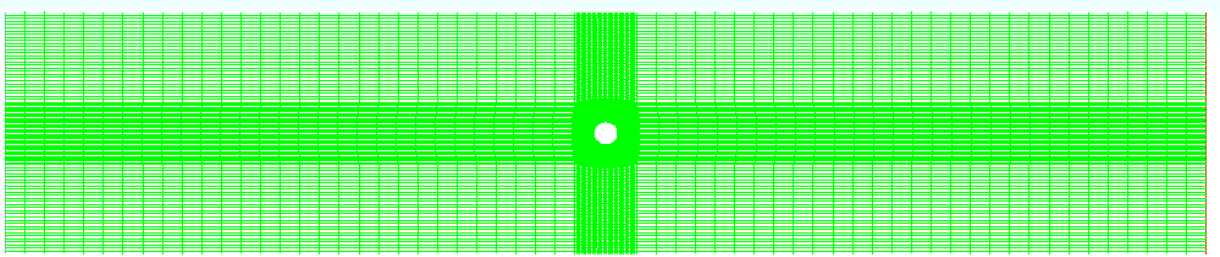


Figure 3-3: Structured mesh around a circular cylinder ($d_t = 38$ mm).

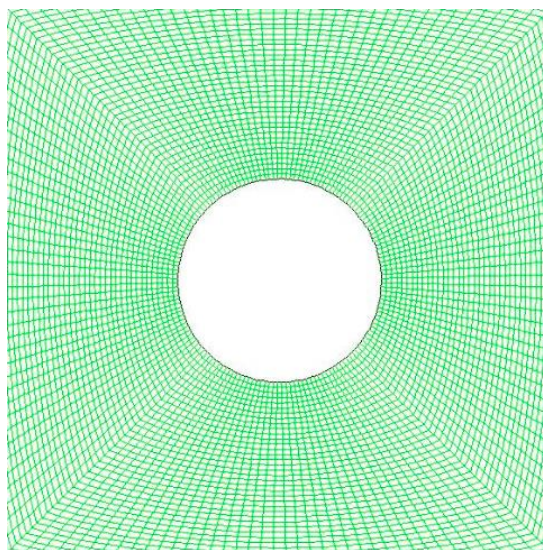


Figure 3-4: Structured mesh magnification around a circular cylinder ($d_t = 38$ mm).

This block-structured mesh has a total of 13972 cells, 28216 faces, 14244 nodes, 156 wall faces on the cylinder. The estimated quality mesh is:

- Minimum Orthogonal Quality= $8.56 \cdot 10^{-1}$ (Orthogonal Quality ranges from 0 to 1, where values close to 0 correspond to low quality).
- Maximum Ortho Skew= $1.43 \cdot 10^{-1}$ (Ortho Skew ranges from 0 to 1, where values close to 1 correspond to low quality).
- Maximum Aspect Ratio= 0.97 (ideally equal to 1).

Later, an unstructured (triangular) mesh was needed to study the grid movement (as will be discussed in section 3.8 and in Chapter 4). This was generated using ANSYS Workbench, software of the same package, easier to use for triangular mesh. In fact, the dynamic mesh option was enabled to simulate the shape of the deposit but the UDF for grid motion with “remeshing” option works only with unstructured mesh (Wacławiak and Kalisz 2011; Garcia Pérez 2016), which does not guarantee the same accuracy. However, this limitation can be overcome refining the mesh close to the cylinder wall to resolve the boundary layer separation and the vortex shedding (Rahman *et al.*, 2008) (Figure 3-5).

Moreover, to fully resolve the viscous sublayer, it is advised to place at least a few cells within $y^+ < 5$ and have $y^+ \approx 1$ for near-wall modelling (Salim and Cheah, 2009) (section A.5).

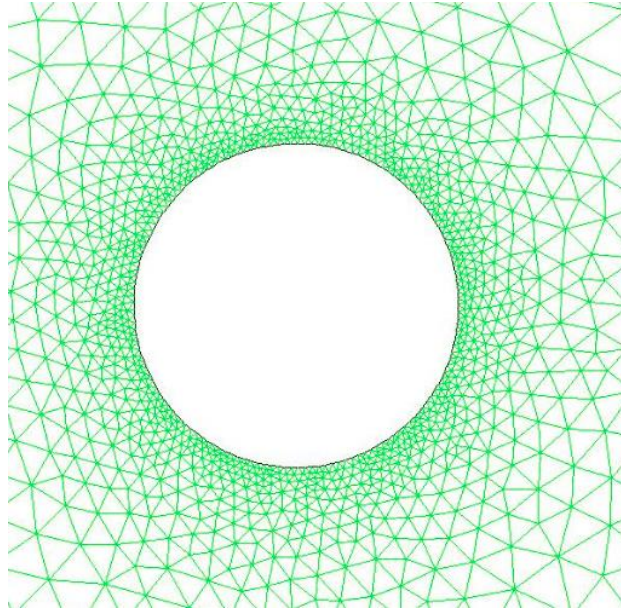


Figure 3-5: Unstructured mesh magnification around a circular cylinder ($d_t = 38$ mm).

Finally, the grid sensitivity is a very important step in the development of CFD modelling as it ensures that the results are independent from the grid size. Ideally, three different grids (coarse, medium, and fine) should be generated to analyse if any differences in the results can be detected (Haugen and Kragset, 2010). The grid sensitivity conducted to study deposition in Cranfield's combustion rig is explained in Chapter 4 and section B.1.

3.4 Simulation set up

The mesh generated and its boundary conditions were imported into Fluent[®] where the CFD simulations were carried out. The definition of appropriate boundary conditions is significant to mimic the real physical representation of the fluid flow in a CFD problem (Tu *et al.*, 2007b). The mass, momentum and energy Navier-Stokes equations were implemented with second-order upwind schemes. A least square cell based method was used to calculate gradients. In Fluent[®] the solver was: pressure based, first-order implicit, double-precision, unsteady, SIMPLE. The default solver's upwind schemes use second order differences in pressure, momentum and energy equations. For the rest of equations (turbulent kinetic, energy and dissipation rate) the default first-order schemes were used. However, in some simulations they were set as second order upwind to improve the convergence. All residuals were one order of magnitude less than default

and fifty iterations per time step were computed. The main parameters to set up the simulations and the boundary conditions are summarised in Table 3-1.

Table 3-1: CFD simulation settings.

Setting	Choice
Geometry	2D
Solver	Pressure based, transient, first-order implicit, double-precision
Pressure velocity coupling	SIMPLE
Spatial discretisation:	
<i>Gradient</i>	Least square cell base
<i>Pressure</i>	Second Order
<i>Momentum</i>	Second Order Upwind
<i>Turbulent kinetic energy</i>	First/Second Order Upwind
<i>Turbulent dissipation rate</i>	First/Second Order Upwind
<i>Energy</i>	Second Order Upwind
Transient Formulation	First Order Implicit
Boundary conditions	
Inlet	Velocity inlet
Outlet	Pressure Outlet
Top wall	Symmetry/wall
Bottom wall	Symmetry/wall
Cylinder	Wall

3.5 Study of the gas flow

The flue gas was approximated to be air entering the domain with a maximum velocity U_0 of 10 m/s (different velocities were tested: 3, 4 and 10 m/s) and temperature of 1273 K, while the tube surface temperature was supposed to be constant (e.g. 700 K). Preliminary simulations were run using some properties from the literature review to describe the flow regime (Yang *et al.*, 2016). For instance, with gas density $\rho_g = 0.245$ kg/m³ and gas viscosity $\mu_g = 46 \cdot 10^{-6}$ Pa·s), the Reynolds number was calculated using the following formula (3-1):

$$Re = \frac{\rho_g U_0 d_t}{\mu_g} \quad (3-1)$$

Where d_t is the tube diameter [m]. According to the Reynolds number obtained (~ 2000), this case study is close to a Von Karman vortex trail (Haugen and Kragset, 2010). In fact, the presence of the obstacle (cylinder) creates some disturbances which are source of turbulent conditions and the Reynolds-Averaged Navier-Stokes (RANS)

equations were used to determine the flow properties (Appendix A, sections A.1 and A.2).

Different turbulent models were used in this work. At the beginning, the turbulent model $k-\varepsilon$ was chosen with standard input data and, at the inlet, the gas had turbulent intensity of 10% (Wacławski and Kalisz, 2014). This is one of the simplest models used in engineering applications, but its performance is quite poor in flow separation and streamline curvature (ANSYS FLUENT, 2006c). Therefore, other turbulence models were applied such as the $k-\varepsilon$ Realizable and $k-\omega$ SST. The latter was used to validate the model since it describes better the boundary layer and the vortex shedding (García Pérez, 2016; Yang *et al.*, 2017) as shown in Chapter 4. (More details are given in Appendix A, section A.2).

Vortex shedding and deposition on heat exchangers have a dynamic nature and only some recent works have studied deposition using a dynamic approach (García Pérez *et al.*, 2016; Yang *et al.*, 2017). In this thesis, transient simulations were carried out and the choice of the time step is crucial to get reliable results and capture the vortex shedding correctly. The vortex shedding frequency was calculated using the Strouhal number, a dimensionless number which is a function of the Reynolds number and gives information about the time step needed to capture the vortex shedding (Lienhard, 1966). However, the time step size is generally defined based on the Courant number in Equation (3-2).

$$C = \frac{U_0 \Delta t}{\Delta x} \leq 1 \quad (3-2)$$

Where: C is the Courant number, U_0 is the free stream velocity [m/s], Δt is the time step size [s] and Δx is the cell size of the domain [m]. The Courant number is a dimensionless number that indicates how the flow moves within the computational domain and compares the time step used in the calculation to the characteristic time that the fluid needs to go through the domain. For instance, if $C \leq 1$, the fluid goes from one cell to the other in (max) one time step, while if $C > 1$, the fluid moves through more cells at each time step. This latter behaviour can compromise the solution convergence (ANSYS Fluent, 2015).

The Courant number is recommended to be ~ 1 and always below 10 (García Pérez, 2016) and the time step size that ensures a Courant number ≤ 1 was calculated using Equation (3-2).

3.6 Discrete phase study

The particle trajectory model was developed using the Discrete Phase Model DPM in Fluent[®] which uses the Euler-Lagrange approach and allows the tracking of the actual position histories of non-zero mass particles using their own inertia (Fluent, 2001). The Eulerian model describes the behaviour of the continuous phase while the Lagrangian model is used to describe the behaviour of the particles. This second phase is assumed to consist of spherical particles dispersed and diluted (volume fraction usually less than 10-12%) in the continuous phase.

Fluent[®] predicts the trajectory of a discrete phase by integrating the force balance on the particle, which is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle (drag, gravity and additional forces) as in Equation (2-31) (more details are given in Appendix A, section A.3).

Particles were assumed to be perfectly spherical inert ash particles. These are injected at the inlet surface boundary where the number of grid faces influences the number of particles injected. The flow rate was scaled by face area and particles injected used face normal direction (see enabled options in Figure 3-7). The model took into consideration the force of gravity acting on the moving ash particles together with the direction of the flue gas (x positive). Thermophoresis was included as additional force term in some of the simulations with the Talbot model (Figure 3-9) (Appendix A, section A.3).

Initially, simulations were run for the fluid without particles. Once the flow was developed around the tube, these were used as the initial fluid field conditions for the transient simulations with particles to study particle deposition.

A two-phase coupled flow was used; this means that in the discrete phase model dialog box the interaction between the two phases was active with 10 iterations of the continuous phase per one discrete phase iteration (Figure 3-6). In fact, this option allows the study of deposit accretion and should be enabled only once the gas flow is quasi steady state. However, inter-particle collisions were neglected since ash particles have a

much higher density than the fluid and the number of these particles is low enough. The maximum number of steps was set to 5000 (at least) with a step length factor of 5. Moreover, the heat transfer between the two phases was included using Law 1 or Law 6 which use a heat balance to relate the particle temperature, $T_p(t)$, to the convective heat transfer and the absorption/emission of radiation at the particle surface (Fluent, 2001) (Appendix A, section A.4) .

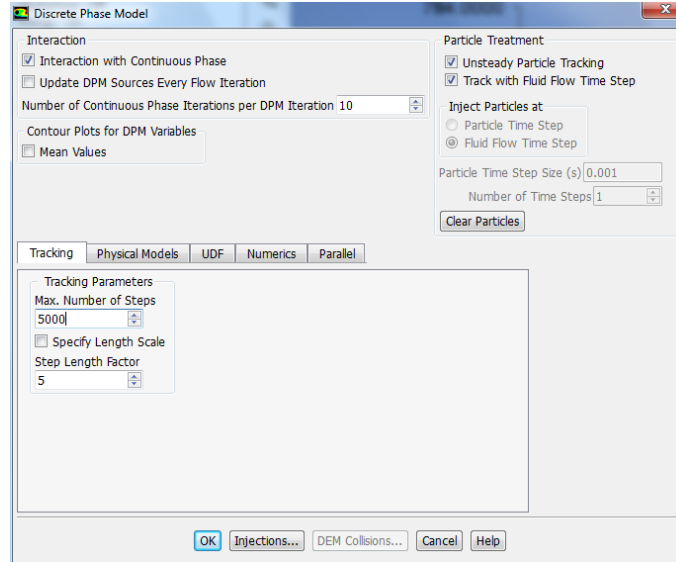


Figure 3-6: Interaction with continuous phase.

The dispersion of particles due to turbulence in the fluid was included by enabling the options for Discrete Random Walk (i.e. DRW) and the Random Eddy Lifetime (with time scale constant 0.15) (Figure 3-7). This permits the prediction of small particle trajectories and their impaction on the backside of the tubes that would not be detected in absence of turbulence (Tomeczek and Waclawiak, 2009; Lee *et al.*, 2014).

Trajectories of different ash particle diameters were studied in steady and unsteady DPM. However, when DPM is unsteady, it is very expensive to track each single particle; therefore Fluent[®] tracks parcels that contain particles with the same properties such as diameter, velocity and position. In this work, ash particle behaviour was studied when injecting either ash particles with uniform diameters (single ash particle diameters) or ash particles with the Rosin-Rammler size distribution model (Fluent, 2001). Once the injections were set, ash particle properties were defined using the Materials' menu.

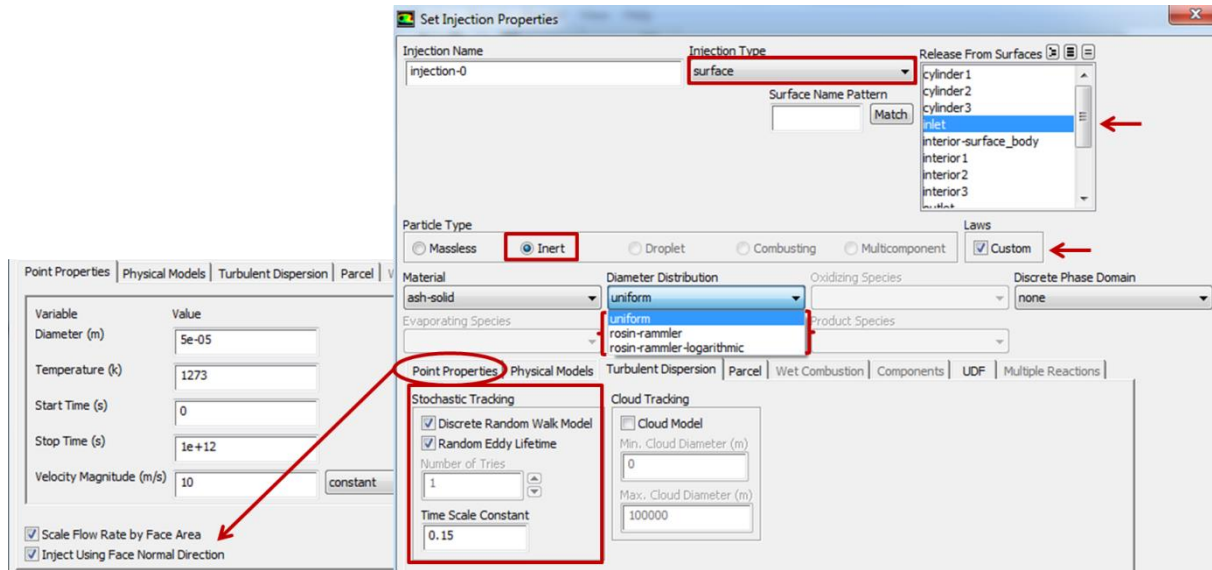


Figure 3-7: Particle injection properties.

The fate of the particle trajectories when a particle hits a boundary condition were left as default (as reported in Table 3-2). In case of walls set as “reflect”, the restitution coefficient was generally left as default (polynomial), however it has been demonstrated to have an impact on particle trajectories (Wacławiak and Kalisz, 2014).

Table 3-2: DPM Boundary conditions.

DPM Boundary conditions	
Inlet	Escape
Outlet	Escape
Top wall	Reflect
Bottom wall	Reflect
Cylinder	Reflect

3.7 Deposition modelling

In this work, deposition on superheaters and reheaters (i.e. fouling) in coal and biomass co-firing was studied and models were developed combining different deposition mechanisms to calculate the total deposition fluxes on heat exchanger surfaces.

Once a particle hits the cylinder wall surface, its probability of sticking and rebounding depends on the particle and surface conditions, expressed with some mathematical correlations (section 2.8.2).

The particle deposition flux $m_{f,A}$ [kg/(m² s)] was calculated with Equation (2-59) as a function of the stickiness probability P_{stick} , the mass flow rate m_p [kg/s] of particulate matter striking the deposition surface A [m²] and the impaction angle γ [rad] (Figure 3-8).

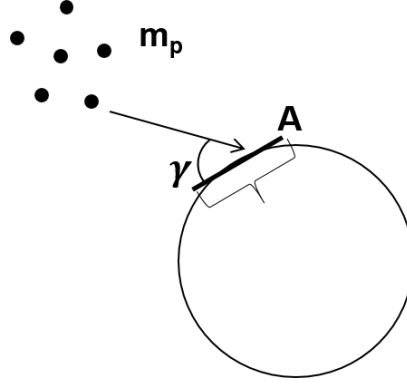


Figure 3-8: Parameters for particle impaction on a tube.

Some preliminary simulations were carried out using single deposition mechanisms. However, since the probability of a particle sticking (P_{stick}) depends on the stickiness of the particle and the surface, a total probability P_{tot} was also calculated (Equation (2-58)). At the beginning of each simulation, the probe surfaces were clean (without deposit), therefore the effect of vapour condensation was considered responsible for the surface stickiness, while the particle stickiness was based on the viscosity model as a function of the particle composition and temperature according to the Urbain model with Kalmanovitch modification (Browning *et al.*, 2003) (Chapter 7). Furthermore, the total deposition flux m_{tot} was calculated including not only the deposition term due to the particles (first term) but also the vapour condensation contribution $m_{c,A}$ in Equation (3-3), which is a modification of Equation (2-59).

$$m_{tot} = P_{tot} \frac{dm_p}{dA} \sin(\gamma) + m_{c,A} \quad (3-3)$$

These assumptions were implemented using a modified version of the DEFINE_DPM_EROSION UDF, which defines the accretion rate as the particle stream strikes a wall surface. This function is called within the model when a particle encounters a reflecting surface (DPM boundary condition) and it is defined as follows: DEFINE_DPM_EROSION (*dpm_accr*, *p*, *t*, *f*, *normal*, *alpha*, *Vmag*, *mdot*).

Where *dpm_accr*, *p*, *t*, *f*, *normal*, *alpha*, *Vmag*, and *mdot* are eight arguments; only the name of the UDF *dpm_accr* is supplied by the user, the other seven are provided by the Fluent[®] solver to the UDF.

The meaning of these parameters is as follows:

- *p* is the pointer to the tracked particle which contains information related to the particle.
- *t* is the pointer to the face thread the particle is currently hitting.
- *f* is the index of the face that the particle is hitting.
- *normal* is the array that contains the unit vector that is normal to the face.
- *alpha* is the variable that represents the impact angle between the particle path and the face [rad].
- *Vmag* is a variable that represents the magnitude of the particle velocity [m/s].
- *mdot* is the flow rate of the particle stream as it hits the face [kg/s]. However, in transient simulations *mdot* is the mass [kg] of particles impacting the surface and the time is not included. Therefore, this must be taken into account considering that flow time [s] = Δt [s/time step] * $n_{\text{time step}}$ [number of time steps].

It is important to highlight that the vapour condensation contribution to the deposition flux, in Equation (3-3) and its simplified versions, was included in the modified DEFINE_DPM_EROSION UDF (~ 200 lines) and the vapour concentration in the flue gas was supposed to be constant during the simulations.

User-Defined Memories (i.e. UDMs) can be used for additional calculations such as: number of particle hits into wall face, average diameter of particles that hit the wall, average radial velocity of particles that hit the wall, etc. Therefore, before compiling the UDF, the number of User Defined Memories Locations needs to be set (Define → User Defined Memory → Number of User Defined Memories Locations).

After the UDF had been compiled (Define → User Defined Functions → Compiled), the name of the UDF was visible in the Discrete Phase Model dialog box when the Interaction with Continuous Phase was enabled (as shown in Figure 3-9).

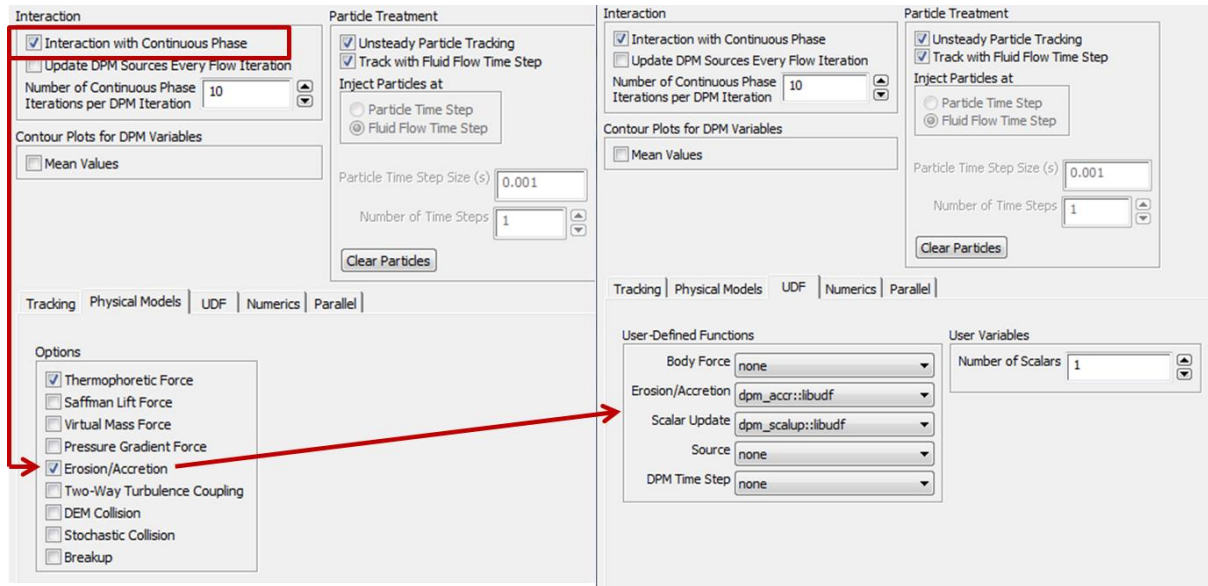


Figure 3-9: Menus for DEFINE_DPM_EROSION set up.

Before starting a simulation, it was important to execute the UDF on demand (Define → User Defined → Execute on Demand). When particles hit the surface, the accretion rates were stored in: $F_STORAGE_R(f, t, SV_DPMS_ACCRETION)$ (“ANSYS FLUENT 12 .0 UDF Manual,” 2009) and the results were visible in Results → Graphics/Plot (XY Plot) → Discrete Phase Variables → DPM Accretion.

It is important to highlight that the value of $F_AREA(A, f, t)$ used in the calculation for the deposition flux was verified. In fact, this returns the face area normal vector of a given face f in a face thread t which always points out of the domain and it is calculated using the right hand rule (Area= face length x depth, with depth=1 m (2D geometry)) (Figure 3-10) (ANSYS FLUENT, 2006a).

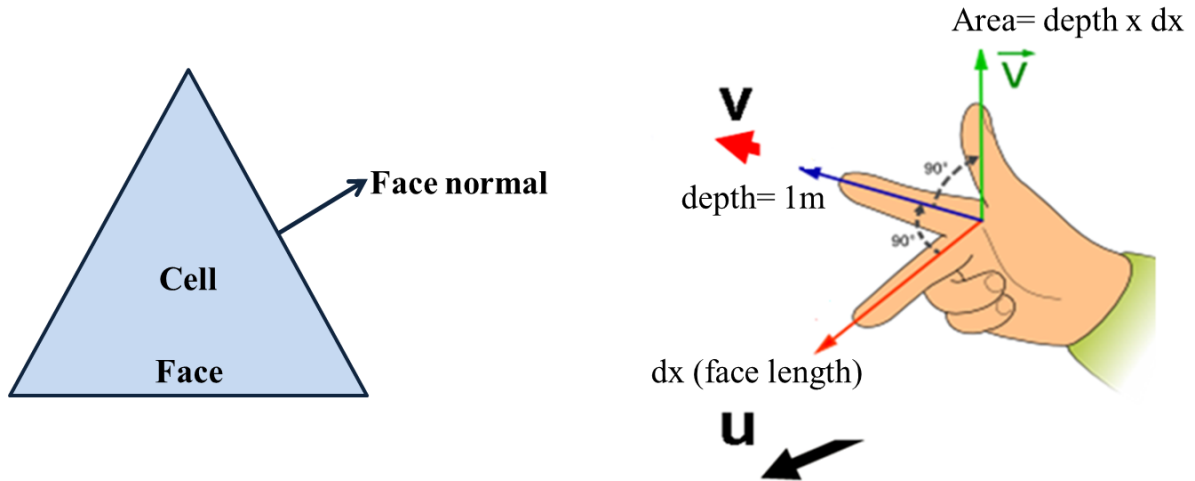


Figure 3-10: Determination of face area normal direction (2D face) (derived from (ANSYS FLUENT, 2006)).

The face area calculated in Fluent[®] (Reports → Surface Integrals) was 0.1225 m² which derives from $2\pi rh$ (with $h=1$ m).

3.8 Deposit shape

Deposit growth was modelled using a modified version of the DEFINE_GRID_MOTION UDF (~ 88 lines). This UDF could shift the nodes' position on each face of the cylinder based on the deposit thickness. This value was obtained from the deposition flux calculated in the modified DEFINE_DPM_EROSION UDF taking into account the exposure time and the deposit density (Wacławiak and Kalisz, 2011; García Pérez *et al.*, 2014).

The procedure used to calculate the node displacement is simplified as follows:

- 1) In the modified DEFINE_DPM_EROSION UDF the deposition flux is calculated on each face of the cylinder according to Equation (3-3), or its simplifications.
- 2) Deposition thickness at each node i of the cylinder and current time step j is calculated as:

$$t_{i,j} = \frac{(m_{f,A})_{i,j}}{\rho_{dep}} \quad (3-4)$$

Where:

$(m_{f,A})_{i,j}$ = deposition flux at node i and time step j [kg/m²];

$t_{i,j}$ = deposition thickness at node i and time step j [m];

ρ_{dep} = deposit density [kg/m³].

The deposition thickness at each node of the cylinder $t_{i,j}$ is used to update the node coordinates and the direction of accretion is computed considering the angle θ normal to each face defined as in Equation (3-5) and in Figure 3-11.

$$\theta = \tan^{-1} \left(\frac{Y_p}{X_p} \right) \quad (3-5)$$

Therefore, the new coordinates of each node can be computed as in Equations (3-6) (Figure 3-11).

$$x'_p = x_p + t_{i,j} \cos \theta \quad (3-6)$$

$$y'_p = y_p + t_{i,j} \sin \theta$$

The final deposit thickness was obtained applying Equation (3-4) for the total number of time steps required to reach the final exposure time.

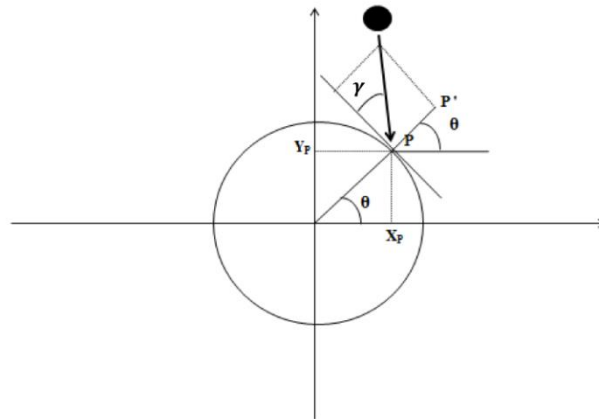


Figure 3-11: Calculation of new node coordinates.

DEFINE_GRID_MOTION(*name,d,dt,time,dtime*) has five arguments: UDF *name*, *d* is the pointer to domain, *dt* which is the pointer to structure that stores the dynamic mesh, real *time* (current time), real *dtime* (time step).

Out of the five arguments, only the *name* is defined by the user, all the others are supplied by the solver to the UDF. Compared to other UDFs, this cannot be interpreted but only compiled. Moreover, as discussed in 3.3, one drawback of using the dynamic mesh with “remeshing” option is the necessity of using a triangular (unstructured mesh) that implies less accuracy in the results (Wacławski and Kalisz, 2011).

After the UDF had been compiled (Define → User Defined Functions → Compiled), the name of the UDF was visible in the Dynamic Mesh dialog box and the procedure used to apply the code at each cylinder face is shown in Figure 3-12.

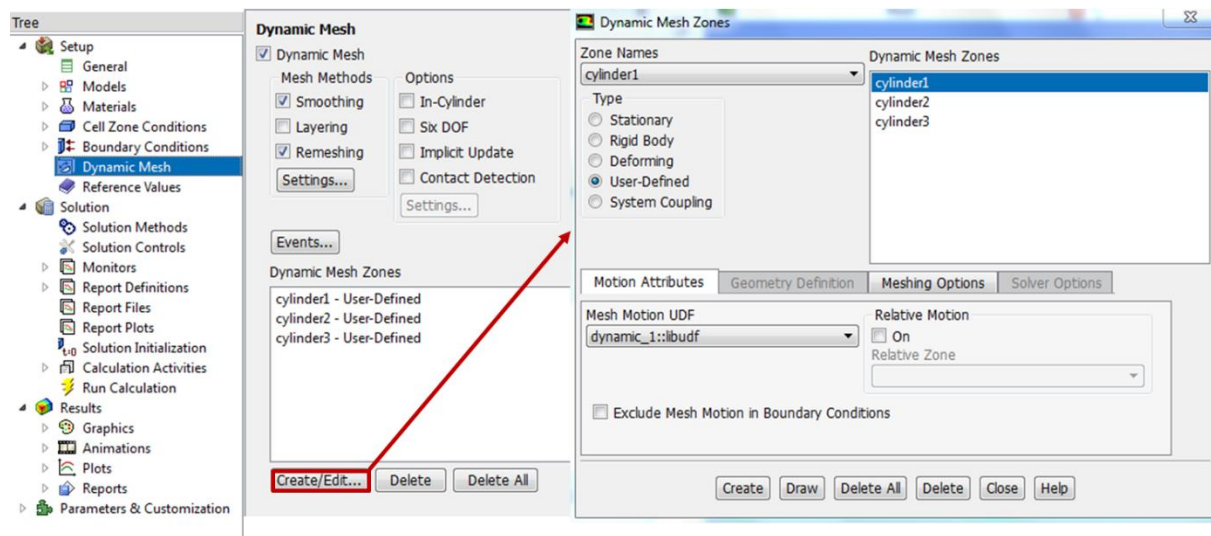


Figure 3-12: Menus for dynamic mesh set up.

3.9 Deposit temperature

In this work, the tube was initially assumed to have a constant surface temperature ($T_{4,s}$). However, deposit formation represents a resistance towards heat transfer between the hot flue gas (T_5) and the coolant inside the tube surface (Figure 3-13). As a consequence, the deposit temperature ($T_{5,s}$) will be higher than the probe surface temperature and Fluent[®] was used to simulate this process with a dynamic approach.

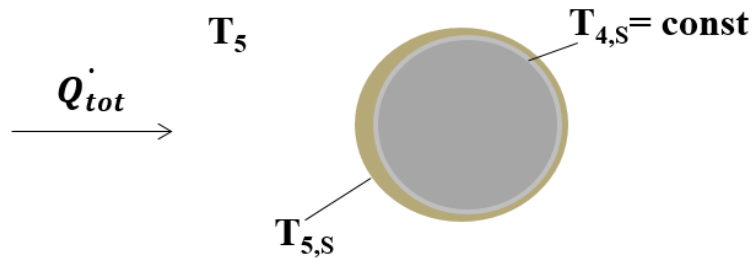


Figure 3-13: Effect of deposit build up on heat transfer.

The deposit thickness, derived from the modified DEFINE_DPM_EROSION UDF, was used in the modified DEFINE_PROFILE UDF (~ 50 lines) to predict the deposit surface temperature according to Equation (2-75). This UDF can specify a custom boundary profile that varies with spatial coordinates or time and it is defined with three arguments: DEFINE_PROFILE (*name*, *t*, *i*).

The *name* is supplied by the user, *t* is the pointer to thread where the boundary is applied and *i* is the index used to define the variable and these two are passed by the solver to the UDF. Once the modified UDF DEFINE_PROFILE has been compiled (Define → User Defined Functions → Compiled), it is visible in the boundary condition panel and can be selected as in Figure 3-14.

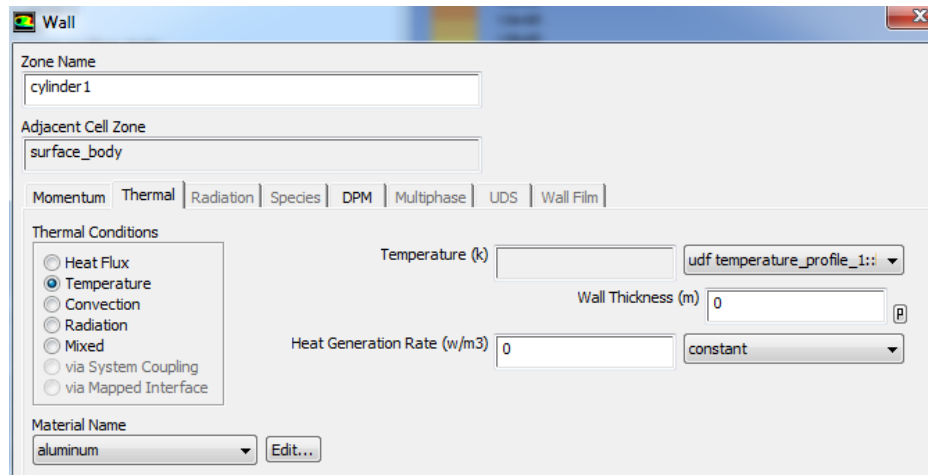


Figure 3-14: DEFINE_PROFILE set up.

In this work, the effect of deposit growth (deposit shape) and deposit temperature on deposition process were considered and the three UDFs, introduced in this chapter, were used simultaneously. Using this method, the probe assumes the deposit shape and

temperature during the simulation, but the gradient of temperature inside the deposit cannot be calculated.

Therefore, for some simulations a mesh with an initial thin layer of deposit around the probe was designed. This allows the simulation of heat transfer between two phases (e.g. solid and fluid) which need to be meshed and identified as separate entities of different materials and thermal properties. The face between the two phases is recognised in Fluent[®] as an interface or double coupled wall. This interface has a wall and wall shadow which represents two faces of the same wall, one looking at the fluid and the other at the solid. As a consequence, more care needs to be spent in the mesh generation. Following this approach, the modified DEFINE_DPM_EROSION and DEFINE_GRID_MOTION UDFs were applied to the interface/doubled coupled wall (Figure 3-15). The coupled thermal boundary condition is available to walls which separate two cell zones and this option is able to compute conduction of heat through solids coupled with heat transfer in fluid (Fluent, 2006). This was enabled as shown in Figure 3-16 and the P1 model in Fluent[®] was used to include the radiation heat transfer.

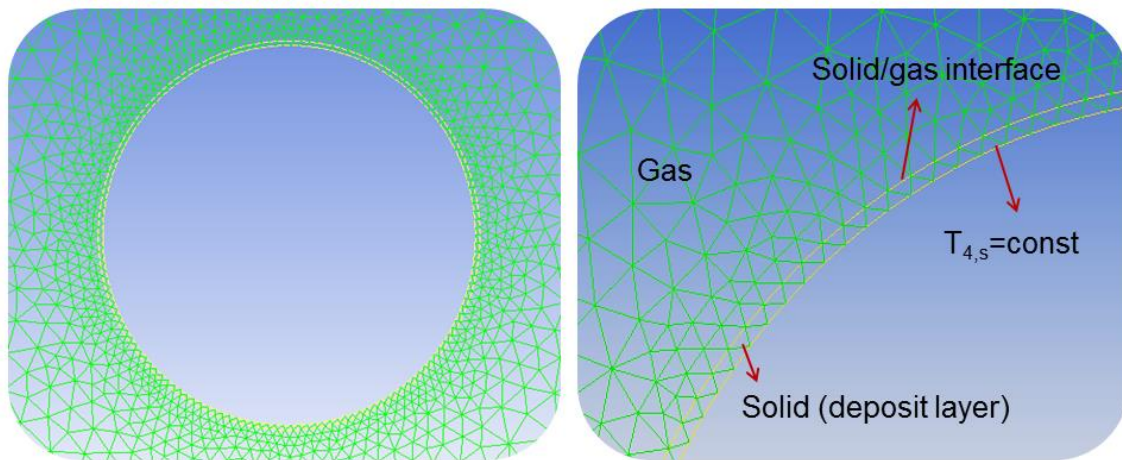


Figure 3-15: Double coupled wall for deposit temperature predictions.

The temperature of the tube wall substrate was assumed to be constant and Fluent[®] could calculate the surface temperature of the deposit knowing the thermal properties of the gas and of the solid as well as the increase in deposit layer thickness.

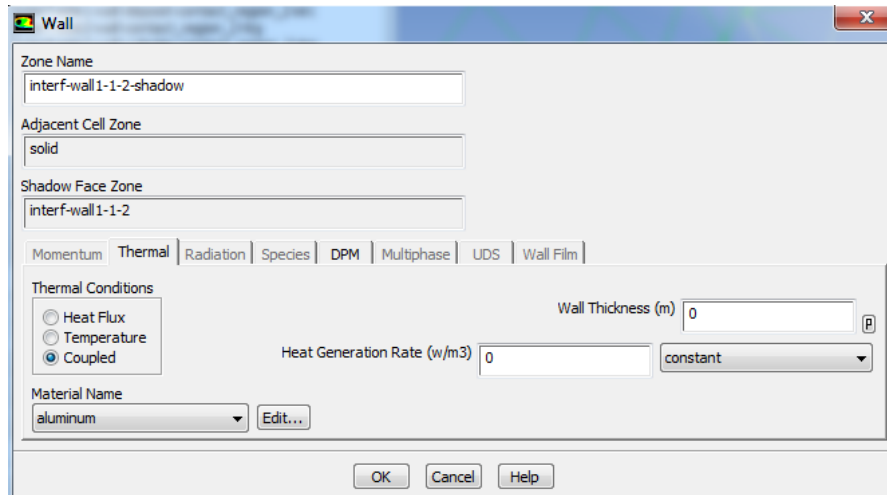


Figure 3-16: Interface boundary conditions.

3.10 Model development strategy

Deposition around heat exchanger tubing was studied using Fluent[®] with custom modified UDFs. Three main UDFs were chosen as starting points for modification to simulate the deposit accretion, the deposit shape and temperature respectively. As explained in sections 3.7-3.9, they were compiled all together in Fluent[®] before enabling the interaction with the gas phase (Figure 3-6). The same methodology was applied to different geometries and their relative meshes.

Once the mesh was imported into Fluent[®], the flue gas was studied without particles until at least partial convergence. However, choices of material properties and boundary conditions, as well as turbulent models and time step size, are necessary to give a real representation of the fluid flow. When the gas flow in the model was stable, particle injections were set (uniform or Rosin Rammler distribution (section 3.6)), they were allowed to develop around the tubes before enabling the interaction between the two phases and, therefore, applying the modified DEFINE_DPM_EROSION UDF. The deposit accretion was monitored during the simulation (using the solution monitor in Fluent[®]) in order to allow the accumulation of a little deposit layer before starting the mesh movement with the modified DEFINE_GRID_MOTION UDF and the deposit temperature simulation with DEFINE_PROFILE.

Moreover, it is important to highlight that after updating the grid, it was necessary to reset the deposition flux on the cylinder wall. For this purpose the code was modified so

that every certain number of time steps the mesh and the surface temperature were updated and the deposition flux would increment starting from zero. Simulations were run until the exposure time of interest was covered. A typical procedure followed to run the simulations is in Figure 3-17.

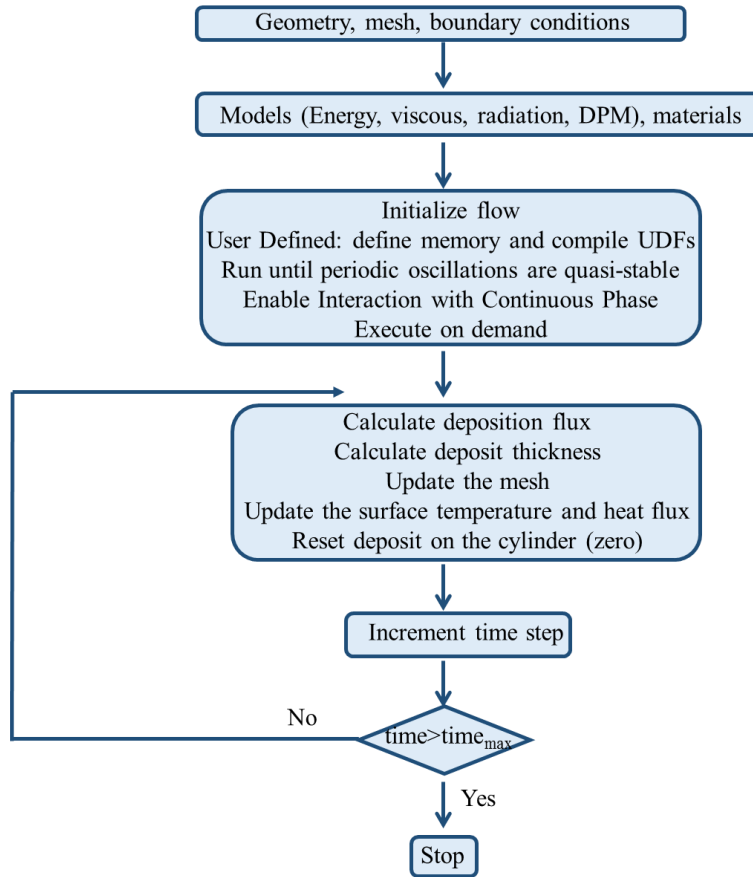


Figure 3-17: Transient procedure to study deposition on heat exchangers.

Preliminary simulations were carried out with an Intel (R) Core(TM) i5-4210 M CPU, 4 GB (RAM), 64 bit, 2 Cores, 4 Logical Processors. Later a workstation was provided to run longer simulations. The main characteristics were: Intel (R) Core(TM) 2, Quad CPU Q9400, 4GB (RAM), 64 bit, 4 Cores, 4 Logical Processors. The length of the simulation varied according to the type of geometry, the type of ash particle injected and the number of UDFs which took up to a week (or more) to be completed (Chapters 4 and 7).

3.11 Summary

Literature studies have shown that CFD is currently the best tool to investigate deposition on heat exchangers and Fluent[®] has been the software used in this work. The methodological procedure has been explained in this chapter and summarised in Figure 3-17. The Reynolds-Averaged Navier-Stokes (RANS) equations were used to describe the flow gas and the Discrete Phase Model (DPM) was applied to predict ash particle behaviour. However, modified User Defined Functions (i.e. UDFs) were created to include some stickiness criteria (DEFINE_DPM_EROSION) and how they affect the surface temperature (DEFINE_PROFILE) and the fluid dynamic around the probe (DEFINE_GRID_MOTION).

4 CFD MODELLING RESULTS AND DISCUSSIONS

4.1 Introduction

The methodology explained in Chapter 3 was used to study the deposition of particles and vapours from hot gas streams onto cooled tube surfaces for different geometries using a series of models. The complexity of the simulations was gradually increased. In fact, at the beginning, single mechanisms were considered to predict deposition on a single tube but later a combination of mechanisms were applied on multiple heat exchanger tubes including the effect of the deposit shape and temperature. The main CFD parameters investigated during the course of the PhD are illustrated in this Chapter as well as some of the challenges met and the approach used to deal with them.

This Chapter presents sensitivity analysis of using different parameters and more details are in Chapter 7. It is important to highlight that this part of the research aimed to employ improved CFD and coding knowledge to get qualitative results using mainly data from the literature. In fact, the lack of available data about fouling in co-firing biomass with coal made the combination of modelling with experimental work necessary to get information for the model boundary conditions and its validation (Chapter 7).

4.2 Case study 1: Single tube

In this section, some of the results presented at the XII International Conference Heat Exchanger Fouling and Cleaning in Madrid (June 2017) are reported.

4.2.1 Geometry and mesh

The geometry shown in Figure 3-2 was one of the first developed for this thesis to learn how to use Fluent[®] for tracking ash particle trajectories with the DPM model. Later, this configuration was slightly modified and the result is in Figure 4-1 with the respective boundary conditions (in claret). Similar geometries were used in previous works (Weber, Mancini, *et al.*, 2013; Yang *et al.*, 2016).

The main difference between the two geometries is the length of the domain which is shorter in Figure 4-1 and, as a consequence, the number of cells is reduced. However,

this length still allows the simulation of vortex shedding but it also reduces the computational costs.

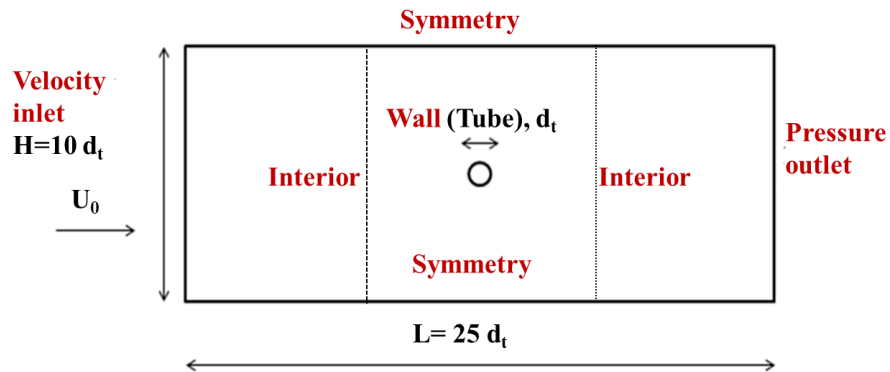


Figure 4-1: 2D geometry and boundary conditions for deposition study around one tube (tube diameter $d_t=38$ mm).

An unstructured mesh (triangular) was generated using ANSYS Workbench, (Figure 4-2 and Figure 4-3) to study the grid movement.

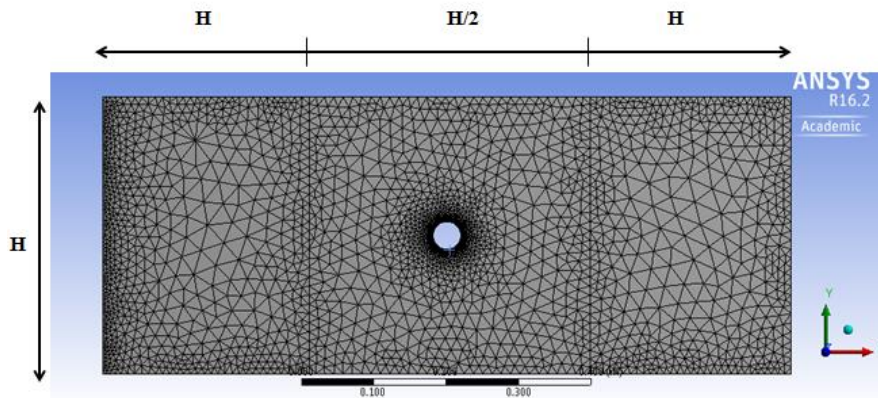


Figure 4-2: Triangular mesh around one tube ($d_t=38$ mm).

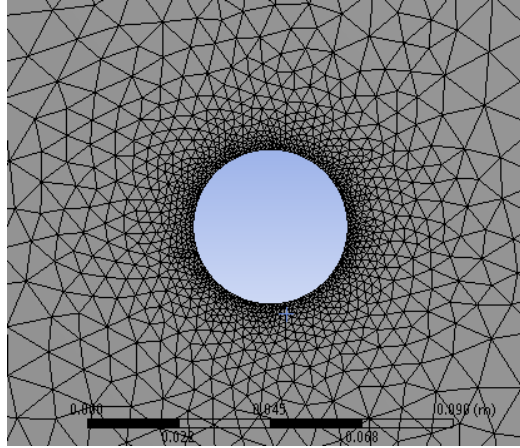


Figure 4-3: Mesh magnification around the tube ($d_t = 38$ mm).

This unstructured mesh has a total of 5841 cells, 8984 faces, 3143 nodes and 150 wall faces on the cylinder. The mesh quality was estimated in Workbench and the main parameters are:

- Average Skewness= $6.09 \cdot 10^{-2}$ (Ortho Skew ranges from 0 to 1, where values close to 1 correspond to low quality).
- Average Aspect Ratio= 1.21 (ideally equal to 1).

The number of nodes at the inlet was increased since this affects the number of particles injected and the geometry was divided into three zones using two vertical “interiors” (faces with fluid cells on both sides). This method was used to avoid the degeneration of the mesh for big domains. Moreover, gradually it makes the mesh finer around the cylinder increasing the accuracy of the vortex shedding formation.

The grid convergence is shown for the real tube configuration of Cranfield combustion rig in 4.3.2 and in Appendix B (section B.1). In fact, these initial simulations were run mainly using data from the literature (e.g. material properties, boundary conditions, etc.); therefore the results were normalised and used to get qualitative information about particle impaction and deposit location, but particularly to create the basic knowledge to build the more extensive model for validation purposes.

4.2.2 Model assumptions

The flue gas was approximated to air and it entered with inert ash particles at the inlet with velocity U_0 of 10 m/s and temperature T_g of 1273 K, while the tube surface

temperature $T_{4,s}$ was fixed at 700 K. The main material properties are reported as follows:

Combusted gas properties (air):

Density $\rho_g = 0.245 \text{ kg/m}^3$ (Yang *et al.*, 2016)

Specific Heat $Cp_g = 1203 \text{ J/(kg K)}$ (*The Engineering ToolBox*, 2018)

Thermal Conductivity $k_g = 0.077921 \text{ W/(m K)}$ (*The Engineering ToolBox*, 2018)

Viscosity $\mu_g = 46 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$ (Yang *et al.*, 2016)

Wall properties (mullite) (AZO Materials, 2018a):

Density $\rho_w = 2800 \text{ kg/m}^3$

Specific Heat $Cp_w = 1050 \text{ J/(kg K)}$

Thermal Conductivity $k_w = 6 \text{ W/(m K)}$

Ash particle properties:

Density $\rho_p = 2200 \text{ kg/m}^3$ (Wacławski and Kalisz, 2012)

Specific Heat $Cp_p = 923 \text{ J/(kg K)}$ (AZO Materials, 2018b)

Thermal Conductivity $k_p = 1.5 \text{ W/(m K)}$ (AZO Materials, 2018b)

With the gas properties, the Reynolds number was calculated according to Equation (3-1) which returned a value of Reynolds equal to ~ 2024 . This means that this case of study is close to a Von Karman vortex trail (Haugen and Kragset, 2010) and the formation of vortices on the rear side of the tube can be appreciated in Figure 4-4.

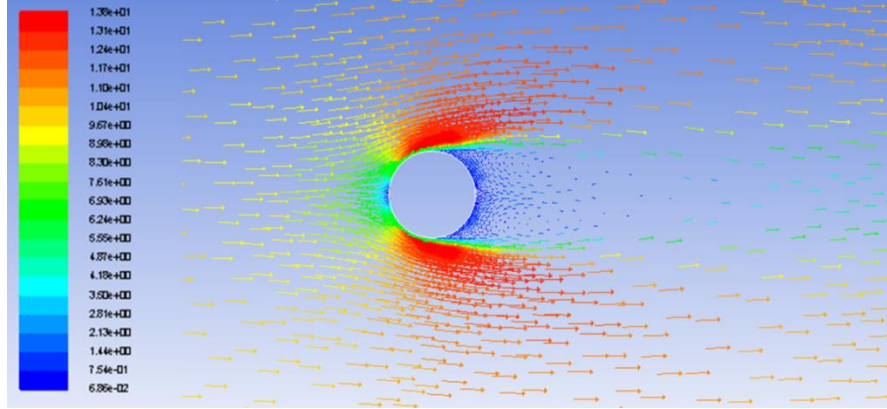


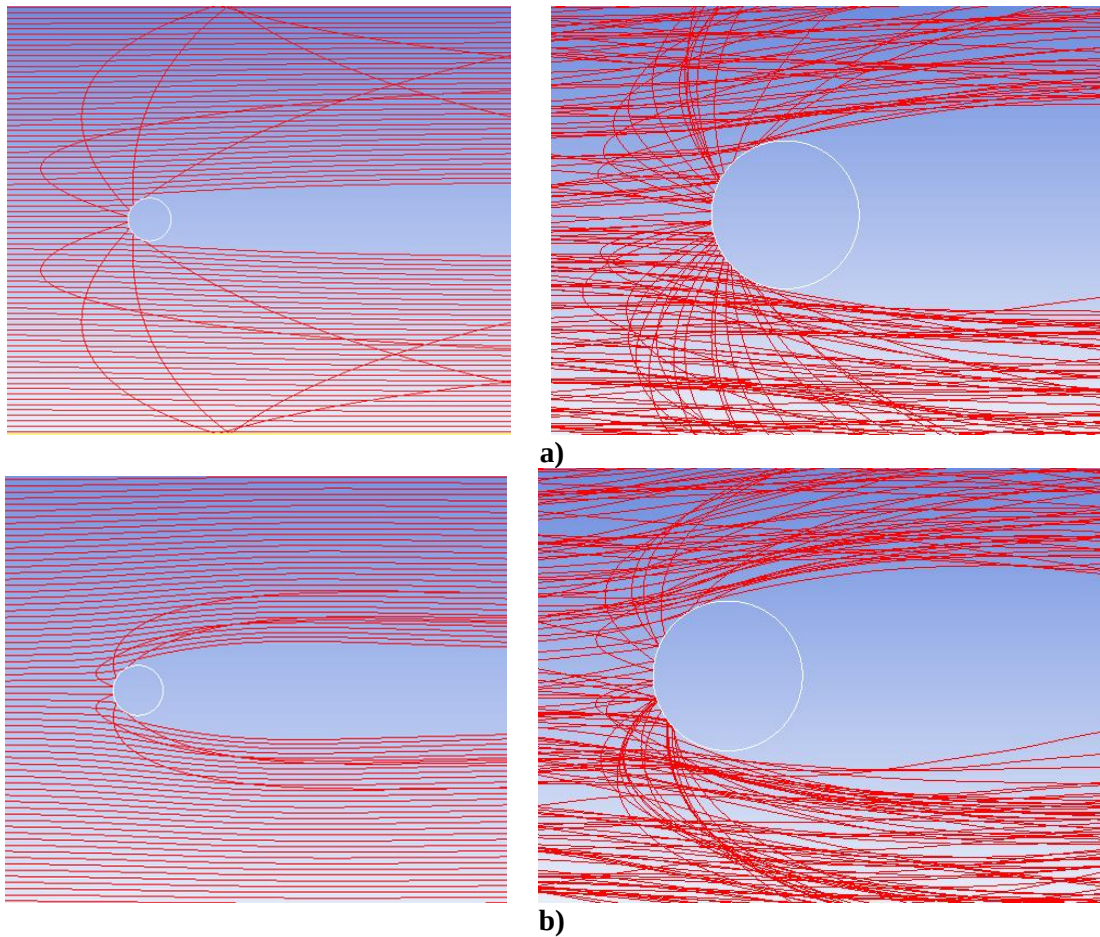
Figure 4-4: Gas velocity vectors [m/s] around a circular cylinder ($U_0 = 10$ m/s, $d_c = 38$ mm).

For this set of simulations, the turbulent model $k-\epsilon$ was chosen with standard input data and, at the inlet, the gas had turbulent intensity of 10% (in line with the model reported by Waclawiak and Kalisz, 2014). The Reynolds-Averaged Navier-Stokes (RANS) equations were used to determine the flow properties. Once the gas oscillations around the cylinder were stable, spherical inert ash particles were injected at the inlet using the Discrete Phase Model as shown in section 3.6. The force of gravity, acting with the same directions of the flue gas (Figure 4-1), was included but no additional force terms (F_x) were considered in these simulations.

4.2.3 Ash particle trajectories

The particle trajectories were calculated for different particle diameters and three examples are given in Figure 4-5 (with DPM being kept steady). As indicated in some previous papers (Baxter, 1993; Waclawiak and Kalisz, 2012; Lee *et al.*, 2014), inertial impaction is the most important particle deposition mechanism for particles larger than $10\text{ }\mu\text{m}$ whose impaction occurs mainly close to the cylinder stagnation point, where they can hit the surface and rebound off because of their higher kinetic energy. Figure 4-5 (left side) shows that the rebound is bigger for $150\text{ }\mu\text{m}$ particles compared to $50\text{ }\mu\text{m}$ particles. In contrast, small particles ($0.5\text{ }\mu\text{m}$) do not have enough inertia to overcome the drag force and tend to follow the flue gas streamlines to the downstream side of the tube where they can deposit because of the Eddy impaction, and, if included, the Thermophoretic and Brownian Forces.

Moreover, when turbulent dispersion was taken into account, it was possible to predict trajectories of small particles and see their impaction on the downstream side of the tube that would not be seen in the absence of turbulence (Figure 4-5 (right side)) (Tomeczek and Waclawiak, 2009; Lee *et al.*, 2014). In addition, when the DPM is steady this option is one way of increasing the number of particles injected by modifying the number of tries (number of times the trajectory is computed) (Fluent, 2001). In contrast, if the DPM is unsteady, then the number of particles or parcels injected may change with the total particle flow rate (which can be set in the Injection dialog box). Simulations were run with steady DPM only at the beginning of this work to track ash particle trajectories of different diameters. Successively, a transient approach was used for both gas and DPM to study deposit formation.



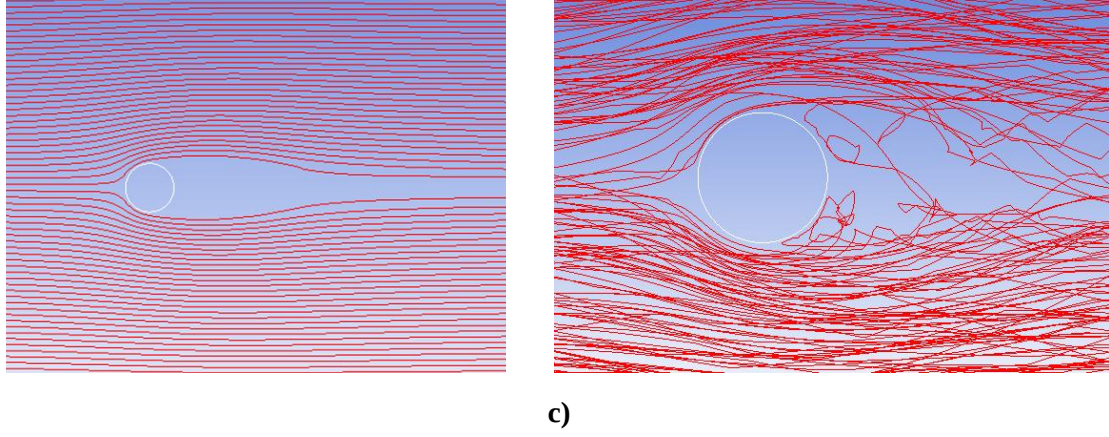


Figure 4-5: Particle trajectories without the effect of the stochastic tracking model (left) and with the effect of the stochastic tracking model (right) for particles with diameters of a) 150 μm , b) 50 μm , c) 0.5 μm ($U_0 = 10 \text{ m/s}$, $d_t = 38 \text{ mm}$).

Results from using a Rosin Rammler ash particle size distribution are shown in Figure 4-6 ($d_{min} = 1 \mu\text{m}$, $d_{max} = 200 \mu\text{m}$, $d_{mean} = 40 \mu\text{m}$, spread diameter $n = 0.8$). This confirms what already observed for single ash particle trajectories in Figure 4-5. In fact, in Figure 4-6, small particles (blue) tend to follow the flue gas streamlines while bigger ash particles (red) hit the upstream side of the tube where they bounce off it and the rebounds are wider for bigger particles (red) than smaller (green).

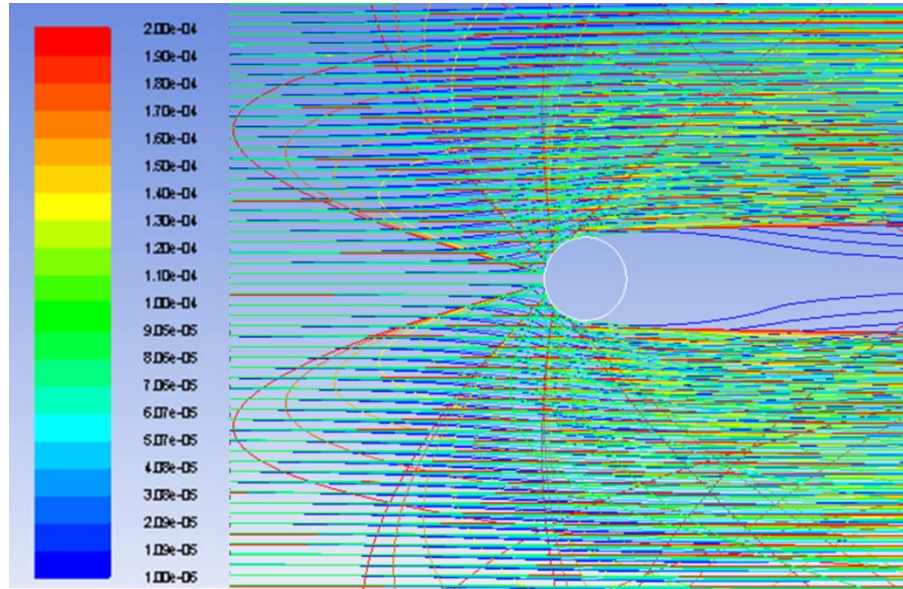


Figure 4-6: Particle trajectories for ash particles described by a Rosin Rammler distribution without the effect of the stochastic tracking model ($U_0 = 10 \text{ m/s}$, $d_t = 38 \text{ mm}$, $d_{min} = 1 \mu\text{m}$ (blue), $d_{max} = 200 \mu\text{m}$ (red), $d_{mean} = 40 \mu\text{m}$, spread diameter $n = 0.8$).

4.2.4 Deposit predictions

The model to predict deposition was developed using modifications to the DEFINE_DPM_EROSION UDF as described in section 3.6. This calculates the deposition flux as a function of the stickiness probability P_{stick} , the mass flow rate m_p of particulate matter striking the deposition surface A and the impaction angle γ (Equation (2-59)). As explained in Chapter 3, m_p , A and γ are all passed by Fluent[®] and only P_{stick} needs to be defined. However, in transient simulations m_p is in kg and in steady state is in kg/s.

Initially, Equation (2-59) was implemented in the UDF to predict deposit accretion on the tube in Figure 4-1 applying two models: “dry impaction”, better known as powdery deposition (due to dry ash particles impacting on a clean surface), and “wet impaction” (due to vapour condensation and sticky particles) (Tomeczek and Waclawiak, 2009; Waclawiak and Kalisz, 2011; Subbarao, Rindt and Van Steenhoven, 2012) by changing the value of P_{stick} .

Firstly, the powdery model was applied without changing the constants and the parameters previously suggested in the literature (section 2.8.2). This model was studied for different particle diameters and it was confirmed that deposition occurs mainly on the front side of the tube for big particles (Figure 4-7). Moreover, it is interesting to highlight that 150 μm particles have more momentum to bounce off once they hit the stagnation point if compared to 50 μm (Figure 4-7 (a and b)), resulting in a reduced amount of deposit on the upstream side of the probe (Figure 4-7 (a)). Differently, small particles deposition was more uniform and took place also on the rear part of the tube (Figure 4-7 (c)).

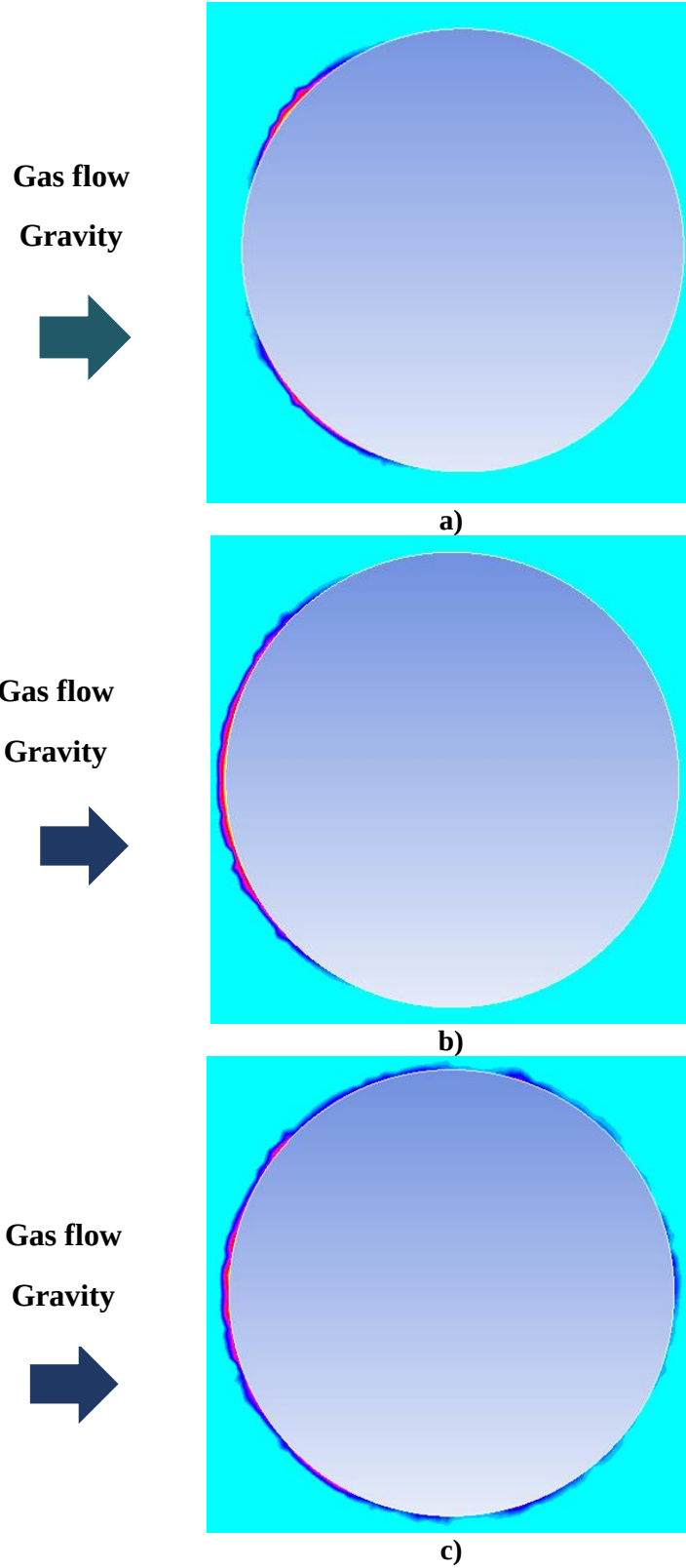


Figure 4-7: Distribution of deposit locations around a tube ($d_t=38$ mm) for particles with diameters of: a) $150\text{ }\mu\text{m}$, b) $50\text{ }\mu\text{m}$, c) $0.5\text{ }\mu\text{m}$ using the powdery deposition model ($U_0 = 10$ m/s, $T_g = 1273$ K, $T_{4,s} = 700$ K).

The deposition flux in Equation (2-59) can also be expressed using the total probability (P_{tot}), which is function of the properties of the wall and of the particles (Kær *et al.*, 2006; Schulze *et al.*, 2011) as in Equation (2-58).

However, in preliminary simulations, only the surface stickiness was taken into account, therefore $P_p = 0$ and Equation (2-58) was simplified as in Equation (4-1) and included in Equation (2-59).

$$P_{tot} = P_s \quad (4-1)$$

For simplicity, Na_2SO_4 [1 ppm] was initially considered to be the only vapour in the hot flue gas. The temperature gradient between the gas and the tube leads to vapour condensation on the surface creating a sticky layer able to enhance the particle deposition. This probability was calculated applying Equation (2-19).

The flux of the condensable vapour i -th was calculated using Equation (2-20). The saturation pressure of the i -th gaseous component at surface temperature, P_{si} [Pa] was obtained from Equation (2-23) and the mass transfer coefficient β_i [m/s] of the i th component from Equation (2-21) where the diffusion coefficient through the gases was $D_i = 0.9 \text{ m}^2/\text{s}$ (Green and Perry, 2008). The dimensionless Sherwood number Sh was calculated using the Froessling equation as follows (Renksizbulut *et al.*, 1991):

$$Sh = 2 + 0.552 Re^{1/2} Sc^{1/3} \quad (4-2)$$

Where Re and Sc are the Reynolds and Schmidt numbers, defined respectively in Equations (4-3) and (4-4).

$$Re = \frac{\rho v d_t}{\mu} = \frac{\text{inertial forces}}{\text{viscous forces}} \quad (4-3)$$

$$Sc = \frac{\mu}{\rho D} = \frac{\text{viscous diffusion rate}}{\text{mass diffusion rate}} \quad (4-4)$$

During these simulations, the effect of the vapour condensation was included in DEFINE_DPM_EROSION UDF and the wall temperature $T_{4,s}$ was kept constant, therefore the effect of deposit growth on the surface temperature was neglected.

The results obtained applying the condensation model (bonded model) to the particle stickiness are reported in Figure 4-8 which represents the normalised mass flux of particles deposited on the tube surface when P_s is a function of the condensation flux.

Predictions from this model are shown and compared to the ones from the dry deposition model for the same particle size in Figure 4-8. This confirms that if the surface becomes sticky because of the vapour condensation, then the bigger particles (e.g. $150\ \mu\text{m}$) hitting close to the centre of the upstream tube face (stagnation point) will stick rather than rebound off as it happens if the surface is initially clean. For simplicity, the x axis range in Figure 4-8 is $-90^\circ/90^\circ$ as $150\ \mu\text{m}$ particles do not hit the rear side of the tube.

Furthermore, for the model validation (Chapter 7) the contribution of the vapour deposition flux was added to the total deposition (Equation (3-3)). This combines both the contribution of the deposition of particles onto a sticky surface and the condensation flux itself.

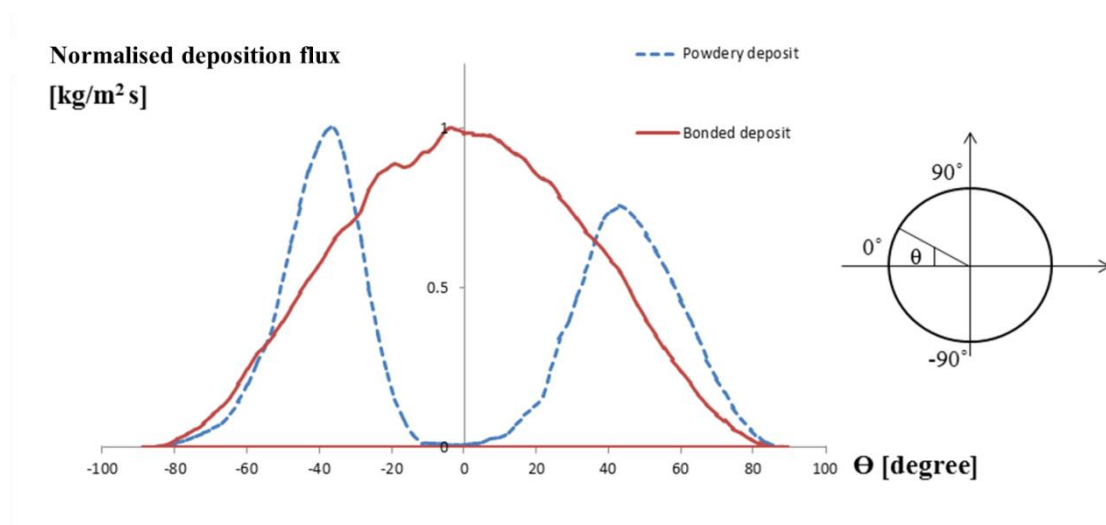


Figure 4-8: Variation of deposit location around a tube ($d_t = 38\ \text{mm}$) between a “dry” and a “sticky” surface for $d_p = 150\ \mu\text{m}$ ($U_0 = 10\ \text{m/s}$, $T_g = 1273\ \text{K}$, $T_{a,s} = 700\ \text{K}$).

4.2.5 Grid motion

In order to simulate the shape of the deposit, DEFINE_GRID_MOTION UDF was modified and used as indicated in section 3.8 with the deposition flux previously

calculated, the time elapsed and the deposit density ($\rho_{dep}= 850 \text{ kg/m}^3$) (Wacławiak and Kalisz, 2011).

The application of this modified UDF has involved many challenges. Trials and errors showed that the mesh resolution and the choice of the time step can both deeply affect the prediction of the shape of deposit formation. Moreover, if the deposit is accumulated for too long before activating the grid motion option, the mesh movements are too big and this can cause an overlap of the neighbouring faces turning into a negative volume error which does not allow the completion of the simulation. An example of typical grid motion with a spiky shape that is going to degenerate in a negative volume is in Figure 4-9 where the powdery deposition model was used with $50 \text{ }\mu\text{m}$ particle diameters and an example of negative volume is given in Figure 4-10.

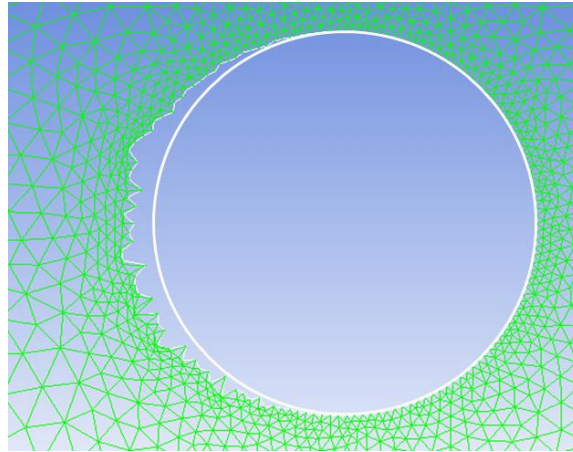


Figure 4-9: Example of grid motion showing the deposit shape on the upstream of the tube ($d_t= 38 \text{ mm}$) applying the powdery deposition model for $d_p= 50 \text{ }\mu\text{m}$ ($U_0= 10 \text{ m/s}$, $T_g= 1273 \text{ K}$, $T_{4,s}= 700 \text{ K}$).

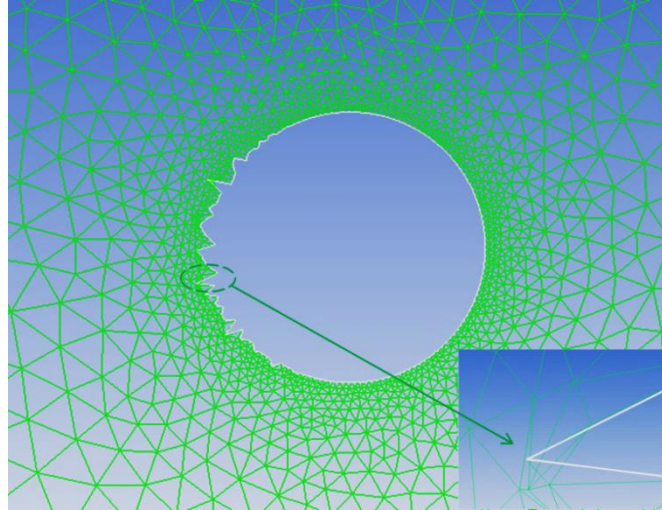


Figure 4-10: Example of negative cell volume created by an overlap of faces (powdery deposition model for $d_p = 50 \mu\text{m}$, $U_0 = 10 \text{ m/s}$, $d_t = 38 \text{ mm}$).

Once the interaction with the continuous phase was enabled, the particles were allowed to accumulate for a few seconds (until deposition flux was $\sim 10^{-7} \text{ kg/m}^2 \text{ s}$) before activating the dynamic mesh (Figure 3-12). In fact, the modified DEFINE_DPM_EROSION UDF saves the deposit accumulation in $F_STORAGE_R(f, t, SV_DPMS_ACCRETION)$ which is an incrementing function and an example is reported below:

```
F_STORAGE_R(f,t,SV_DPMS_ACCRETION)+((((Ps+Pp-Pp*Ps)*mdot)/(area))*sin(alpha))
```

The amount of deposit accumulated in each time step was extrapolated and the mesh was updated every time step. However, this technique was found to be less efficient since in a single time step, the amount of deposit accumulated was not significant, especially for small time step sizes. Moreover, this approach would not be feasible to simulate deposition over hours as shown in Chapter 7.

Therefore, the code was further modified so that every certain number of time steps (depending on the accretion model), the amount of deposit accumulated was used to calculate the deposit thickness over that period of time and the modified DEFINE_GRID_MOTION UDF was executed to move the grid. However, it was important to make sure that every time the mesh was revised the deposit accumulation would start from zero on the new surface without taking into account the deposit

previously accumulated. In fact, if this does not happen, the grid will generate in a negative volume as an increasing amount of deposit accumulates in a short time.

4.3 Case study 2: Multiple tubes

4.3.1 Geometries and mesh

In section 4.2 a 2D geometry with one tube in the middle of the domain was generated. Later, the CFD model was enabled for deposit predictions onto ceramic probes in the combustion rig at Cranfield (Figure 1-2 and Figure 4-11). More details about the rig are reported in Chapter 5. The real geometry (Figure 4-11) was simplified to a 2D domain with probe diameters $d_t = 39$ mm.

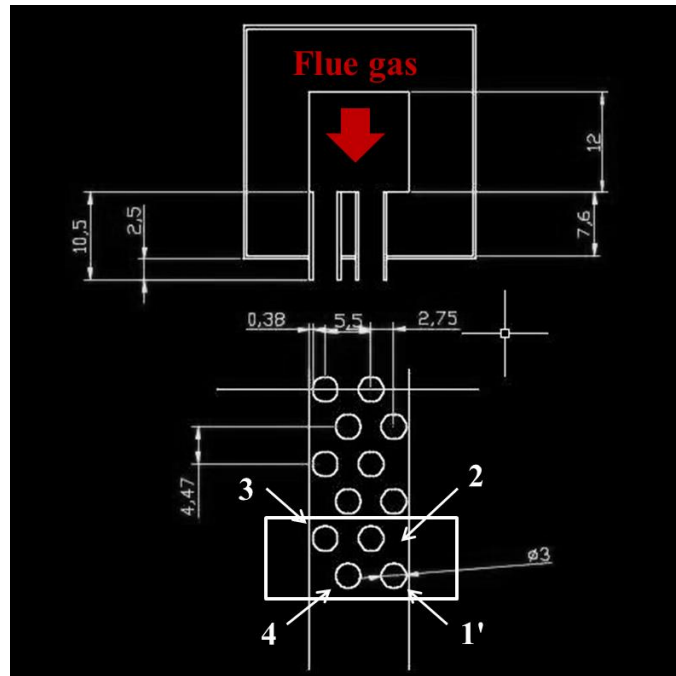


Figure 4-11: Drawing of the vertical section of the combustor chamber with identification of the ports used to study deposition on ceramic probes ($d_t = 39$ mm, the dimensions in the drawing are in inches).

A periodicity in the port distribution can be identified and, firstly, the attention was focussed on four tubes (1', 2, 3, 4) (Figure 4-11). Several tube configurations were realised with a 90° rotation anticlockwise of the geometry (Figure 4-12 and Figure 4-13) (others in Appendix F). In this work, the geometry has a fixed width and its length was a degree of freedom. For the CFD model, the inlet was placed at $20d_t$ from the first tube

and the outlet at $40d_t$ from the last tube to avoid the flow reflection (causing reversed flow) and to allow the vortex shedding to be developed enough (Dröge, 2007; Rahman *et al.*, 2007).

The first geometry with its boundary conditions for the tube 2 is in Figure 4-12. The choice was mainly due to the similarity between this configuration and the one used in section 4.2 (Figure 4-1). The boundary conditions are the same as before except for the top and bottom walls that needed to be defined as “wall” and not “symmetry” since the geometry is not symmetric anymore. This study represented a step forward in the model development as the probe location and the presence of other tubes were considered.

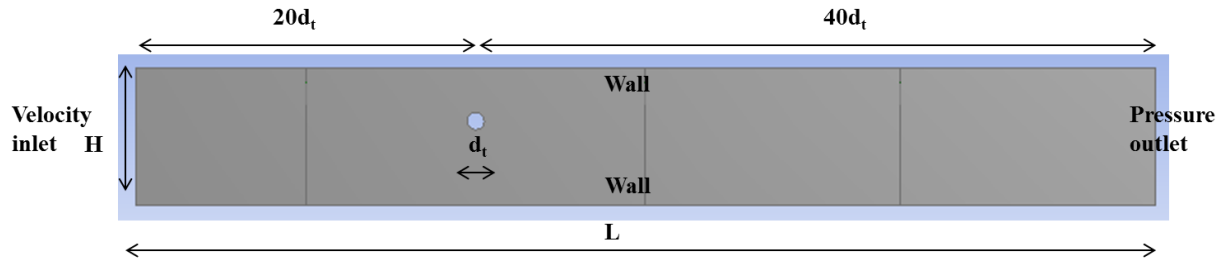


Figure 4-12: 2D geometry and boundary conditions for deposition study around probe 2 (tube diameter $d_t = 39$ mm) in Cranfield combustion rig ($L = 2340$ mm, $H = 305.054$ mm).

Some other configurations were generated and an example is in Figure 4-13. However, this does not represent the configuration used in the experiments but rather was used to understand the particle behaviour and deposition mechanisms in the presence of more tubes. In fact, at this stage, the experimental activity had not yet started, but training to learn how to use the combustion rig were being carried out.

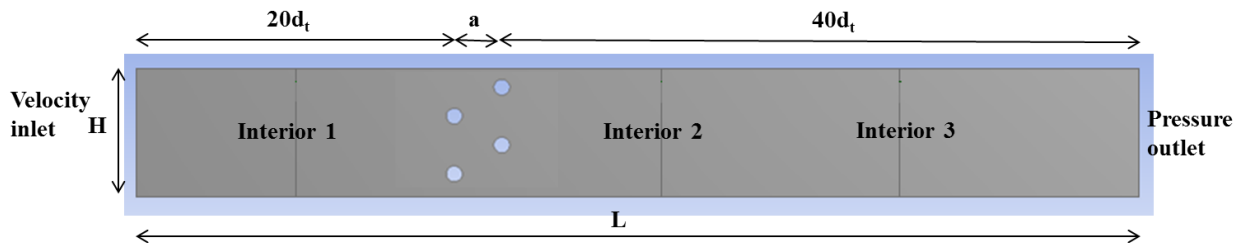


Figure 4-13: Tube configuration 1', 2, 3, 4 ($d_t = 39$ mm) in Cranfield combustion rig ($L = 2453.54$ mm, $H = 305.054$ mm, $a = 113.538$ mm).

All the meshes were unstructured (triangular) to study the grid movement (Wacławski and Kalisz 2011; Garc Pérez 2016). The meshes with tube 2 and with four tubes are

shown in Figure 4-14 and Figure 4-15 respectively. They were all realised using ANSYS Workbench.

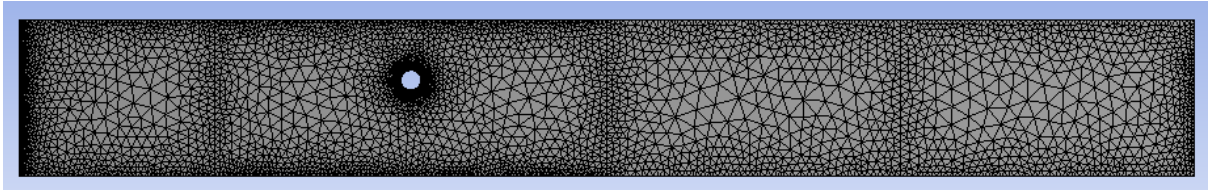


Figure 4-14: Triangular mesh (tube 2, $d_t= 39$ mm).

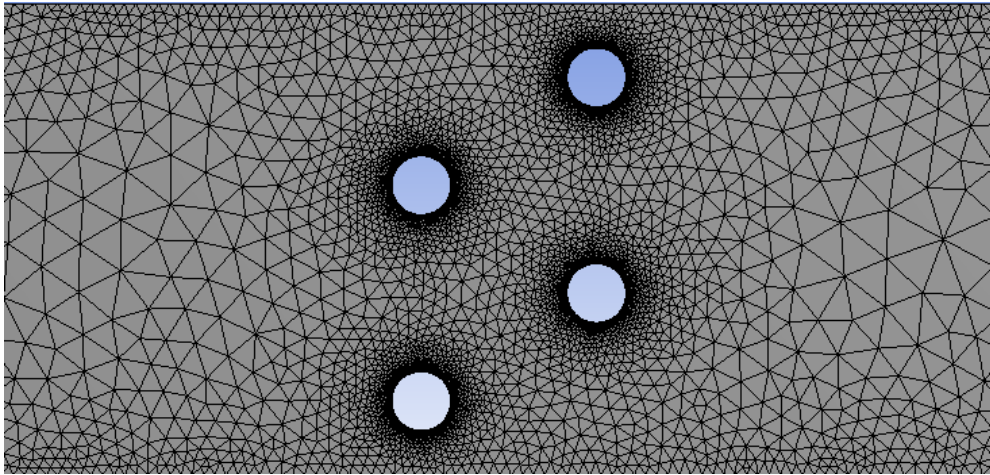


Figure 4-15: Triangular mesh (tubes 1', 2, 3, 4, $d_t= 39$ mm).

In this case, as well as in section 4.2.1, the number of nodes was increased at the inlet (since this affects the number of particles injected) and around the cylinder (to increase the accuracy of the results in the boundary layer). Moreover, as the domain was quite long, the geometry was divided into four zones with three interiors (vertical lines) to avoid the degeneration of the mesh and to make the mesh finer gradually around the tubes (Figure 4-13).

4.3.2 Grid convergence

Testing the grid is a very important step in the development of a CFD model as it ensures that the results are independent of the grid size. Three different grids were applied to the configuration in Figure 4-12. As this example is for an external flow case, the grid sensitivity was studied mainly by changing the number of nodes around the cylinders where the deposition takes place; the mesh characteristics are in Table 4-1 and Table 4-2.

A first set of simulations were run with the $k-\varepsilon$ standard turbulence model and all residuals were one order of magnitude less than the default values.

Table 4-1: Mesh features.

Mesh	Cylinder nodes	Nodes	Elements/Cells	Faces
1	100	4869	8954	13823
2	150	5276	9718	14994
3	200	5691	10500	16191

Table 4-2: Grid characteristics.

Mesh	y ⁺			Aspect ratio			Skewness		
	Max	Min	Ave	Max	Min	Ave	Max	Min	Ave
1	3.33	0.25	1.55	2.30	1	1.22	0.53	$2.42 \cdot 10^{-6}$	$6.18 \cdot 10^{-2}$
2	2.55	0.13	1.04	2.30	1	1.22	0.53	$3.32 \cdot 10^{-7}$	$6.22 \cdot 10^{-2}$
3	2.12	0.11	0.82	2.41	1	1.22	0.55	$2.42 \cdot 10^{-6}$	$6.22 \cdot 10^{-2}$

The second mesh was chosen because it represents a good compromise for its value of y^+ , the quality and computational costs. More information about the y^+ value is in Appendix A (section A.5). It should be noted that, y^+ needs to be lower than 5 (ideally 1) for the model to have a good description of the near wall region (Fu *et al.*, 2017).

Initially, the mesh was chosen considering only the flue gas without particles. In fact, the grid sensitivity is time consuming and it was not feasible to carry it out for all the geometries and models used in this work. Therefore, the results presented in this chapter were only taken as qualitative. However, once the model was settled, the grid convergence was verified for probe 2 using the model validated as reported in Chapter 7 and Appendix B (section B.1).

4.3.3 Model assumptions

Three different turbulence models were applied and a comparison is given in Figure 4-16 where the velocity profiles are represented at different distances from the cylinder 2 (interiors in Figure 4-13). They are all comparable except for the interior 2, which was located downstream from the cylinder and therefore was more affected by the vortex shedding formation.

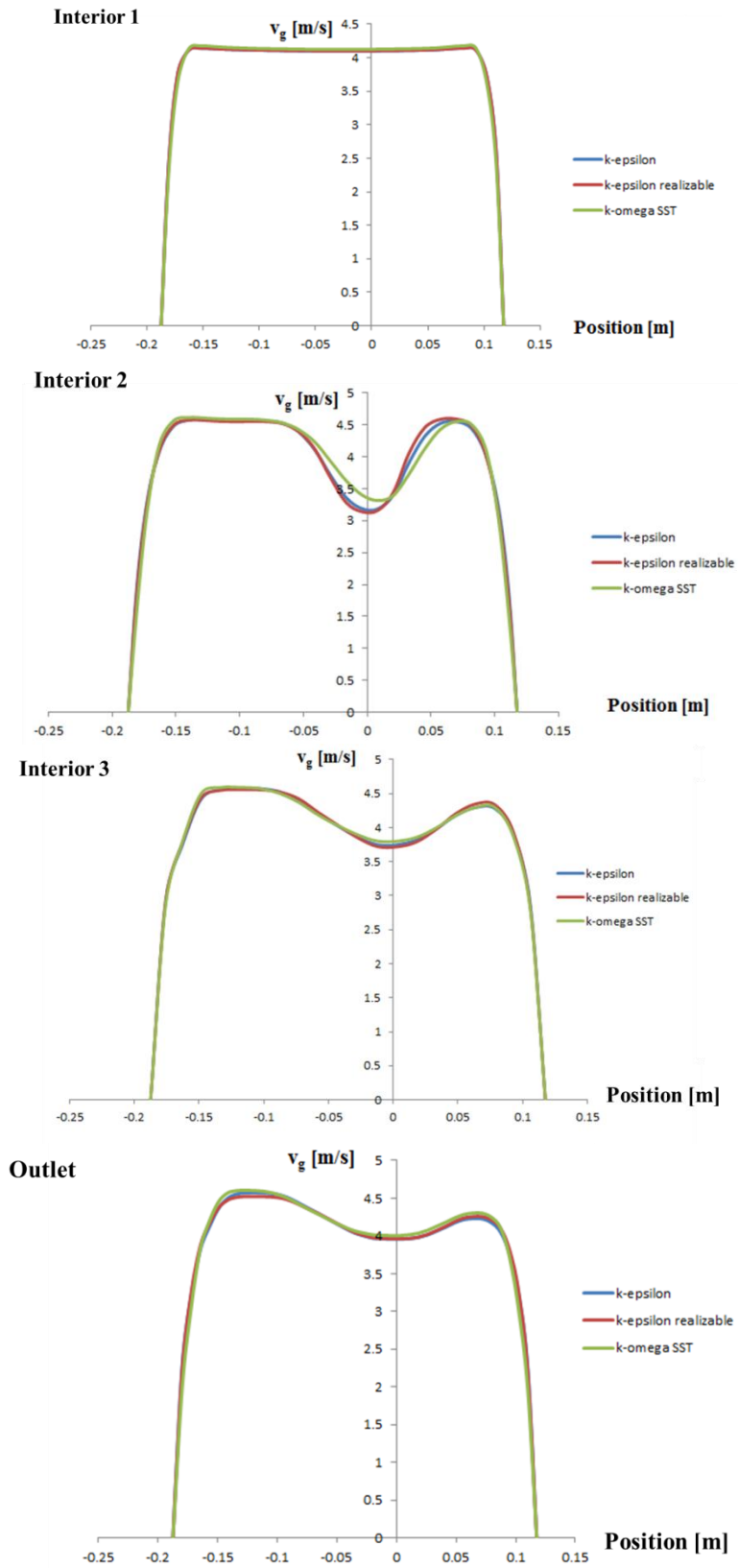


Figure 4-16: Velocity profile at Interior 1, Interior 2, Interior 3 and Outlet (tube 2, $d_t = 39$ mm, $U_0 = 4$ m/s, $T_g = 1273$ K, $T_{4,s} = 773$ K).

The velocity profile at the outlet is not too different from Interior 3 and it shows that the flow is still not fully developed. However this is out of the scope of this research since, for external flow, the length of the domain should guarantee the flow separation.

The velocity contours around the cylinder 2 for three different turbulence models ($k-\varepsilon$ with standard input, the $k-\varepsilon$ Realizable and $k-\omega$ SST) are shown in Figure 4-17 for simulations all using gas velocity 4 m/s, 1273 K and 773 K temperatures of the gas at the inlet and of the probe 2 respectively. For the following simulations, the $k-\omega$ SST model was used as it is generally recognised to better simulate the boundary layer and the vortex shedding (Rahman *et al.*, 2008; García Pérez, 2016; Yang *et al.*, 2017).

The flue gas was approximated to air and its velocity was based on some values of primary, secondary and pilot air from previous combustion rig operations. The inlet gas velocity was fixed to 4 m/s, as was the inlet particle velocity and the tube surface temperature was set to 773 K.

The main material properties were the same as reported in section 4.2.2, except for the gas, which were slightly modified and are reported below:

Combusted gas properties (air) at $T_g = 1273$ K (*The Engineering ToolBox*, 2018):

Density $\rho_g = 0.345 \text{ kg/m}^3$

Specific Heat $Cp_g = 1146 \text{ J/(kg K)}$

Thermal Conductivity $k_g = 0.069 \text{ W/(m K)}$

Viscosity $\mu_g = 44.07 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$

In this case the Reynolds number, based on the gas properties and tube diameter, was $Re \sim 1221$; therefore this case study is close to a Von Karman vortex trail which is turbulent (Haugen and Kragset, 2010) as confirmed in Figure 4-18.

Fluent[®] solved the equations of fluid motion, better known as Reynolds-Averaged Navier-Stokes (RANS) equations to determine the flow properties. Initially, simulations were run for the fluid without any particles. Once the flow was almost steady state, these simulations were used as the fluid field initial condition for the transient simulations with particles.

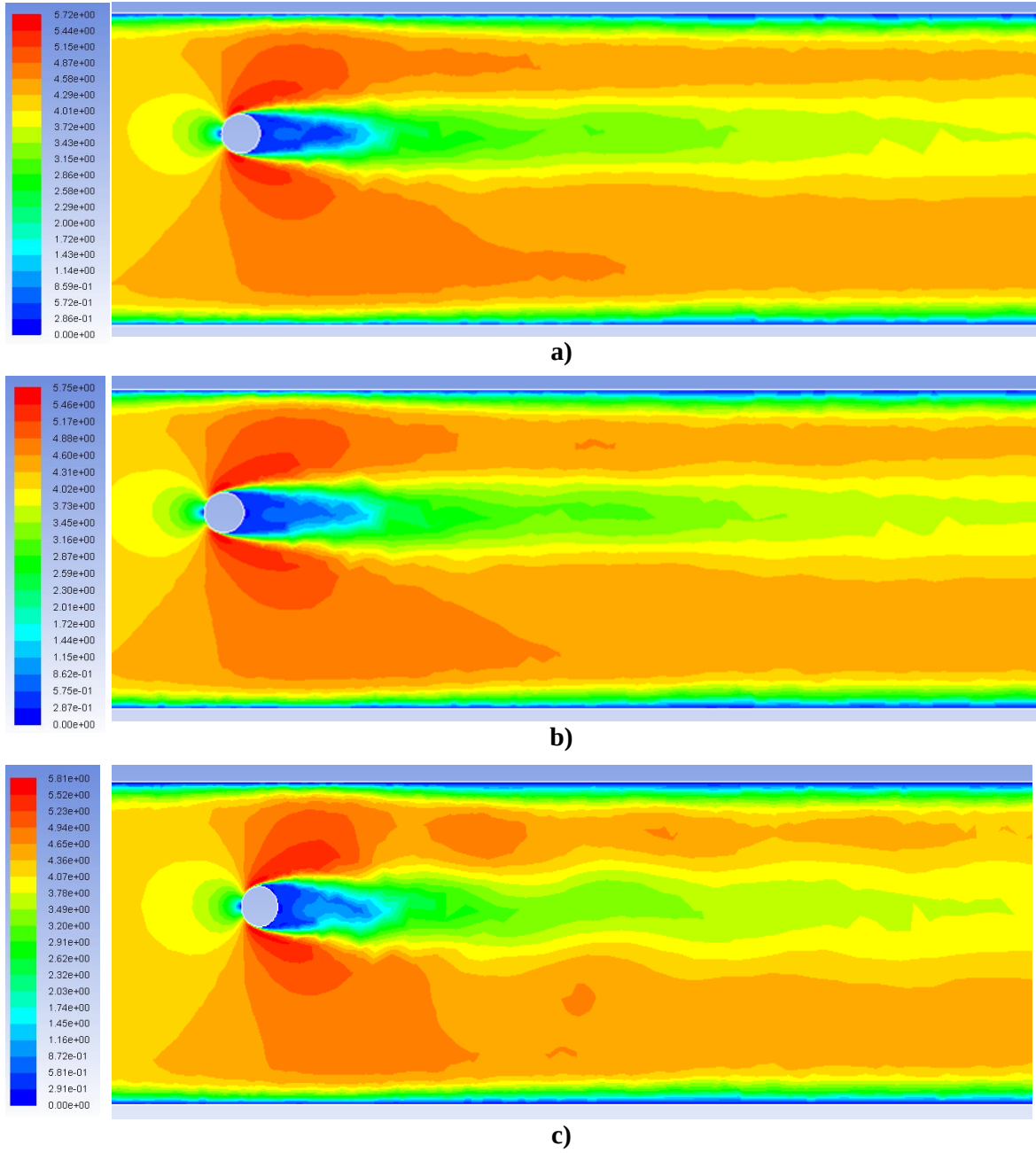
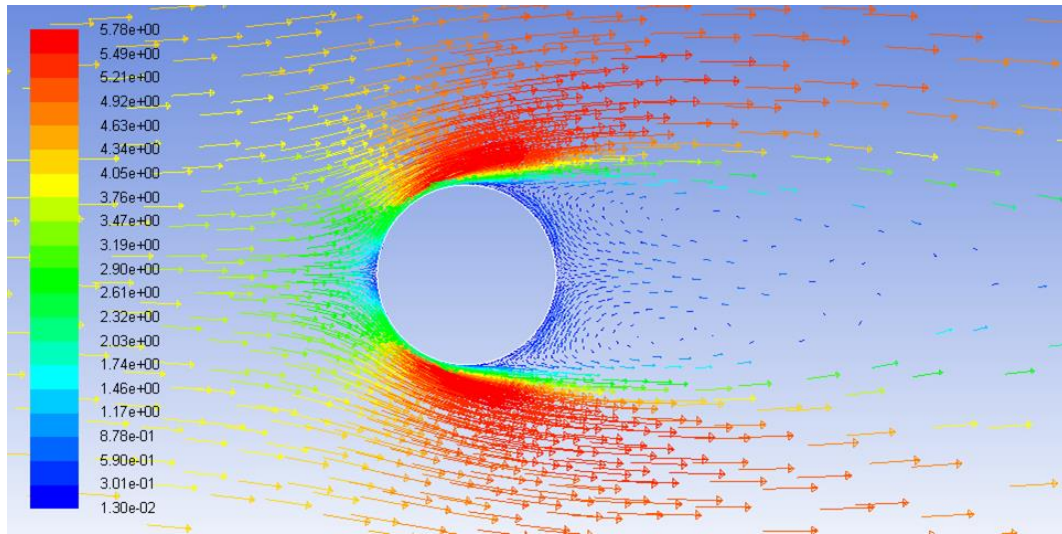
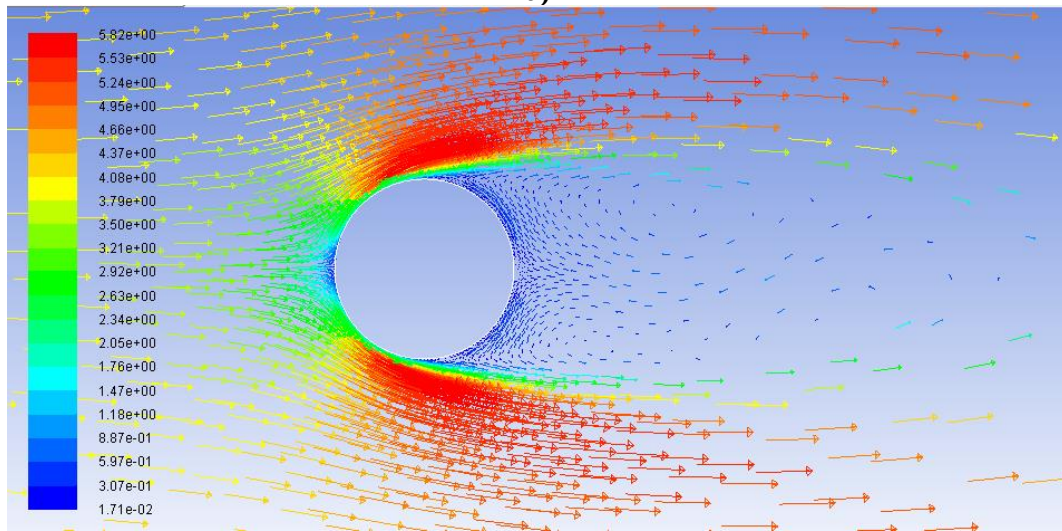


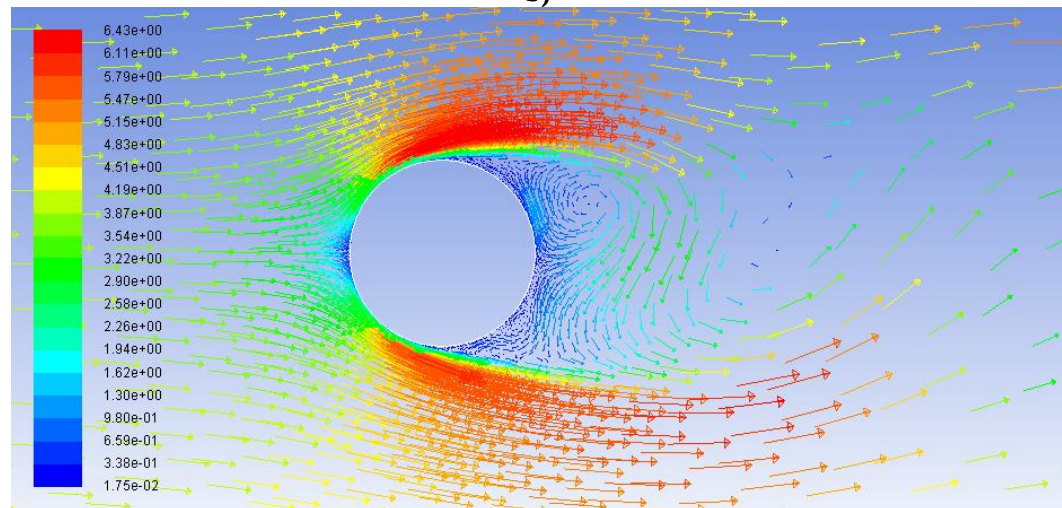
Figure 4-17: Velocity contours [m/s] around tube 2 ($d_t=39$ mm) for different turbulent models a) $k-\varepsilon$ standard, b) $k-\varepsilon$ realizable c) $k-\omega$ SST ($T_g=1273$ K, $T_{4,s}=773$ K, $U_0=4$ m/s).



a)



b)



c)

Figure 4-18: Gas velocity vectors [m/s] around tube 2 ($d_t = 39$ mm) a) $k-\epsilon$ standard, b) $k-\epsilon$ realizable c) $k-\omega$ SST ($T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

In this work, transient simulations were carried out and the time step that ensures a Courant number ≤ 1 was chosen. In fact, this is crucial to get reliable results and to capture the vortex shedding correctly as it affects some of the particle deposition behaviours.

The frequency of vortex shedding behind the cylinder was characterised by the Strouhal number (St) which is function of the Reynolds number (Lienhard, 1966) (Appendix A, section A.6). Once the Reynolds number had been calculated, the Strouhal number was obtained ($St \sim 0.22$) and used to get the frequency of vortex shedding (f) as in Equation (4-5) and, as a consequence, the time period (T) in Equation (4-6):

$$f = \frac{St u_g}{d_t} = 23.09 \text{ s}^{-1} \quad (4-5)$$

$$T = \frac{1}{f} = 0.043 \text{ s} \quad (4-6)$$

In order to capture the shedding correctly, it was important to have at least 20-25 time steps (n) in one shedding cycle (Fluent, 2017). Therefore, the time step size (Δt) needed to be at most:

$$\Delta t = \frac{T}{n} = \frac{0.043}{25} = 0.0017 \text{ s} \quad (4-7)$$

The lift coefficient over the cylinder 2 was obtained during the simulation in Fluent[®] using the $k-\omega$ SST model and it was reported in Figure 4-19. Its behaviour is typical of a transient simulation periodically converged and the period between two consecutive oscillations is not too different from the one calculated in Equation (4-6).

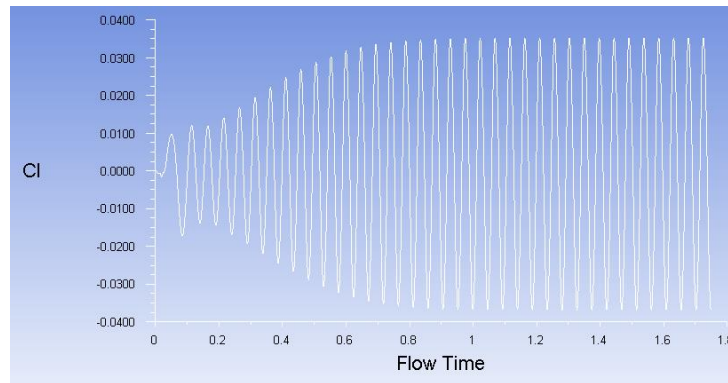


Figure 4-19: Time history of the lift coefficient (tube 2, $d_t = 39$ mm, $k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

4.3.4 Ash particle trajectories

The unsteady Discrete Phase Model DPM in Fluent[®] was used to inject perfectly spherical inert ash particles at the inlet. The model took into consideration the force of gravity acting along the moving ash particles with the direction of the flue gas (x positive) and the interaction between the two phases.

In Figure 4-20 ash particle tracking is reported for different diameters. Small particles tend to follow the flue gas streamlines because they do not have enough inertia to overcome the drag force. In contrast, particles with bigger diameters tend to rebound and possibly hit the neighbouring tubes (Tomeczek and Waclawiak, 2009; Waclawiak and Kalisz, 2012; Lee *et al.*, 2014).

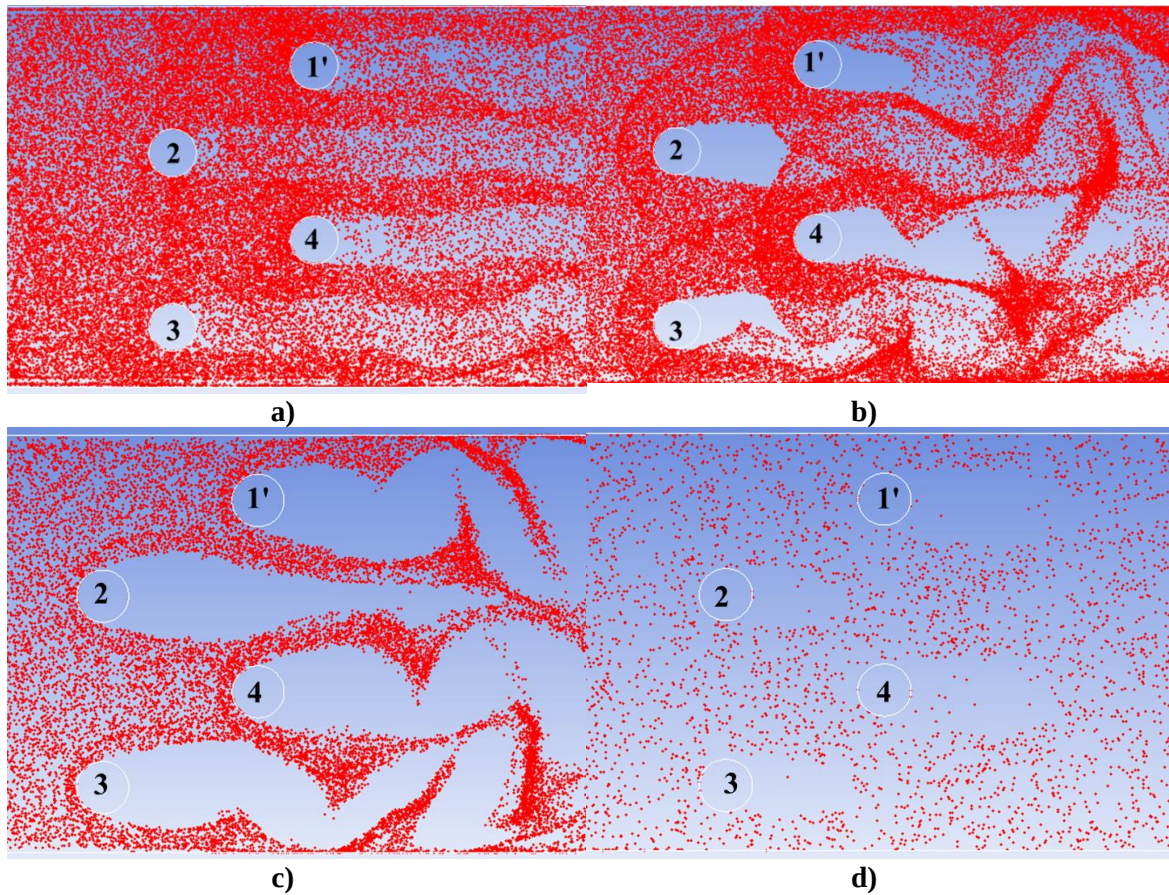


Figure 4-20: Tracking of different ash particle diameters a) 200 μm , b) 100 μm , c) 50 μm , d) 1 μm ($d_t = 39 \text{ mm}$, $k-\omega$ SST, $T_g = 1273 \text{ K}$, $T_{a,s} = 773 \text{ K}$, $U_0 = 4 \text{ m/s}$).

In particular, it can be seen in Figure 4-20 (a) that 200 μm particles hit the rear side of tubes 2 and 3 because of the high energy of the rebounding particles from tubes 1' and 4 and, as a consequence, this can affect their deposition behaviour.

Finally, an example of trajectories for an ash particle distribution following the Rosin-Rammler model is given in Figure 4-21 and it confirms what has already been stated above for single ash particles in Figure 4-20. In fact, particles with $d_p > 10 \mu\text{m}$ hit the front of probes and their rebound increases with their diameters. Figure 4-21 confirms that bigger particles are able to hit the rear side of probes 2 and 3 because of their rebound from the top of probes 1' and 4. In contrast, small particles tend to follow the gas on the downstream side (e.g. probes 1' and 4) (Figure 4-21).

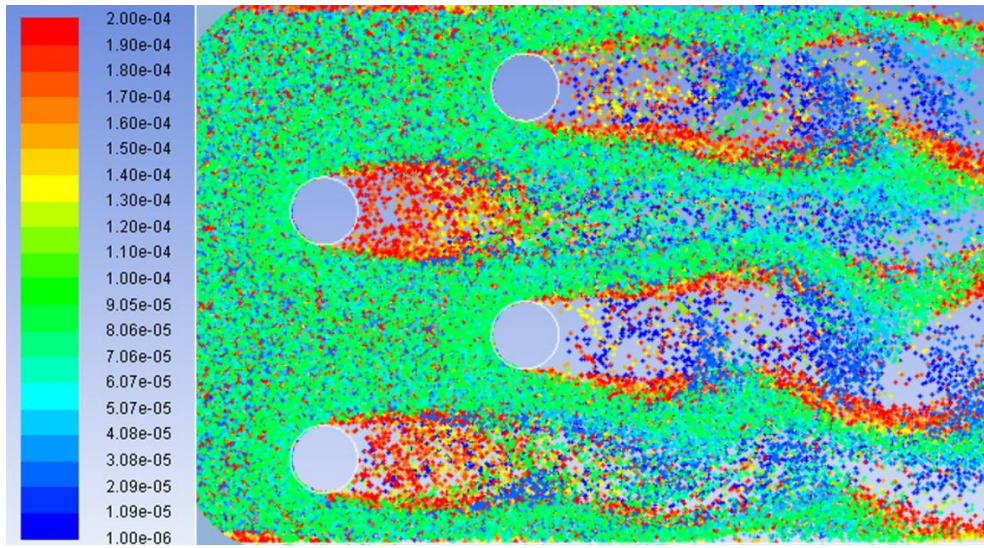


Figure 4-21: Tracking of ash particles following a Rosin Rammler size distribution ($d_{min}= 1 \mu\text{m}$, $d_{mean}= 40 \mu\text{m}$, $d_{max}= 200 \mu\text{m}$, polydispersion parameter $n= 0.8$, $d_t= 39 \text{ mm}$, $k\text{-}\omega$ SST, $T_g= 1273 \text{ K}$, $T_{4,s}= 773 \text{ K}$, $U_0= 4 \text{ m/s}$).

4.3.5 Deposition predictions

Predictions of deposition were obtained using the powdery deposition model for different ash particle diameters. This confirmed that deposition occurred mainly on the front side of the tube for big particles. In contrast, small particles also deposited on the rear part of the tube (consistent with results reported by Waławiak and Kalisz, 2012).

As in previous studies (Fu et al., 2017; Hosseini et al., 2017), the deposition flux was studied as a function of the gas velocity (3, 4 and 10 m/s) for different particle diameters (100, 50, 1 μm) around tube 2 (Figure 4-12 and Figure 4-22). The results are shown in Figure 4-23 to Figure 4-25. These figures show that at higher velocities, the bigger

particles (in particular 100 μm and 50 μm) have more momentum to rebound from the surfaces and this reduces the deposition flux.

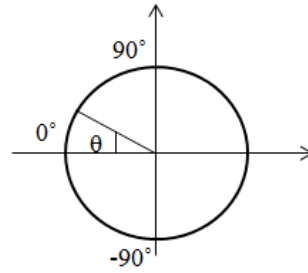


Figure 4-22: Angle around a circular cylinder.

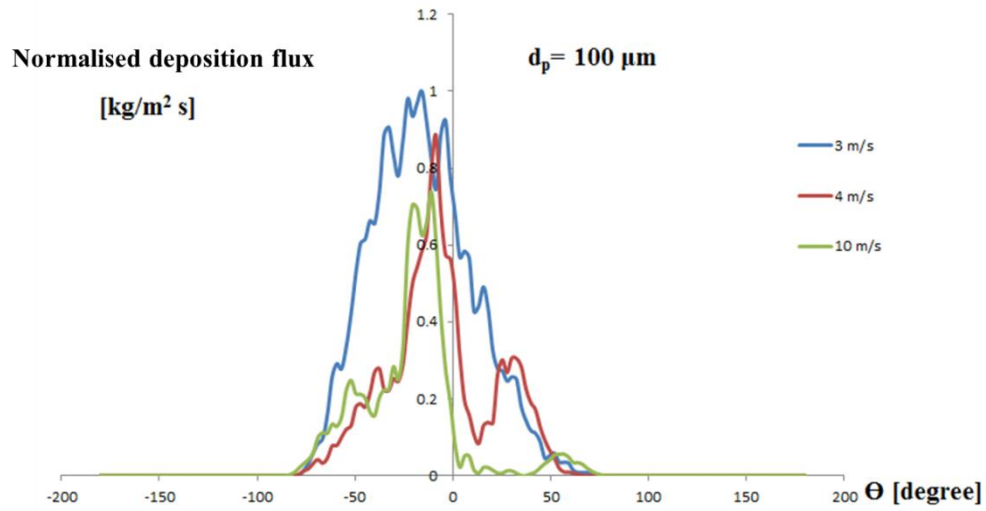


Figure 4-23: Normalised deposition flux around probe 2 ($d_t = 39 \text{ mm}$) using the powdery model at different gas velocities ($k-\omega$ SST, $T_g = 1273 \text{ K}$, $T_{4,s} = 773 \text{ K}$, $U_0 = 4 \text{ m/s}$, $d_p = 100 \mu\text{m}$).

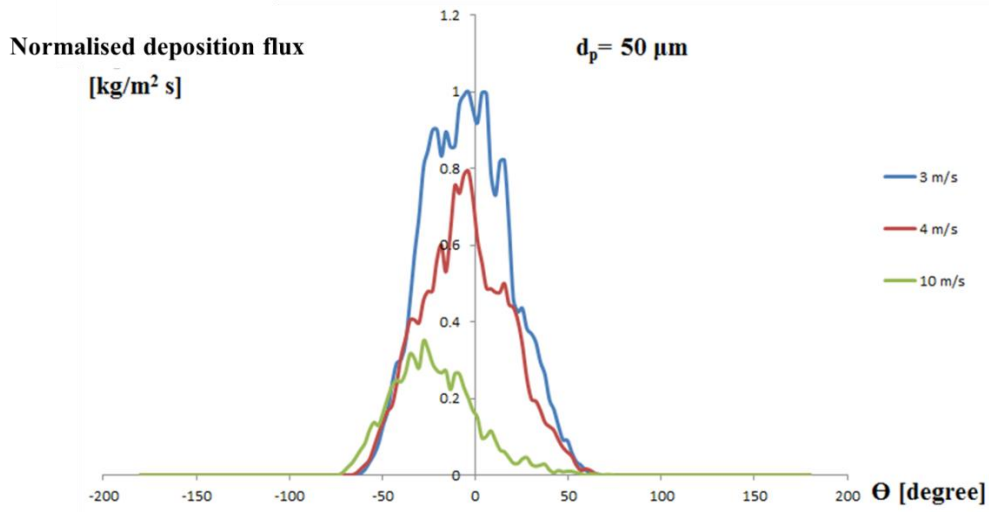


Figure 4-24: Normalised deposition flux around probe 2 ($d_t = 39 \text{ mm}$) using the powdery model at different gas velocities ($k\text{-}\omega$ SST, $T_g = 1273 \text{ K}$, $T_{4,s} = 773 \text{ K}$, $U_0 = 4 \text{ m/s}$, $d_p = 50 \mu\text{m}$).

The trend was similar for $150 \mu\text{m}$ and $50 \mu\text{m}$ particles but it was different for smaller particles which were more likely to deposit all around the probe and their deposition flux was found to be less affected by the gas velocity (Figure 4-25).

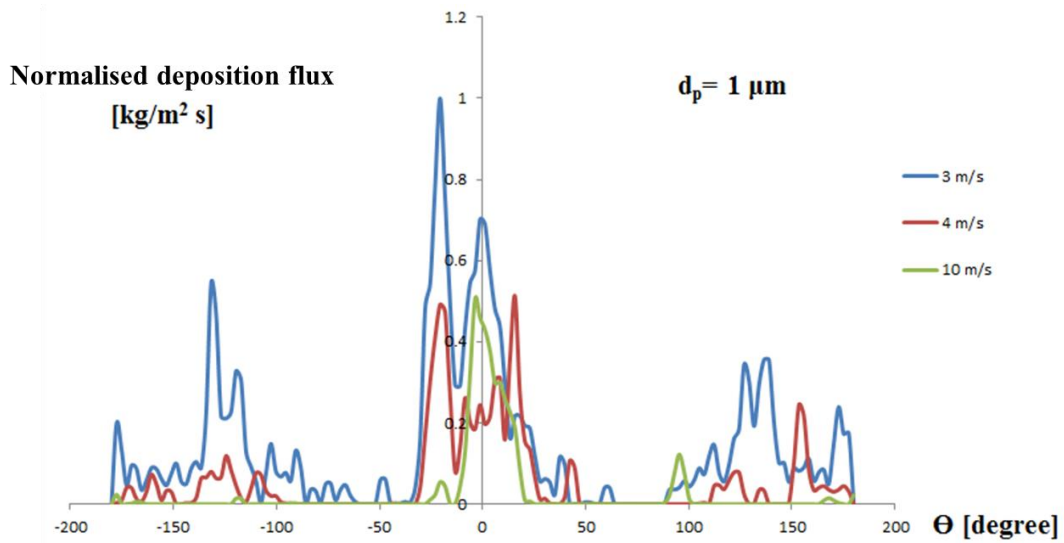


Figure 4-25: Normalised deposition flux around probe 2 ($d_t = 39 \text{ mm}$) using the powdery model at different gas velocities ($k\text{-}\omega$ SST, $T_g = 1273 \text{ K}$, $T_{4,s} = 773 \text{ K}$, $U_0 = 4 \text{ m/s}$, $d_p = 1 \mu\text{m}$).

A comparison between the powdery model applied to study deposition on tube (2), in Figure 4-1 and Figure 4-12 in sections 4.2 and 4.3 respectively, shows that bigger particles ($d_p \geq 10 \mu\text{m}$) have more energy to rebound, in particular at the stagnation point.

However the deposition flux profile in Figure 4-8 is more symmetric around $\Theta = 0^\circ$ than in Figure 4-23. This could be due to the position of tube 2 which is located in the middle of the domain in Figure 4-1 and closer to the wall in Figure 4-12. Moreover, $50\ \mu\text{m}$ particles have less energy to rebound and their tendency of sticking at the stagnation point is higher as can be observed in Figure 4-7 (b) and Figure 4-24. Finally, smaller particles ($d_p \leq 1\ \mu\text{m}$), with low inertia, are more likely to deposit all around the probe as given in Figure 4-7 (c) and Figure 4-25.

This model is more suitable for dry ash particles hitting a clean surface which only happens at the beginning of the deposition process and it does not take into account the vapour condensation.

Therefore, a step forward was to include the stickiness of the surface and of the particles including (P_{tot}) in Equation (2-59).

The surface stickiness P_s depending on Na_2SO_4 [1 ppm] was considered as in section 4.2.4 and the wall temperature was fixed to 773 K. Moreover, the propensity of a particle to stick to the tube surface P_p was calculated with the reference viscosity model function of the particle chemical composition and temperature (section 2.8.2).

However, at this stage of the research data of ash chemical composition were not available yet and previous correlations suggested by Beckmann *et al.*, (2016) for Middelburg coal were used as in Equation (4-8):

$$\log(\mu_p) = \log(a) + \frac{b}{T_p} \quad (4-8)$$

Where $\log(a)$ and b were obtained from some experimental graphs in which the log of ash viscosity μ_p was plotted versus the reciprocal of temperature.

The values used in this particular case were:

$$\log(a) = -8.07;$$

$$b = 14100.72;$$

$$\mu_{ref} = 17\ \text{Pa s}.$$

However, these parameters strongly depend on the fuel and ash composition and were only used in a preliminary stage of the research to calculate the total deposition flux (m_{tot}) including the total stickiness probability (P_{TOT}) (function of the particle and surface stickiness).

This model was applied to study deposition around four tubes (Figure 4-26) for three different particle diameters (200, 100 and 1 μm as shown in Figure 4-27, Figure 4-28 and Figure 4-29 respectively). In the following figures, the brown line represents the deposit accumulated on the probe surface (black line). Deposits were accumulated until the deposition flux was stable (a few seconds in case of single injections) and the values were exported to simulate the shape around the probes. However, these results are only qualitative since deposition was simulated for single ash particles (not ash distribution) and with models and parameters taken from the literature.

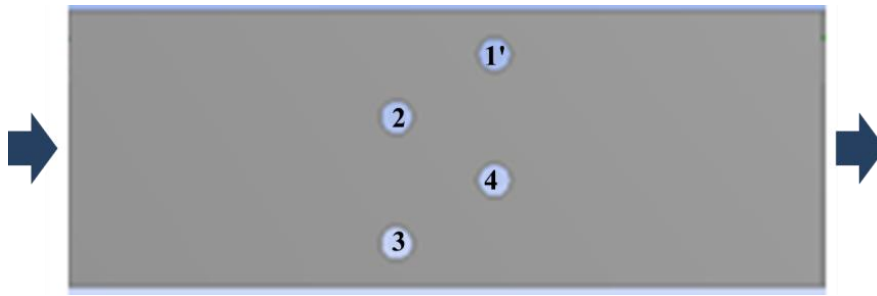


Figure 4-26: Configuration with four tubes: 1', 2, 3, 4 ($d_i = 39$ mm) in Cranfield combustion rig.

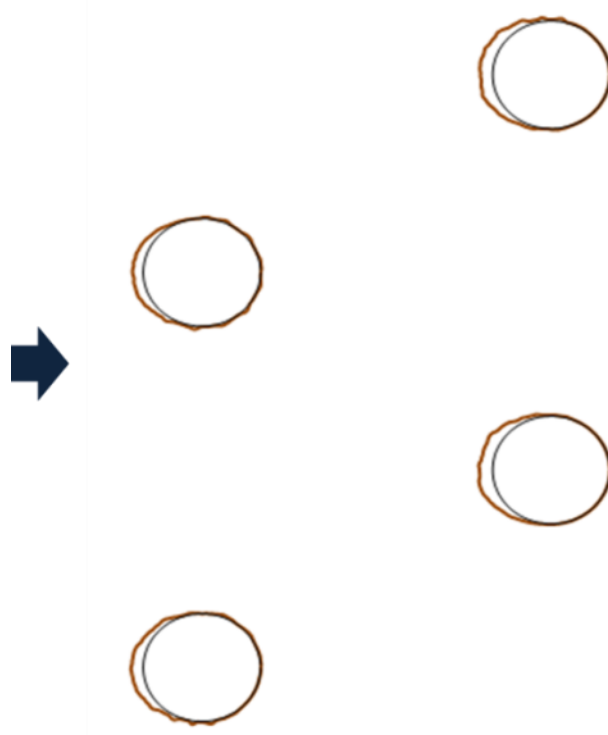


Figure 4-27: Deposit location around tubes 1', 2, 3, 4 ($d_t = 39$ mm), using P_{tot} ($d_p = 200$ μm , $k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

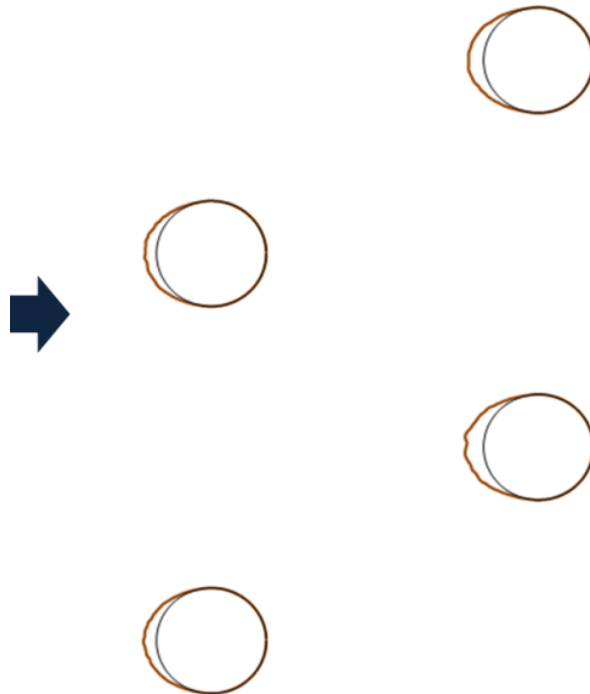


Figure 4-28: Deposit location around tubes 1', 2, 3, 4 ($d_t = 39$ mm), using P_{tot} ($d_p = 100$ μm , $k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

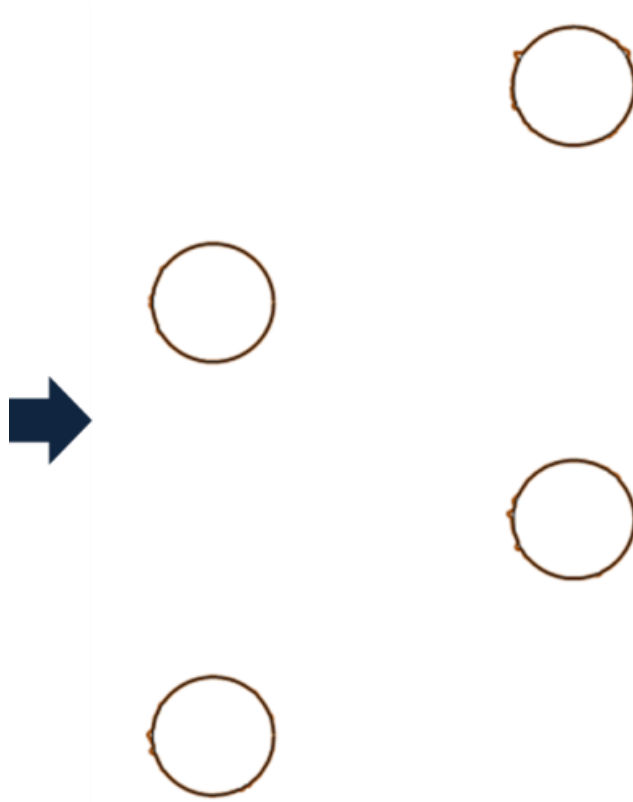


Figure 4-29: Deposit location around tubes 1', 2, 3, 4 ($d_t = 39$ mm), using P_{tot} ($d_p = 1$ μm , $k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

The deposition occurred mainly on the upstream face for bigger particles. However, some deposits can be identified on the rear side of tubes for small particles (1 μm) and 200 μm particles as they rebound from tubes 1' and 4 to the rear of 2 and 3 which confirms what already noticed in the ash particle behaviour in section 4.3.4.

In addition, the effect of the alkali vapour concentration on the deposition flux (P_{TOT}) was studied varying level of Na_2SO_4 (1, 10 and 100 ppm) in the configuration in Figure 4-26. The results of deposition flux around the probes as function of the vapour concentration in the presence of a Rosin Rammler ash particle size distribution were plotted in Figure 4-30-Figure 4-33.

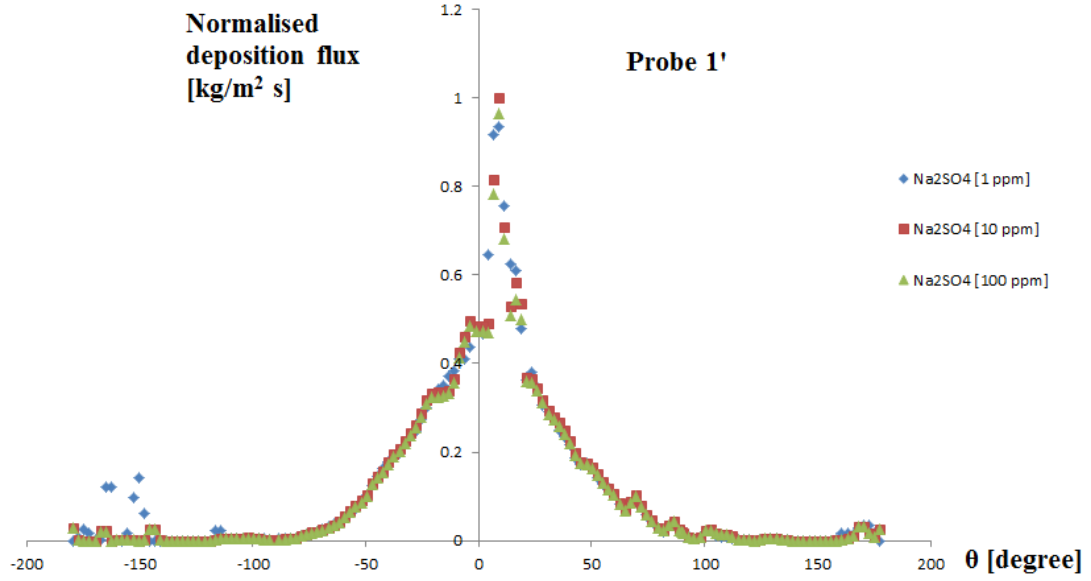


Figure 4-30: Normalised deposition flux around probe 1' ($d_t = 39$ mm) using P_{tot} at different Na_2SO_4 concentrations ($k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s, Rosin Rammler size distribution $d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$).

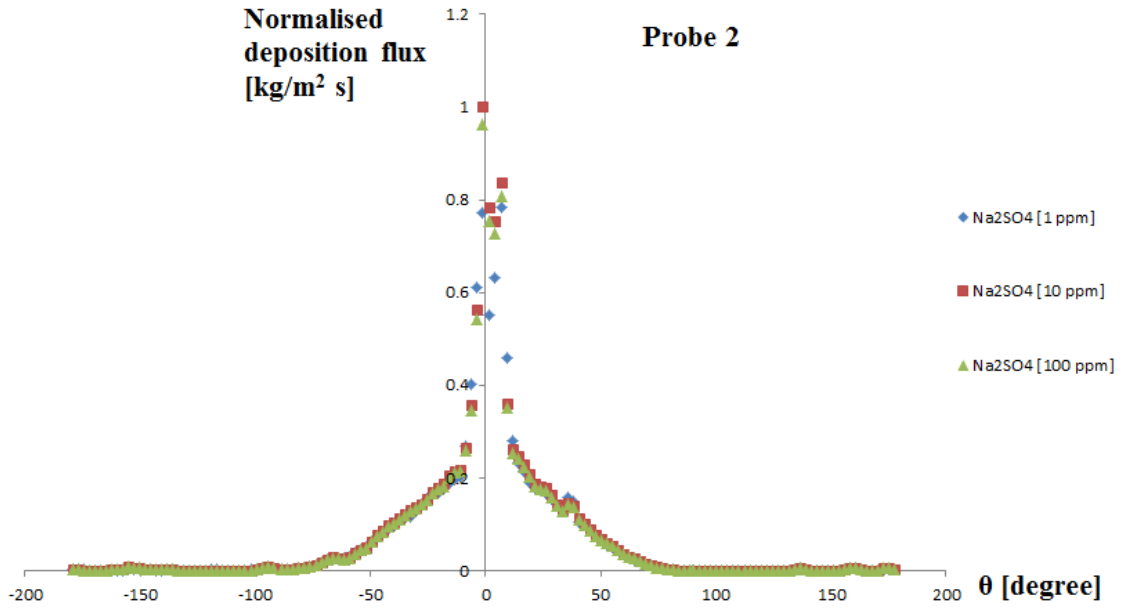


Figure 4-31: Normalised deposition flux around probe 2 ($d_t = 39$ mm) using P_{tot} at different Na_2SO_4 concentrations ($k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s, Rosin Rammler size distribution $d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$).

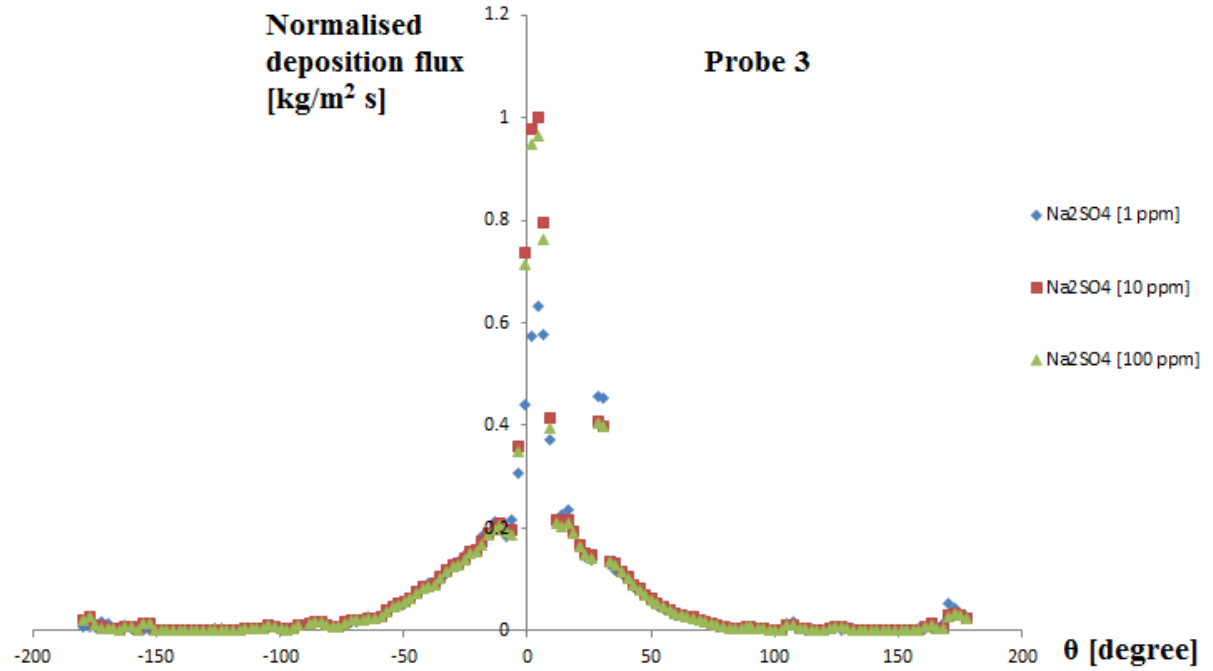


Figure 4-32: Normalised deposition flux around probe 3 ($d_t = 39$ mm) using P_{tot} at different Na_2SO_4 concentrations ($k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s, Rosin Rammler size distribution $d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$).

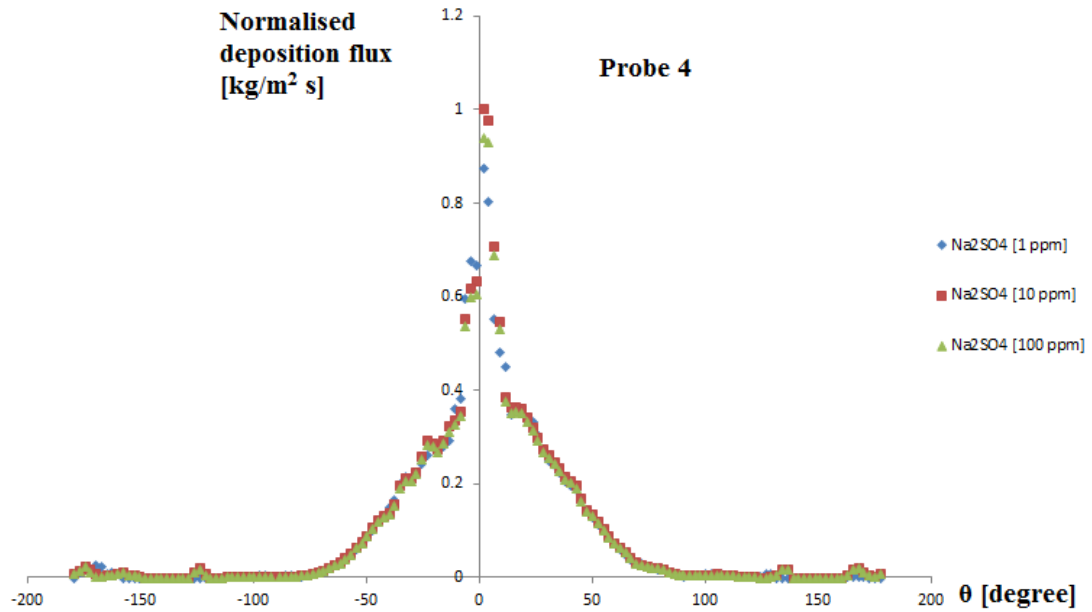


Figure 4-33: Normalised deposition flux around probe 4 ($d_t = 39$ mm) using P_{tot} at different Na_2SO_4 concentrations ($k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s, Rosin Rammler size distribution $d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$).

The simulations were run in the same conditions (e.g. gas velocity $U_0 = 4$ m/s, inlet gas temperatures $T_g = 1273$ K and probe temperatures $T_{4,s} = 773$ K, turbulence model $k-\omega$ SST and ash particle size distribution $d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$), varying only Na_2SO_4 concentration (1, 10 and 100 ppm).

The results showed that deposition occurred mainly on the top of the probes and only a little deposition flux was identified on the side and downstream for all the probes. However, variable concentration of Na_2SO_4 in the flue gas did not significantly affect the deposition flux values. Therefore, it can be stated that vapour concentration contributes to the formation of a thin sticky layer which supports deposition especially on a clean tube and for bigger particles that would be more likely to rebound as shown in section 4.2.4.

4.3.6 Deposit temperature

The methodology explained in section 3.9 was applied to the tube in Figure 4-12 to predict the effect of deposit formation on its surface temperature. Preliminary results were obtained assuming a constant tube temperature (773 K) and external heat flux $\dot{Q}_{tot}$.

First of all, the deposit thickness calculated from the modified DEFINE_DPM_EROSION UDF was exported to update the mesh and the temperature using Equations (2-75). As already mentioned in section 4.2.5, if the grid movements are too big, the grid can degenerate in a negative volume and it can also cause temperature divergence errors. An example of results obtained combining the three modified UDFs for deposit accumulation, grid motion and deposit temperature is reported in Figure 4-34 which was realised for 100 μm particles and powdery deposit. The following figures are temperature contours around the probe 2 (Figure 4-12) where the lowest temperature is in blue (773 K) and the highest is in red (1273 K).

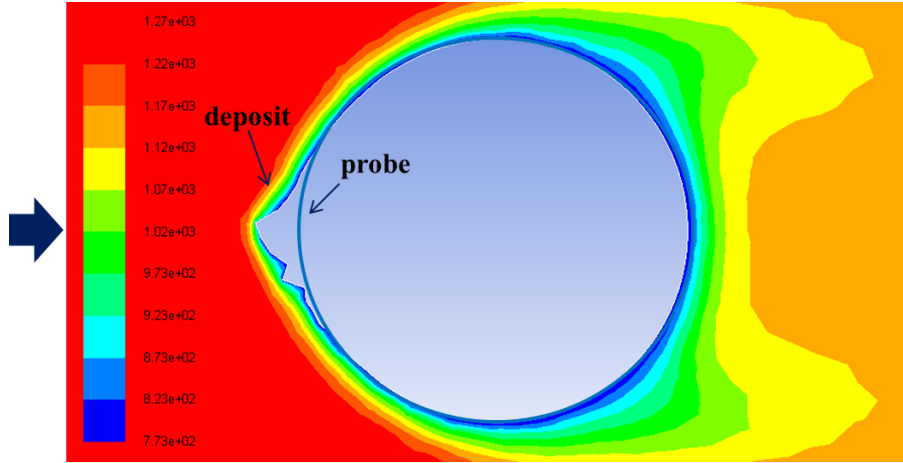


Figure 4-34: Temperature contour [K] around probe 2 ($d_t = 39$ mm) with powdery deposit model ($d_p = 100$ μm , $k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

This confirms that this size of particle deposit mainly on the upstream side of the tube and it creates an insulating layer which results into a higher surface temperature. Moreover, Figure 4-35 shows the combination of deposit shape and temperature prediction around probe 2 for a distribution of ash particles in terms of the total deposition flux (i.e. including both particle and surface stickiness).

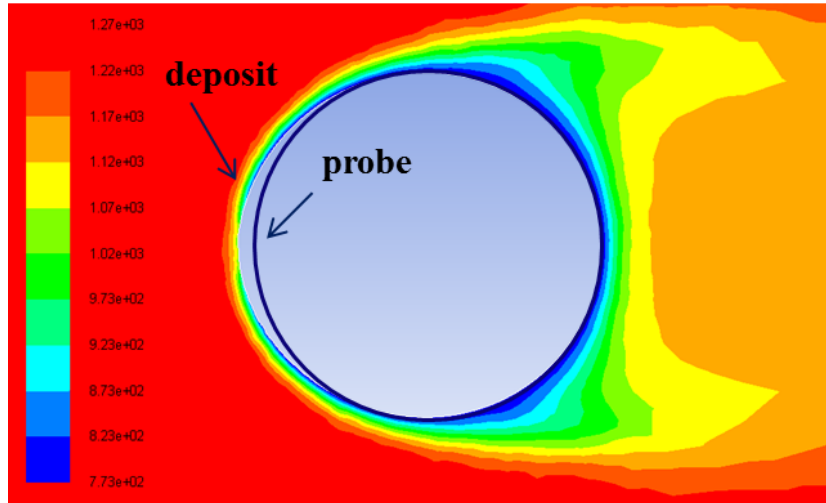


Figure 4-35: Temperature contour [K] around probe 2 ($d_t = 39$ mm) after ~ 2 hours exposure including P_{tot} with Rosin Rammler size distribution ($d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$, $k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s, Na_2SO_4 at 1ppm).

With this method, the tube assumes the shape of the deposit and the gradient of temperature into the deposit layer cannot be appreciated.

Another technique was considered for simulations with probe 2. It required the presence of an initial thin deposit layer (max 1 mm) with the properties of a solid surrounded by fluid gas (section 3.9). DEFINE_DPM_EROSION and DEFINE_GRID_MOTION UDFs were applied to the interface between the two phases and the temperature contours, before the deposition started, are in Figure 4-36 and Figure 4-37. This latter figure shows a detail of the gradient inside the deposit where the layer side closer to the cylinder wall has a lower temperature compared to the one exposed to the hot flue gas.

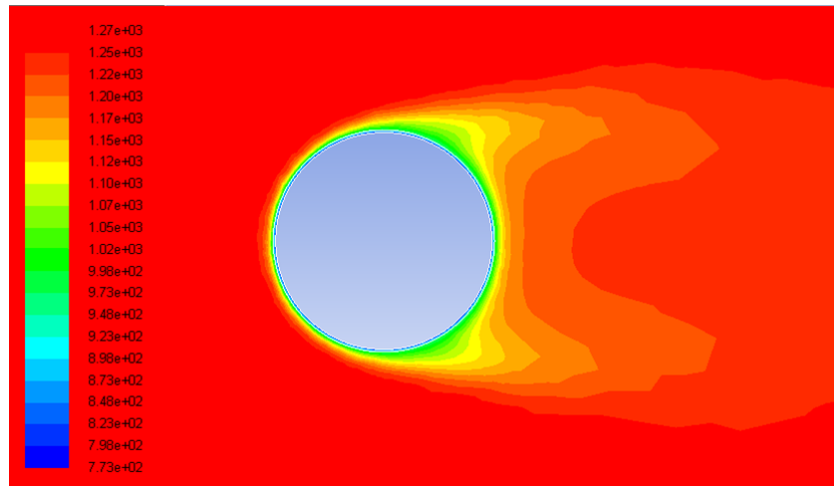


Figure 4-36: Contour of temperature [K] around tube 2 ($d_i = 39$ mm) at $t = 0$ s ($k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

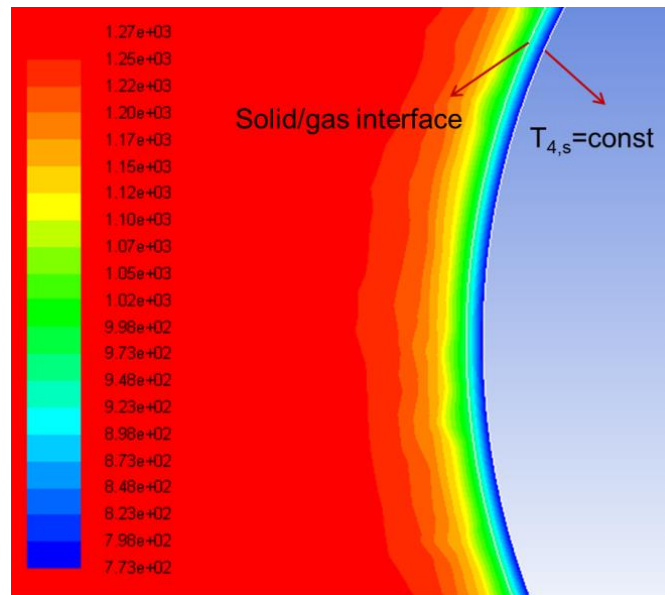


Figure 4-37: Detail of temperature contour [K] in a thin deposit layer around tube 2 at $t = 0$ s ($k-\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s).

Once the deposit accumulated on the surface of the tube, the grid motion was enabled. Examples are shown in Figure 4-38 which gives a detail of the shape of the deposit and its increasing surface temperature. In fact, when the deposit thickness grows, its surface tends to the surrounding gas temperature (Figure 4-38, b).

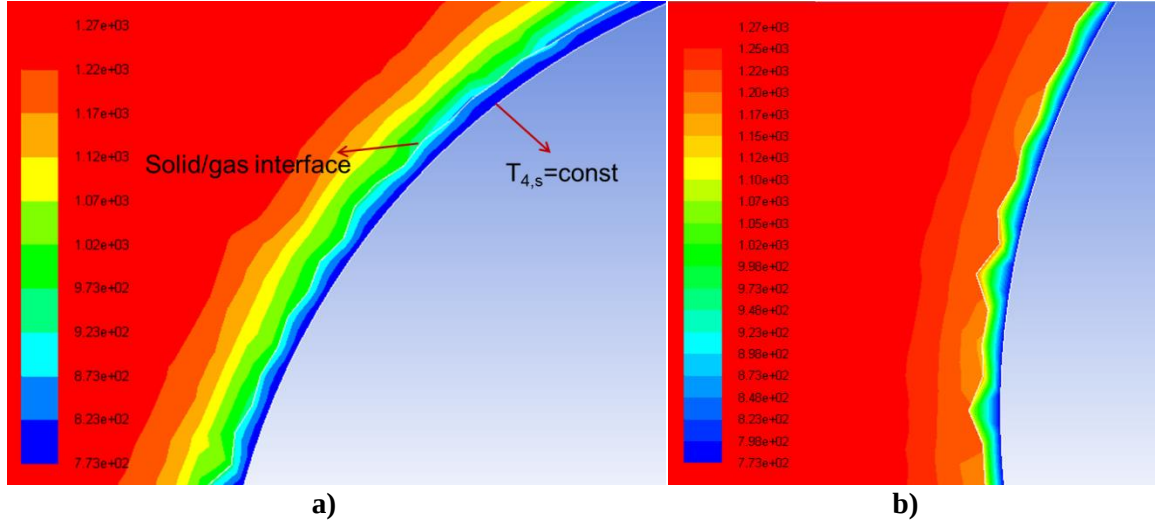


Figure 4-38: Grid motion applied to the solid/fluid interface to simulate the deposit temperature [K] around tube 2 ($d_t = 39$ mm) with powdery deposit model ($d_p = 100$ μm , $k\text{-}\omega$ SST, $T_g = 1273$ K, $T_{4,s} = 773$ K, $U_0 = 4$ m/s) a) after ~ 30 s, b) after ~ 200 s.

The use of this method has been demonstrated to depend highly on the deposit thermal conductivity and on the mesh resolution into the deposit layer. Therefore, it needs further study and, for this reason, it was not used to validate the model (Chapter 7).

4.4 Summary of key findings

In this chapter, the methodology described in Chapter 3 was applied to run several simulations for deposit predictions. Previous models from the literature were used for comparison in terms of qualitative information about ash particle behaviour as function of the geometry, tube arrangement, gas velocity and sticking models.

The main observations can be summarised as follows:

- 1) Ash particles trajectories were studied with single particle injections and using an ash particle size distribution with the Rosin Rammler model ($d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , polydispersion parameter $n = 0.8$). In both cases, bigger particle diameters hit the upstream side of the tubes and they are more likely to rebound because of their high momentum. Small particles follow the

flue gas streamlines and hit the rear part of the tube, in particular if the stochastic tracking model is enabled.

- 2) Ash particle trajectories are influenced by the tube location in the computational domain, the vicinity of the walls and the presence of other tubes, which can modify the trajectory of ash particles. For example larger particles can rebound from the upstream faces of downstream tubes to produce deposition on the downstream parts of the upstream tubes.
- 3) Different deposition models were included in the modified DEFINE_DPM_EROSION UDF with an increasing complexity. These ranged from single deposition mechanisms to a combination of them (including the stickiness of particles and surface). The presence of vapour phase species (Na_2SO_4) led to a sticky surface which enhanced the deposit accretion, especially on a clean tube. This was studied at different levels of concentration (1, 10 and 100 ppm) but it demonstrated not to have a significant impact on the total deposition flux.
- 4) The grid motion code was able to predict the shape of the deposit and some suggestions of how to run the code were provided in order to avoid computational errors.
- 5) The shape of the deposit and the increasing surface temperature due to the deposit built up were simulated. In fact, the presence of the deposit can modify the flow dynamic around the cylinder and the deposition mechanisms, in particular those depending on the surface temperature (Chapter 7).

Finally, it is remarkable that examples like the ones investigated in this chapter have not been used to get quantitative descriptions of the phenomena. However, due to the high degree of complexity, it has been necessary to make many simplifications. Some simulations were run with single ash particle diameters to understand specific particle behaviour; however they do not represent the real situation in boilers where ash particle distributions are encountered. Moreover, injections of single ash particles can overestimate the amount of deposits (Figure 4-34). Therefore, experimental results were necessary to provide boundary conditions for the models and data for their validation (Chapter 7).

5 EXPERIMENTAL METHODOLOGY

5.1 Introduction

In this chapter, the methodology used to run the experiments of ash deposition on air-cooled ceramic probes in a pilot scale pulverised combustion rig is described. A detailed description is given of the facility and the fuel used in this work, as well as the main analytical techniques adopted for gas, temperature and ash deposit characterisation. A procedure to run the experiments was written and is summarised in section 5.7 and Appendix E.

The same methodology was applied to all the experiments to ensure consistency and to allow the comparison of results. Moreover, some calculations and preliminary considerations were done and the methodology was planned to provide the information necessary for the model boundary conditions and for its validation. The main data to be generated can be summarised as follows:

Model set-up and boundary conditions:

- Geometry of the PF combustor (Figure 5-2)
- Probe configurations (Figure 5-21)
- Probe temperatures (section 5.6)
- Gas properties (velocity and temperature) (section 5.5)
- Ash particle size distribution and chemical composition (section 5.8 and Chapter 6)

Model validation:

- Deposition flux results (Chapter 6)
- Deposit shape and thickness (Chapter 6)

5.2 Rig description

The tests were conducted in a 100 kW_{th} capacity downward firing pulverised fuel (PF) pilot-scale combustion rig at Cranfield University (Figure 5-1). It consisted of a fluidised bed combustor (FB) up to 1.24 m (left) and a pulverised fuel combustor (PF), 3.71 m height (right) (Khodier, 2011; Jurado Pontes, 2014) (Figure 5-1 and Figure 5-2).

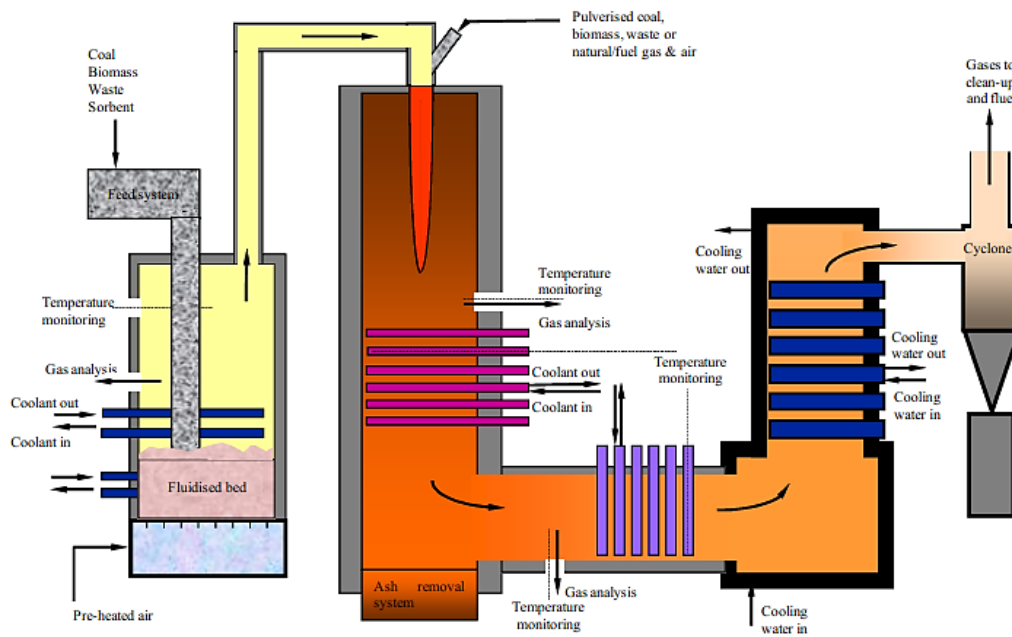


Figure 5-1: Schematic of the FB (left) and PF (right) combustors at Cranfield (Khodier, 2011).

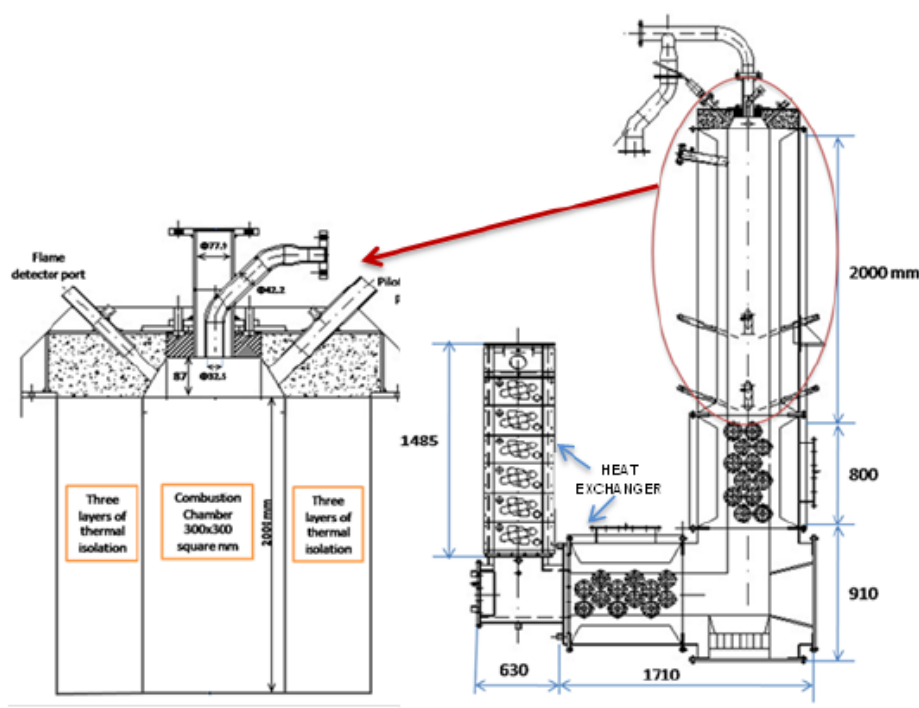


Figure 5-2: Drawing of the PF combustor at Cranfield with dimensions (Jurado Pontes, 2014).

The combustor has a square cross-section (0.3 x 0.3 m) and three layers of thermal isolation. The rig was heated up to $\sim 800^{\circ}\text{C}$ overnight with natural gas before switching to pulverised fuels (Khodier *et al.*, 2012). The paths of air and flue gas are indicated by the orange and red arrows respectively in Figure 5-3 and by the black arrows in Figure 5-1. The fluidised bed

was not used as reactor, in fact, primary and secondary air, pre-heated in a gas burner, passed through the fluidised bed and then up to the top of the vertical chamber where the pulverised fuel was fed into the downward firing burner and the combustion took place. After leaving the combustion chamber, the flue gas passed through the water cooled heat exchangers, entered the cyclone to remove suspended ash particles, then passed to the ID (i.e. Induced Draft) extraction fan and finally to the stack (Khodier, 2011). During the tests, the PF combustion chamber pressure was kept slightly negative (by changing the ID fan frequency) to avoid the flue gases escaping in the laboratory.

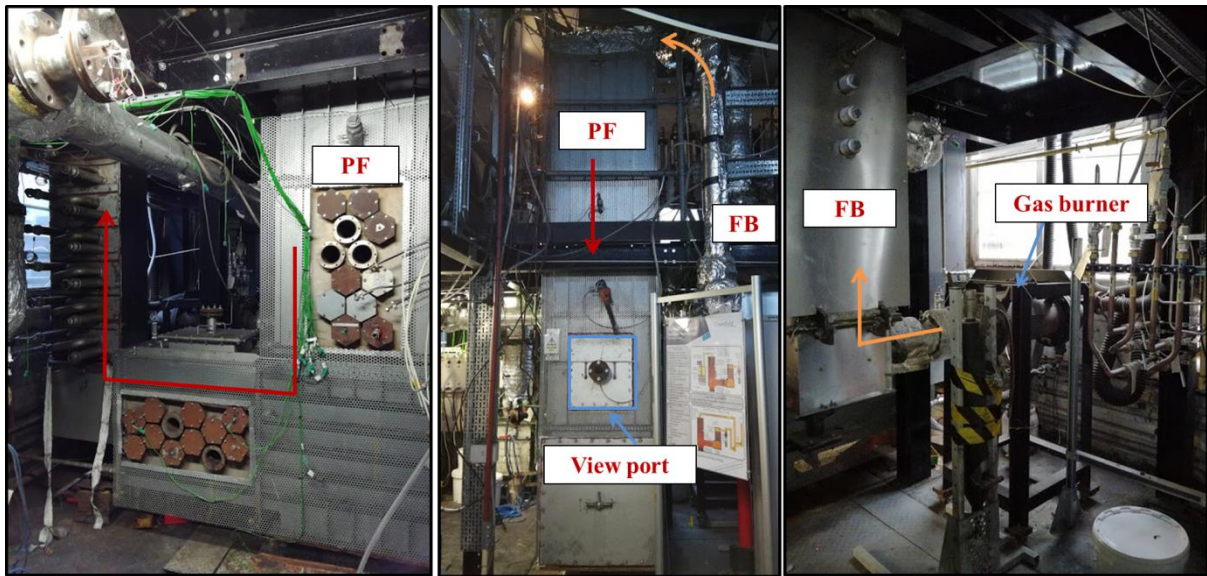


Figure 5-3: Air (orange) and flue gas (red) paths through the FB and PF combustors (look from right to left).

The combustor operation was guaranteed by the presence of a pilot flame and a flame detector (Figure 5-2) (Jurado Pontes, 2014). A multi-fuel excess air burner was used to ensure complete combustion and four view ports were located along the rig for optical access to the combustion zone, to monitor the flame, the ash particles and for image acquisition (Khodier *et al.*, 2012). A detail of the upper part of the PF combustor with all the inlets is shown in Figure 5-4.

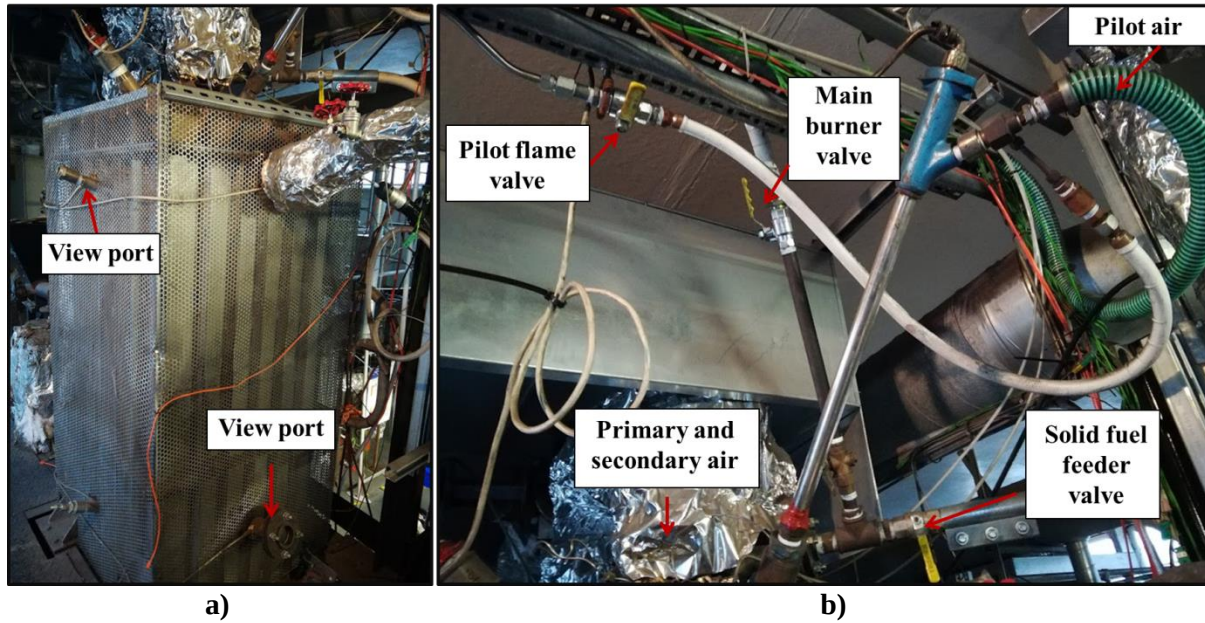


Figure 5-4: a) Upper part of the PF combustor with view ports; b) detailed location of the main inputs (pilot, primary and secondary air, solid fuel feeder, pilot and main gas).

Several ports were accessed for online gas analysis (5.5.1), temperature measurements (5.5.2) and fly ash and deposit collection (5.8) (Khodier *et al.*, 2010). In fact, the temperature was monitored with R type thermocouples in ceramic sheaths and infra-red pyrometers in the hotter areas and K type thermocouples in metal sheaths in the cooler parts of the rig (Hussain *et al.*, 2013).

5.3 Fuel feed system

The fuel feed system had a metering screw, a vibratory tray (to prevent the fuels from slumping and agglomerating) and a Venturi eductor (Figure 5-5) (Jurado Pontes, 2014). The feeder had three purge points located at the main refill hopper (first floor), at the feeder material hopper and at the end of the vibratory tray feeder. Once the pulverised fuel reached the Venturi eductor, it was fluidised with nitrogen (30 L/min) and sent to the burner (Figure 5-6).

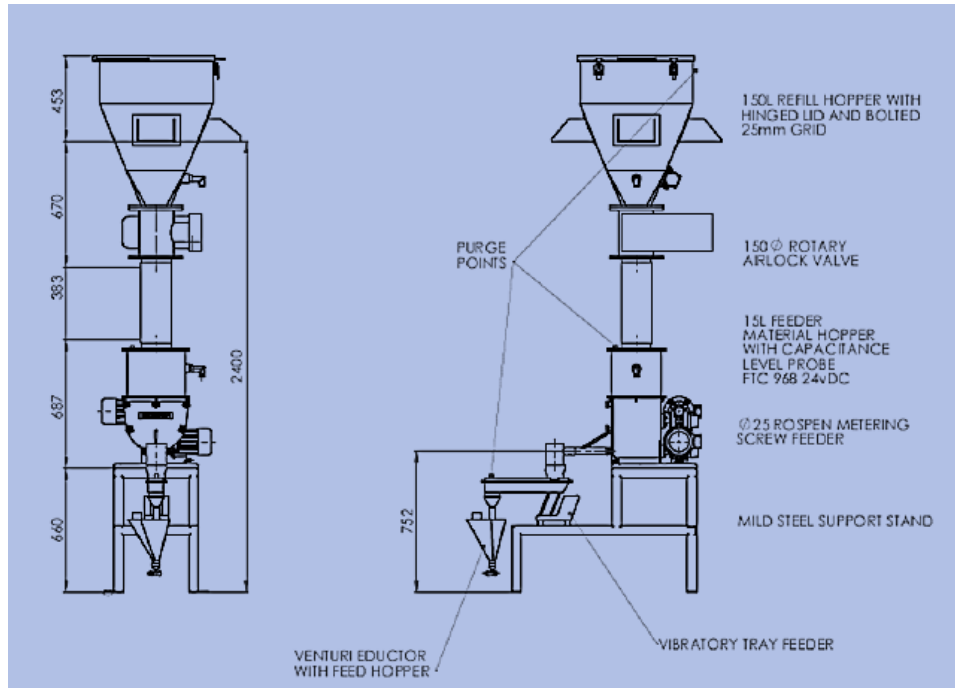


Figure 5-5: Drawing of the fuel feeding system (Jurado Pontes, 2014).

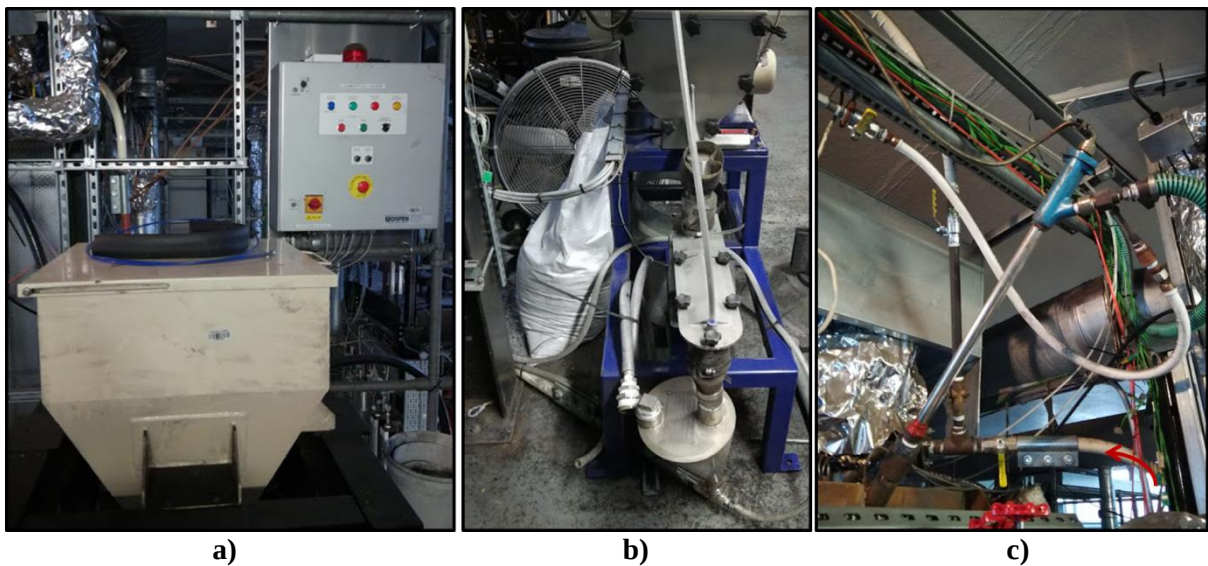


Figure 5-6: Fuel feeding system: a) refill hopper; b) vibration tray and venturi eductor; c) feeding pipe.

The calibration of the fuel feed system was carried out weighing the amount of fuel (collected in a bucket of known weight) every 10 minutes at different feeder speeds (from 6 to 18) and the corresponding results are in Figure 5-7.

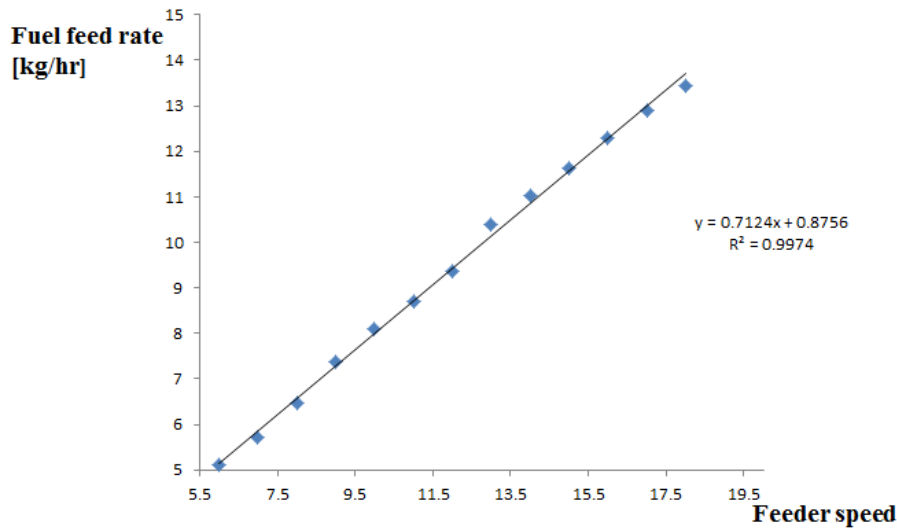


Figure 5-7: Pulverised fuel feeding calibration.

During the tests, a knob was used to adjust the feeder speed (therefore the fuel feed rate) to keep the oxygen concentration about 4%_{vol} which is a common value in coal fired boilers. The feeder speed values were converted into fuel feed rate [kg/hr] using the equation in Figure 5-7 and varied between 7 and 9 kg/hr during the combustion experiments.

5.4 Daw Mill coal and Miscanthus properties

The fuels used in this study were Daw Mill Coal and Miscanthus, both provided by E.ON Engineering plc (Technology Centre, Ratcliffe-on-Soar, Nottingham, UK) (Khodier *et al.*, 2012) (Figure 5-8). Daw Mill is a British coal whose mine was located in Arley (Warwickshire), but closed in 2013 because of a fire (Taylor, 2013). Miscanthus is an Energy Crop, also known as Elephant Grass that grows up to 3 m and can be used to produce a crop every year without replanting. This characteristic, with its low mineral content, makes Miscanthus a candidate alternative fuel for energy production (SEIL, 2012).



Figure 5-8: a) Daw Mill colliery in Arley, Warwickshire (Waddington, 2015); b) Miscanthus (Wyevalleyenergy, 2018).

The proximate, ultimate and ash analyses of both fuels are in Table 5-1 whose values were found in some databases (BCURA, 2018; Phyllis, 2018b, 2018a). Miscanthus has a higher moisture content and a lower ash content and calorific value compared to Daw Mill coal. The ultimate analysis of the fuels shows that Miscanthus has a lower carbon, sulphur and chlorine content but higher oxygen content than Daw Mill which confirms the typical biomass characterisation explained in section 2.3.2.

Table 5-1: Daw Mill and Miscanthus characterisation (wt. %) on as received (AR) basis (BCURA, 2018; Phyllis, 2018b, 2018a).

	Daw Mill Coal	Miscanthus	Daw Mill-12 wt.% Miscanthus
<i>Proximate analysis (wt % AR)</i>			
Moisture	3.20	40.00	7.62
Ash content	12.39	2.85	10.93
Volatile matter	27.59	-	-
<i>Calorific value (kJ/kg)</i>			
Gross calorific value	25,300	9,740	23,432.8
Net calorific value	26,290	11,440	24,508
<i>Ultimate analysis (wt % AR)</i>			
Carbon	67.08	28.75	61.88
Hydrogen	4.16	3.30	4.10
Nitrogen	1.16	0.33	1.04
Oxygen	10.32	24.60	12.97
Sulphur	1.43	0.07	1.23
Chlorine	0.23	0.11	0.21
Fluorine	0.02	-	0.01
<i>Ash composition (wt % of total ash)</i>			
SiO ₂	36.80	63.00	38.06
Al ₂ O ₃	23.90	0.45	22.77
Fe ₂ O ₃	11.20	0.36	10.68
TiO ₂	1.10	-	1.05
CaO	12.00	7.10	11.76
MgO	2.50	2.85	2.52
Na ₂ O	1.50	0.18	1.44
K ₂ O	0.50	14.80	1.19
Mn ₃ O ₄	0.40	-	0.38
P ₂ O ₅	< 0.30	1.75	0.08
SO ₃	12.90	3.70	12.46

The fuels were pulverised and a blend of Daw Mill-12 wt.% Miscanthus was used for the following study with an average fuel feed rate of ~ 8 kg/hr. An example of the appearance of the prepared fuel before combustion is given in Figure 5-9. The proximate, ultimate and ash analyses of the blend were calculated from the pure fuel analysis and are reported in Table 5-1.



Figure 5-9: Pulverised Daw Mill-12 wt. % Miscanthus in a bucket before combustion.

However, measurements of the ash and moisture contents for the blend of fuel were carried out at Cranfield University for comparison with the calculated data and a revised fuel composition was calculated (Table 5-2).

5.4.1 Fuel ash content

The ash content analysis for the blend of Daw Mill-12 wt.% Miscanthus was conducted at Cranfield University. The ASTM (i.e. American Society for Testing and Materials International) Standards for coal and biomass (ASTM International, 2012, 2015) were assessed and a compromise between the two procedures was required. For example, for biomass, it was suggested to keep the temperature below $575 \pm 25^{\circ}\text{C}$, lower than the maximum temperature allowed for coal which can be heated up to 950°C .

Two different horizontal furnaces were used but the same experimental procedure was followed. The fuel was dried overnight and ~ 1 g of it was weighed in a dry ceramic crucible (of known weight) and placed in a cold furnace. Later, it was exposed to a gradual increase of temperature to avoid flaming (ASTM International, 2015) (Figure 5-10). In fact, the temperature was increased up to 250°C at 10 K/min (first ramp), then it was kept constant for 30 minutes (first dwell) and brought up to $575 \pm 25^{\circ}\text{C}$ at 6 K/min (second ramp). This final temperature was kept constant (second dwell) and the sample was weighed generally every hour until it was stable ($\pm 0.001\text{ g}$) (ASTM International, 2012).

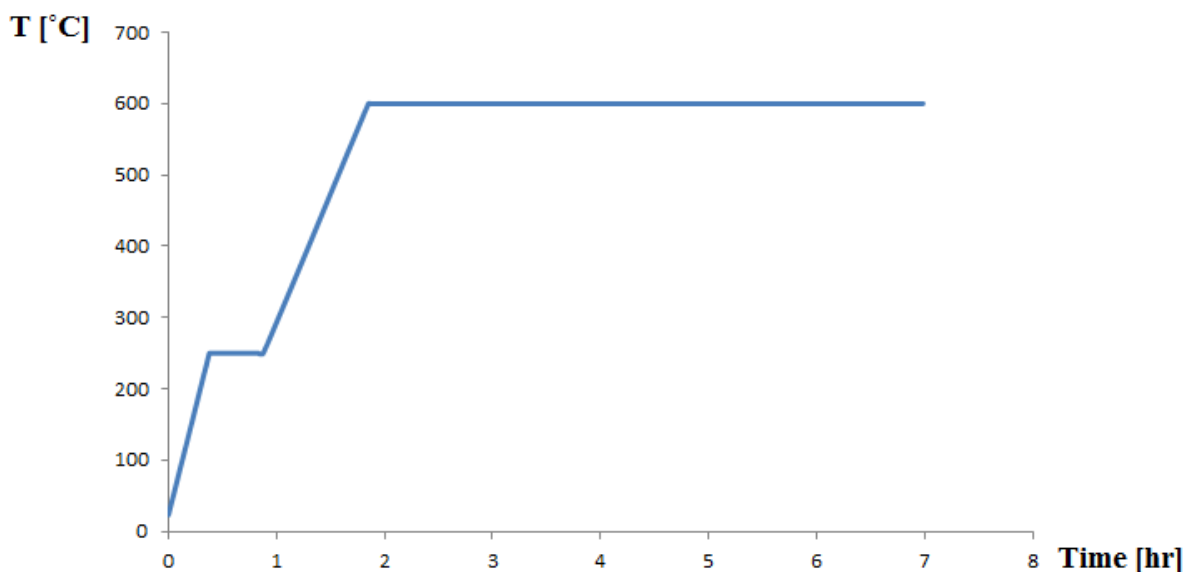


Figure 5-10: Temperature profile during fuel ash content tests.

The first tests were carried out in the horizontal furnace in Figure 5-11. It consisted of a horizontal furnace, a valve and a pre-furnace container; a box that can be independently purged and is mainly used to load and unload samples. Before the test, the valve was open, the crucible with the fuel sample was placed in a metallic boat located in the pre-furnace container and it was pushed into the horizontal furnace with a long metallic stick (Figure 5-11). The valve was open during the combustion tests (but the door of the pre-furnace container was bolted) and was closed when the sample was pulled out to be weighed to avoid the hot combustion gas escaping into the laboratory. The tests were conducted in air with a flow rate of 100 mL/min. Moreover, a flow of pure nitrogen ($200 \text{ cm}^3/\text{min}$) was sent into the pre-furnace container for safety and to cool the sample down before weighing it. Moreover, a thermocouple was located in the metallic boat in order to monitor the sample temperature once extracted (Figure 5-11).

However, the system used to insert and extract the sample proved not to be reliable since it required opening/closing the valve and dragging the crucible with a long stick through quite a long and rough path which caused some sample loss. Moreover, this method needed some time (~ 30 minutes) to take the sample out, cool it down, weigh, load it again and put it back into the furnace. Therefore, it was difficult to run tests for more than 3 hours at $575 \pm 25^\circ\text{C}$. In fact, only one test (the third) was run for nine hours but this lasted for two days and the results were not reliable already after 4 hours for ash loss.

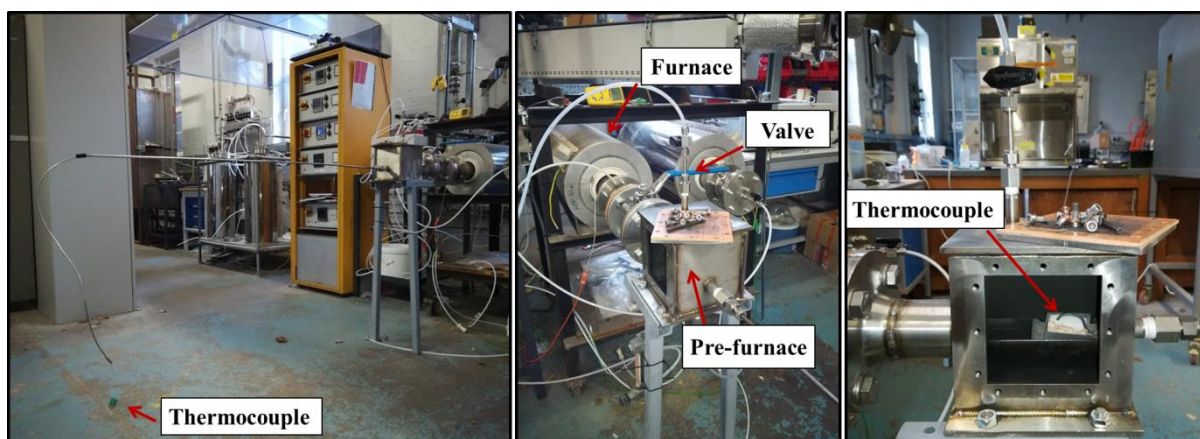


Figure 5-11: First horizontal furnace used for ash content test in Daw Mill-12 wt.% Miscanthus.

As a consequence, another horizontal furnace, of the same design but with easier access at its end, was used to run more tests and the results from the different tests were compared. In this case, the sample was placed directly into the horizontal furnace, with negligible sample loss, and it burned with a compressed air flow rate of 4.5 L/min. However, in absence of a pre-furnace container to cool the sample down, it was necessary to use protective gloves and a refractory surface to take the hot crucible out (Figure 5-12).

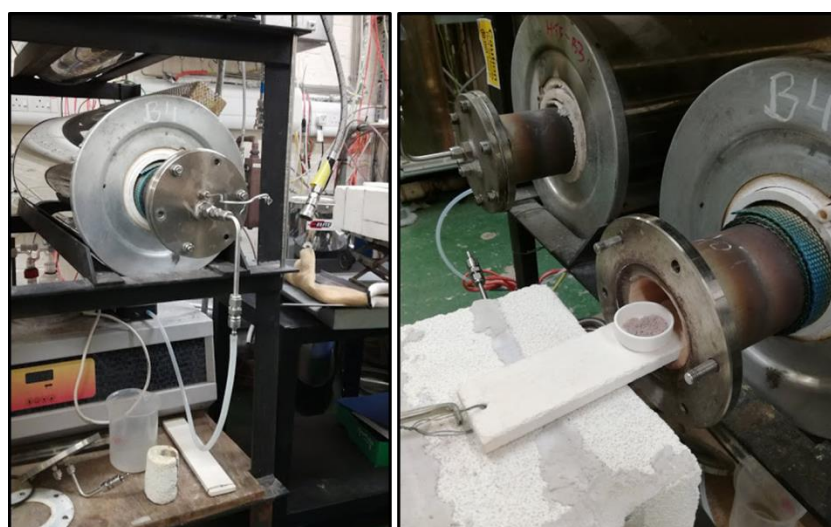


Figure 5-12: Second horizontal furnace used for ash content test in Daw Mill-12 wt.% Miscanthus.

Examples of samples before and after tests in the two furnaces are shown in Figure 5-13 and Figure 5-14. Apart from the weight loss, the most evident difference is the colour of the fuel which turns into a light sand colour ash sample.

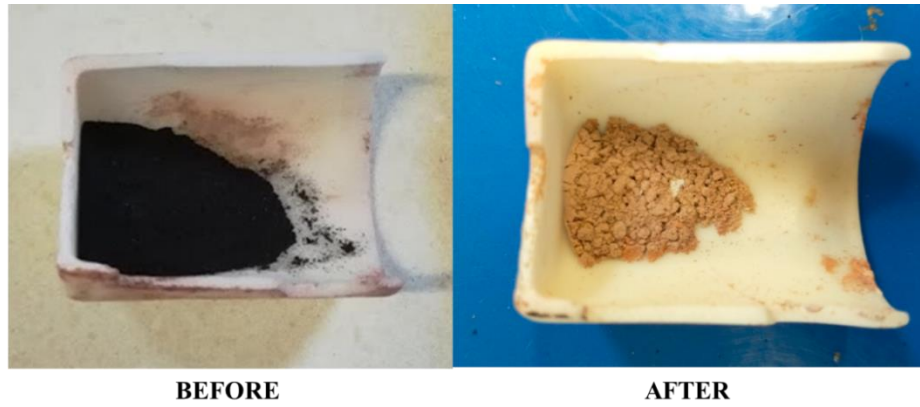


Figure 5-13: Sample before and after the ash content test in Daw Mill-12 wt.% Miscanthus using the first furnace.

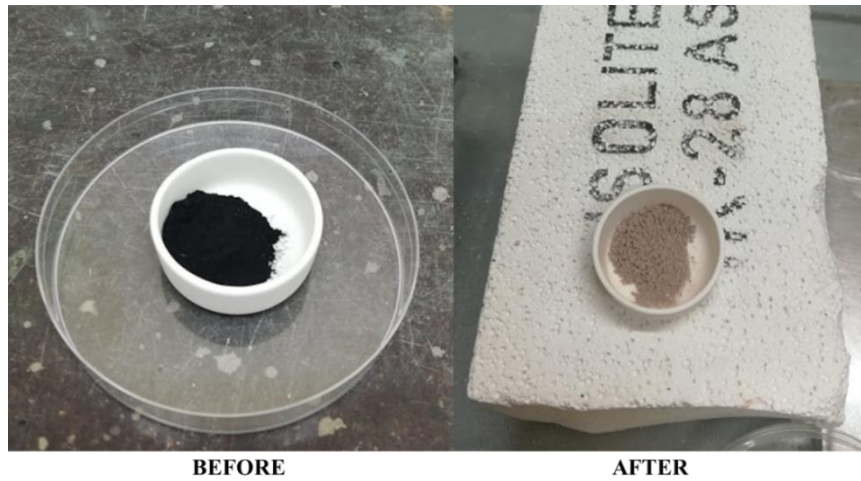


Figure 5-14: Sample before and after the ash content test in Daw Mill-12 wt.% Miscanthus using the second furnace.

The ash content was calculated with Equation (5-1) (ASTM International, 2012):

$$\%ash = \frac{(A - B)}{C} 100 \quad (5-1)$$

Where:

A = sample and crucible weight after exposure [g]

B = dry crucible weight [g]

C = sample weight before exposure [g]

The sample weight loss obtained during the tests using both furnaces is reported in Figure 5-15 and Figure 5-16. A comparison shows that the second test is more reliable and efficient as the weight was already stable after one hour.

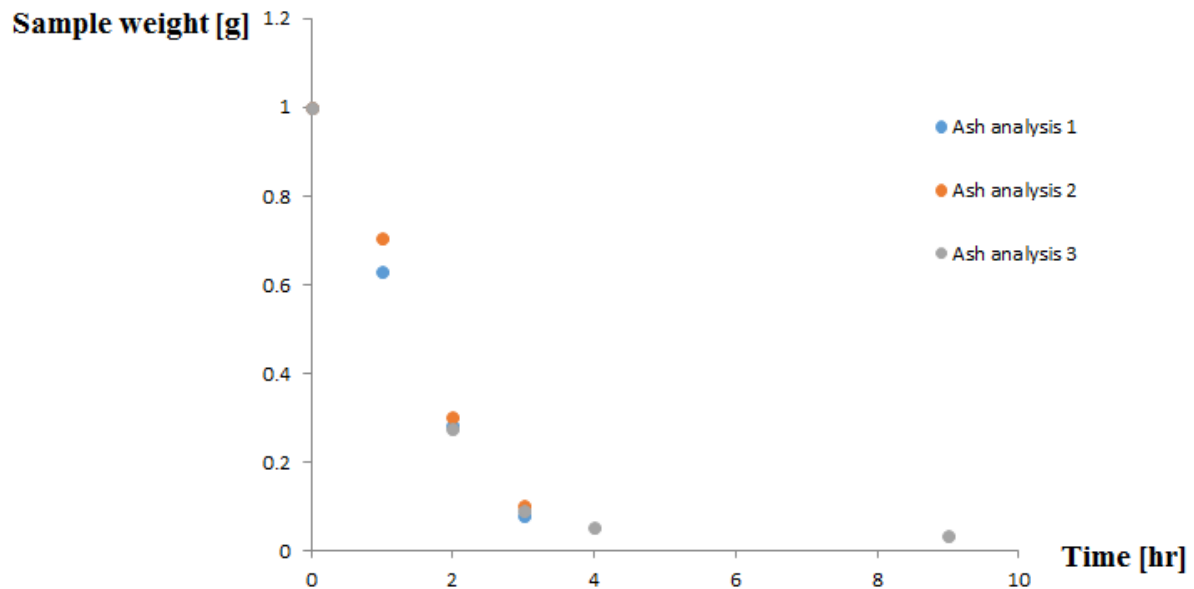


Figure 5-15: Normalised sample weight loss in the first furnace.

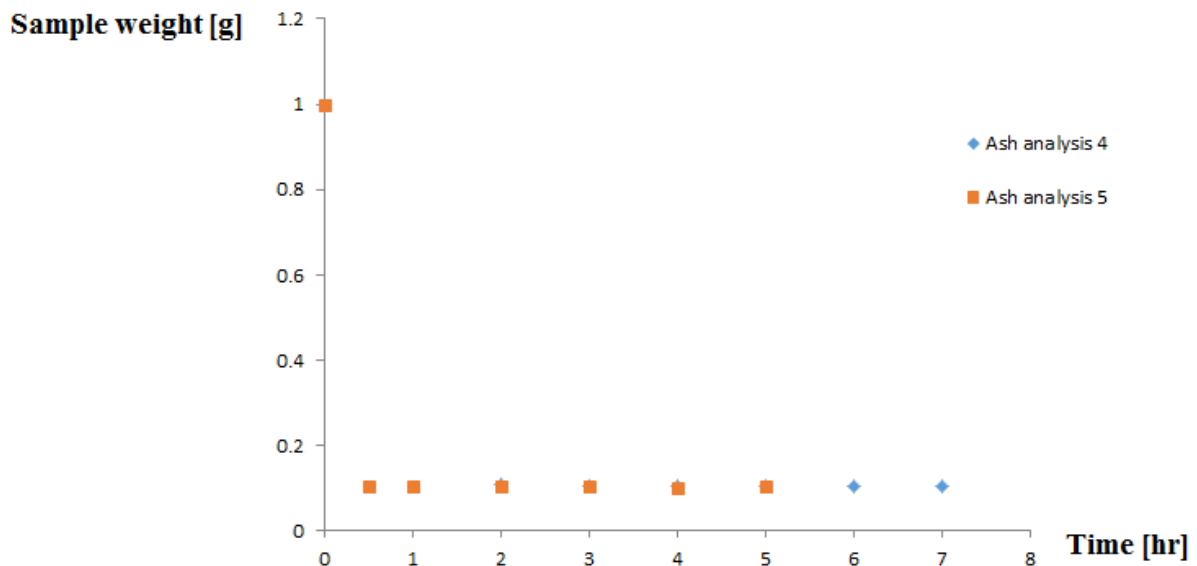


Figure 5-16: Normalised sample weight loss in the second furnace.

The results of the ash content in the fuel calculated with Equation (5-1) for the two horizontal furnaces are illustrated in Figure 5-17. They were not too different from each other; however the ash content percentages obtained using the first furnace were more scattered (and lower

due to sample spillage) compared with the second one which gave more constant and reliable values. Therefore an average of the fuel ash content obtained from the second furnace was calculated (10.33 wt.%). In fact, this is similar to the calculated value that was given in Table 5-1.

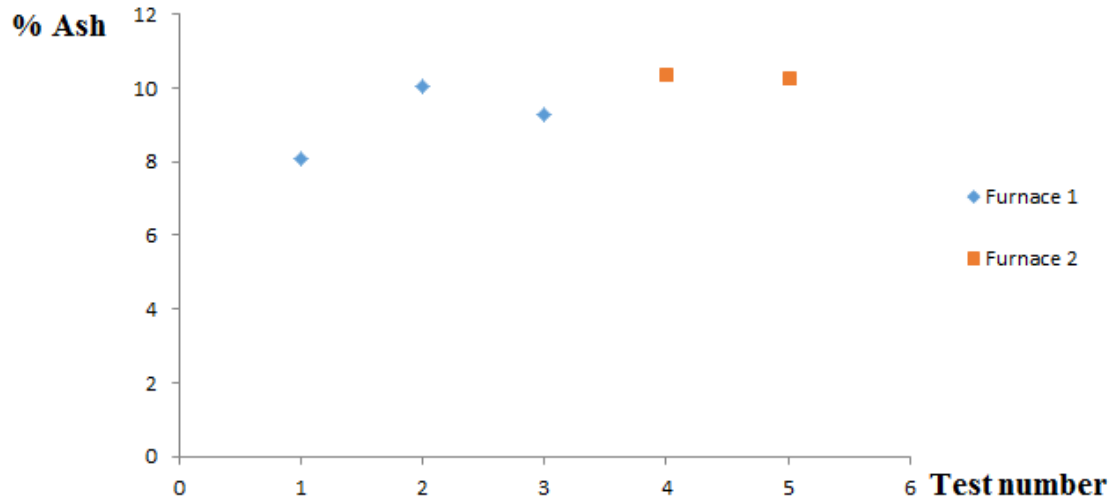


Figure 5-17: Ash content in Daw Mill-12 wt.% Miscanthus after tests in two different horizontal furnaces.

5.4.2 Fuel moisture content

The fuel moisture content was measured in order to get a comparison with the calculated data given in Table 5-1. A known amount of fuel was put in a beaker, previously weighed, and dried in a heater at 100 °C for one day. The moisture content was calculated with Equation (5-2).

$$\%moisture = \frac{(A - B)}{C} 100 \quad (5-2)$$

Where:

A = weight of sample before drying [g]

B = weight of sample after drying [g]

C = weight of sample before drying [g]

The results are plotted in Figure 5-18 for three tests; the average value is 3.17%. This value is significantly lower than the one calculated in Table 5-1 and this could be due to the fact that the fuel dried out over time as it was stored in bags in the laboratory.

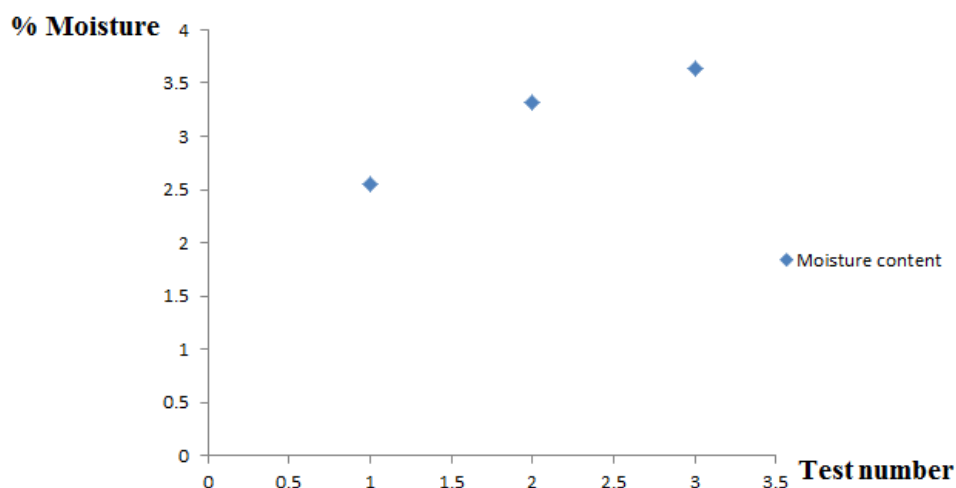


Figure 5-18: Measurements of moisture content in Daw Mill-12 wt.% Miscanthus.

The moisture content (3.17%) and the dry ash content previously obtained (10.33%) were used to recalculate the as-received (AR) ultimate analysis for the blend starting from the daf (i.e. dry ash free) fuel analysis and a comparison is given in Table 5-2.

Table 5-2: Comparison between Daw Mill-12 wt.% Miscanthus characterisation (wt. %) on as received (AR) basis (BCURA, 2018; Phyllis, 2018b, 2018a) (Table 5-1) and the ultimate analysis recalculated with the real ash and moisture contents in the fuel blend.

	Daw Mill-12 wt.% Miscanthus	Recalculated Daw Mill-12 wt.% Miscanthus
<i>Proximate analysis (wt % AR)</i>		
Moisture	7.62	3.17
Ash content	10.93	10.00
<i>Ultimate analysis (wt % AR)</i>		
Carbon	61.88	65.96
Hydrogen	4.10	4.37
Nitrogen	1.04	1.11
Oxygen	12.97	13.83
Sulphur	1.23	1.31
Chlorine	0.21	0.23
Fluorine	0.01	0.01

5.5 Gas characterisation

5.5.1 Gas composition

An online gas analysis was provided by a high-resolution multi-component Fourier Transform Infra-red (FTIR) gas analyser [Protir 240M Mobile FTIR Multi-component gas analyser, Protea Ltd., Cheshire, UK] (Khodier, 2011) (Figure 5-19).

A sampling port was located in the vertical chamber near the deposition probes and its position was never changed during the tests. The gas was sucked through a pipe (595 mm length, 12 mm internal pore size) bounded by glass wool, filter, and a heated line ($\sim 180\text{ }^{\circ}\text{C}$) to avoid the water condensation before and in the instrument which could compromise its operation. A 5 m heated line was attached to ensure that the gas would reach the analyser at a constant temperature. In the gas analyser pure N_2 was used as a zero gas for calibration and to purge before and after sampling. The flue gas was sucked through the FTIR using a vacuum compressor and it was vented to the atmosphere after the analysis (Khodier, 2011; Legrave, 2012).

In the FTIR system, the combusted gas goes through the gas cell where absorption for the different species takes place. In the data logging system the spectra obtained are compared to standard spectra to quantify the species in the flue gases. The FTIR contains an electrochemical (zirconia-based) oxygen sensor which allows quantification of the oxygen concentration (Khodier, 2011).

The main flue gas components (CO_2 , O_2 , H_2O , CO , NO , NO_2 , N_2O , NH_3 , SO_2 , HCl , HF and CH_4) were displayed on a dedicated laptop and data were represented numerically and graphically (Figure 5-19).

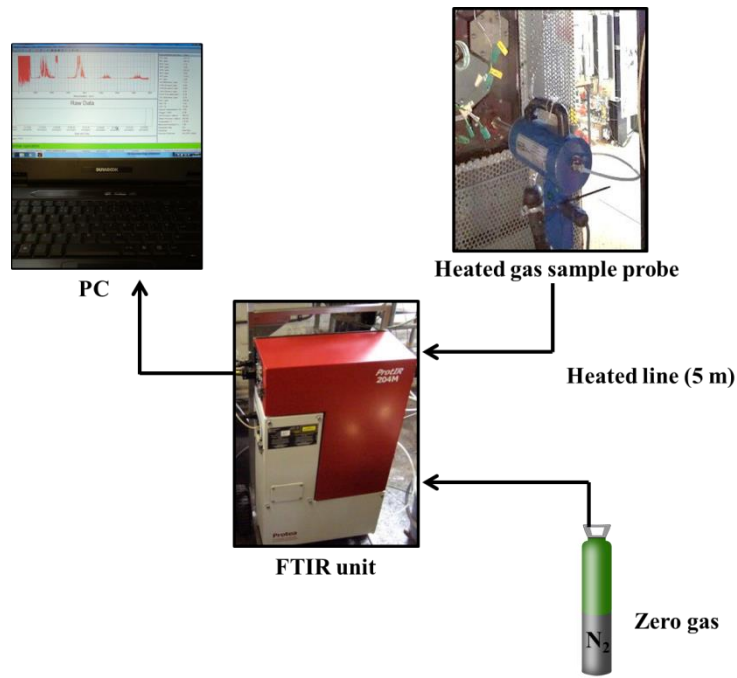


Figure 5-19: Main components of FTIR gas analyser (modified from (Khodier, 2011; Legrave, 2012)).

5.5.2 Gas temperature

The temperature was monitored at different locations along the combustor with thermocouples; the data acquisition system used during the tests was built up from several Pico Logger TC-08 units (Jurado Pontes, 2014).

Before starting the experimental campaign, thermocouples were positioned and opportunely labelled. Moreover, it was important to ensure the correspondence between each thermocouple (Figure 5-20 (a)) and the channel number (Figure 5-20 (b)). The temperature was recorded at different heights along the PF combustor, at the air inlet and outlet of the deposition probes as well as at the surface of the probes. The temperatures at the thermocouple locations in the PF combustor were generally $\sim 1000\text{-}1100\text{ }^{\circ}\text{C}$ and $\sim 700\text{ }^{\circ}\text{C}$ around the deposition probes. The data were recorded on a dedicated computer and displayed numerically and graphically as shown in Figure 5-20 (c).

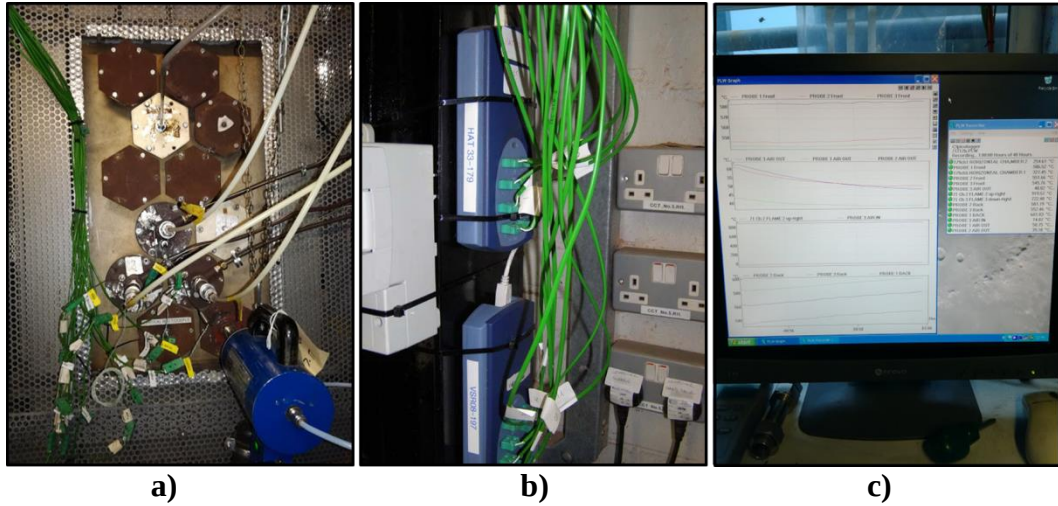


Figure 5-20: Pico Logger temperature record: a) thermocouples; b) connection between the channel and the thermocouple; c) display of results.

5.5.3 Gas velocity

The gas velocity U_0 around the deposition probes was calculated applying Equation (5-3) which takes into account the air flow rate (Table 5-3), the combustor section and the thermal dilatation (Khodier, 2011):

$$U_0 = \frac{\text{air flow rate}}{\text{combustor cross sectional area}} * \frac{T}{T_{ref}} \quad (5-3)$$

Where:

$$\text{air flow rate} \sim 0.041 \text{ m}^3/\text{s}$$

$$\text{combustor cross sectional area} = (0.3)^2 \text{ m}^2$$

$$T = 1273 \text{ K}$$

$$T_{ref} = 298 \text{ K}$$

Table 5-3: Typical values of air flow rate used during the experiments.

Pilot air [L/min]	Primary air [L/min]	Secondary air [L/min]	Tot [L/min]
100	750	1600	2450

Considering the values of primary, secondary and pilot air, the gas velocity was $\sim 1.9 \text{ m/s}$, which was the gas and particle velocity at the inlet of the computational domain for the model validation (Chapter 7). In the reality, the gas velocity would be slightly higher taking into

account the combustion gases produced (2450 L/min + ~ 3%) and the error of the rotameter reading.

5.6 Deposition probes

In this study, some of the ports located in the vertical section of the combustion chamber were used to study the formation of deposits on probes during combustion of pulverised fuels as highlighted in the combustion drawing in Figure 5-21. Two different configurations were investigated whose main difference was the position of probe 1 which was closer to the chamber wall in Configuration 1 and further away in Configuration 2 (Figure 5-21).

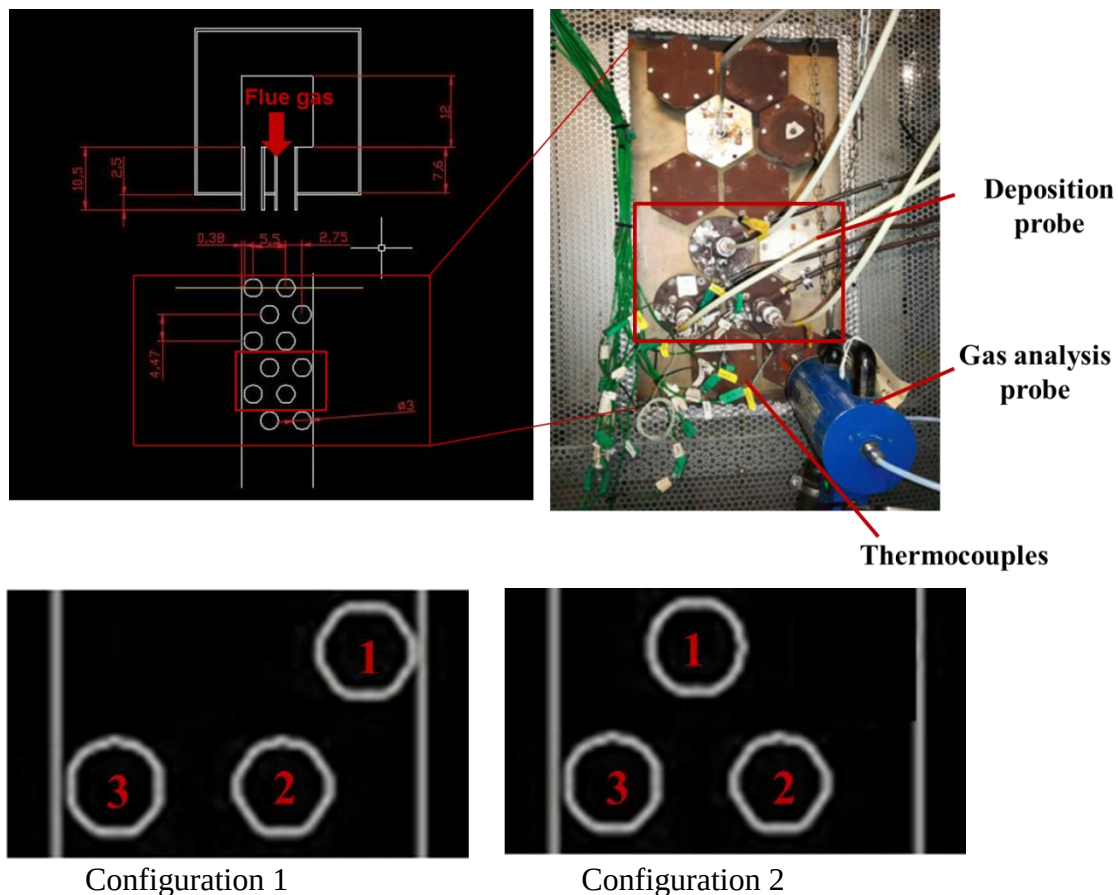


Figure 5-21: Vertical section of the combustor chamber drawing with ports for deposition probes and the configurations used during the experiments (dimensions are in inches).

Three annular air-cooled ceramic probes were used and an example is shown in Figure 5-22 and Figure 5-23. Compressed air entered the inner tube (at room temperature and 4 bar in the rotameter (as it loses pressure after the needle valve)), reached the end of the tube and left it through some holes to go into the outer tube in the opposite direction towards the outlet. The

outer part of the probes was made of a ceramic ring (OD= 39 mm; ID= 32 mm; length= 61 mm) placed between two stainless steel rings.

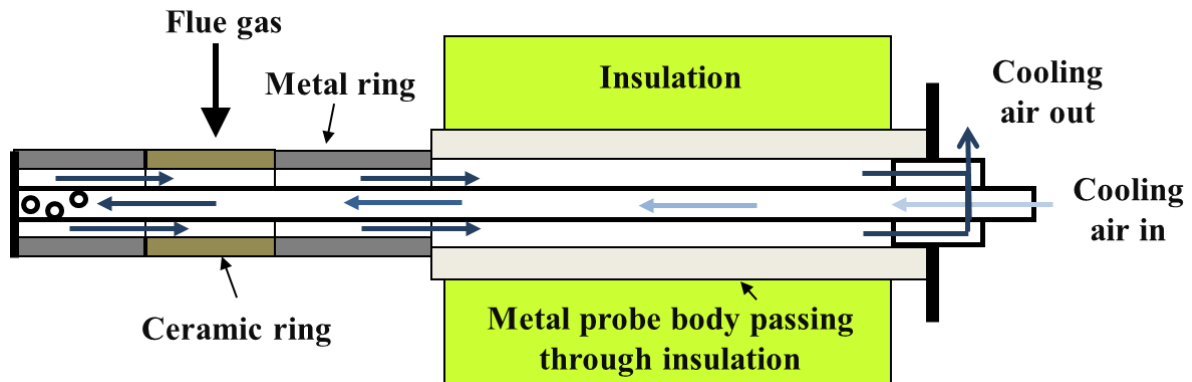


Figure 5-22: Schematic of the deposition probe in the combustion chamber (modified from (Coleman, 2008)).

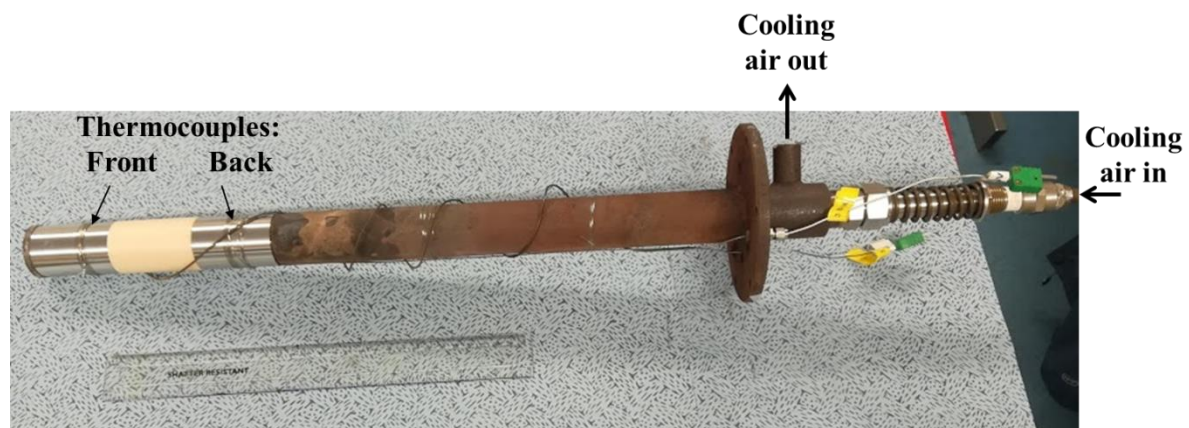


Figure 5-23: Deposition probe with thermocouples.

Deposition was studied onto ceramic (mullite) rings because their properties were similar to the deposit surfaces of real power plants. Before each test, the metal rings were washed with laboratory water and isopropanol and assembled with a new ceramic ring. Two thermocouples were fixed with locking wire, one on each metal ring (labelled as front and back), to monitor the probe temperature and finally placed in the cold combustor before starting the experiments. During the tests, the cooling air flow rate was adjusted with calibrated rotameters in order to keep the probe temperature constant at $\sim 500^{\circ}\text{C}$ and 600°C , which are realistic surface temperatures of superheaters and reheaters (Figure 5-24).

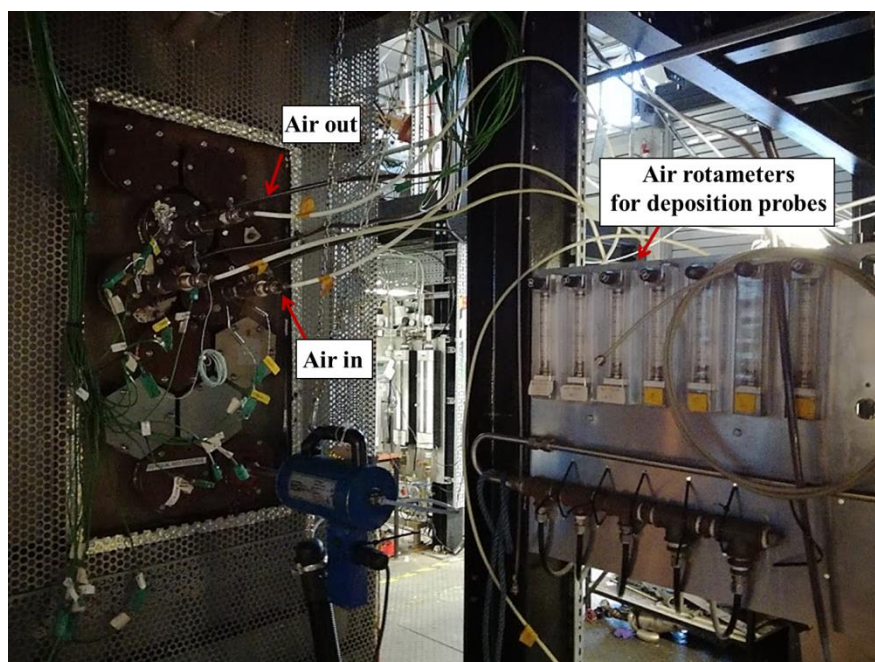


Figure 5-24: Air rotameters to control the deposition probe temperatures.

The deposition flux [$\text{mg}/(\text{cm}^2 \text{ hr})$] was defined as the amount of deposit [mg] on the surface area of the ceramic probe [cm^2] accumulated over the exposure time [hr]. Before starting the experimental campaign, the deposition flux calculations were planned carefully. In fact, different zones were identified on the probe surface (upstream, downstream and sides, Figure 5-25 (b)); their lengths were measured with a calliper and the area of each of them was calculated considering the total surface area of the probe and the % of each zone length over the entire perimeter (Figure 5-25 and Table 5-4). In particular, the side zones were identified as right and left as specified in Figure 5-25 (a).

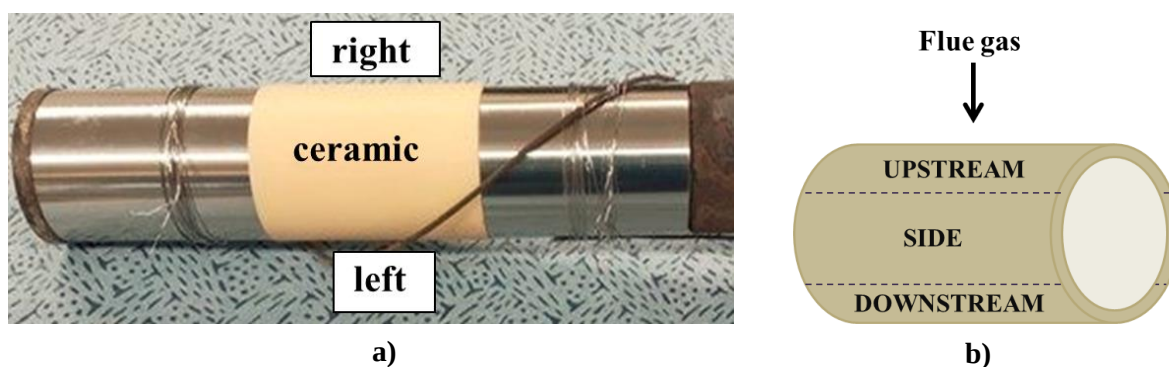


Figure 5-25: Top view of an air cooled ceramic probe for deposition studies: a) Detail of a ceramic ring placed between two metal rings; b) schematic of ceramic ring with identification of the different zones for deposit collection.

Table 5-4: Ceramic probe dimensions.

	Dimension	%Length_i=(Length_i/p)·100	A_i=A·%Length_i/100
OD= 2r	3.9 cm		
L	6.1 cm		
Area (A)= 2πrL	74.70 cm ²		
Upstream	5 cm	40.83	30.5 cm ²
Left side stream	1.9 cm	15.51	11.59 cm ²
Right side stream	1.9 cm	15.51	11.59 cm ²
Downstream	3.45 cm	28.14	21.02 cm ²
Perimeter (p)= 2πr	12.25 cm		

5.7 Experimental procedure

Before starting the experimental campaign, several training runs were done to learn how to use the combustion rig. Moreover, the main thermocouples were checked and the horizontal section of the combustor was cleaned so as not to compromise the experimental results. However, to keep it clean, at the end of each test, ash was hoovered from the ports along the horizontal section of the combustion chamber.

Generally, a test took three days from starting the rig up to switching it off. The main steps followed during the experiments are summarised below and more details are in Appendix E:

- 1) Assemble the deposition probes and place them in the combustor
- 2) Fix the probes' thermocouples (air in and out, probe front and back)
- 3) Start the combustor and warm it up overnight

The main values to set the rig up are in Table 5-5.

Table 5-5: Main parameters used to set the rig up. Abbreviations: ID= induced draft; FD= forced draft; MB= main burner; FBP= fluidised bed primary air; FBS= fluidised bed secondary air; FB= fluidised bed.

P	ID	FD	MB	PILOT AIR	FBP	FBS	FB
[Pa]	[Hz]	[Hz]	[L/min]	[L/min]	[L/min]	[L/min]	[L/min]
>100	15	25	30	120	400	800	16

- 4) Warm the combustor up the morning after

The main reference parameters at this stage are in Table 5-6.

Table 5-6: Main parameters used to warm the rig up. Abbreviations: ID= induced draft; FD= forced draft; MB= main burner; FBP= fluidised bed primary air; FBS= fluidised bed secondary air; FB= fluidised bed.

P [Pa]	ID [Hz]	FD [Hz]	MB [L/min]	PILOT AIR [L/min]	FBP [L/min]	FBS [L/min]	FB [L/min]
~200-300	↑↓(~19)	35	35	120	600	2000	16

- 5) Start feeding solid fuel
- 6) Cool down overnight
- 7) Switch off

In the following Table 5-7, the main actions taken during one of the tests are reported. Different colours were used to highlights some of the main actions.

Table 5-7: Main steps followed during one of the experiments with Daw Mill-12 wt.% Miscanthus (highlighted with different colours).

Step/Action	Time	P [Pa]	ID [Hz]	FD [Hz]	MB [L/min]	PILOT AIR [L/min]	FBP [L/min]	FBS [L/min]	FB [L/min]	O ₂ %vol	T _{flame} up right [°C]	Feeder speed
Warm up	9:47	261	19.5	35	35	120	600	2000	16	5.04	750	0
Stop feeding gas	10:59	~200	19.5	35	0	100	750	1600	0	-	780	0
Start feeding solid fuel	11:00	~100	19.5	35	0	100	750	1600	0	-	850	8.7
ID fan was adjusted to keep P ~100 Pa	11:16	↓100	20	35	0	100	750	1600	0	4.11	866	8.7
	11:39	↓100	21.5	35	0	100	750	1600	0	3.86	895	8.7
	12:24	~100	24.5	35	0	100	750	1600	0	4.81	931	8.7
Feeder speed was adjusted to keep ~ 4% O ₂	12:29	~100	24.5	35	0	100	750	1600	0	~4.81	~950	8.8
	12:51	↓100	25	35	0	100	750	1600	0	4.27		8.9
	13:25	↓100	25.5	35	0	100	750	1600	0	4.61	975	9

	14:37	↓100	29	35	0	100	750	1600	0	4.78	~1000	9.1
	14:42	↓100	29	35	0	100	750	1600	0	4.12	~1000	9.2
	14:50	↓100	31	35	0	100	750	1600	0	4.69		9.4
	14:54	↓100	31	35	0	100	750	1600	0	4.33		9.5
	15:48	↓100	34	35	0	100	750	1600	0	4.17	1048	9.5
Fuel off	15:55											0
Cool down overnight	15:56	~200	15	25	0	30	200	0	0			0

5.8 Deposit/fly ash collection and analysis

Ash collection from the probes was possible the following day, after cooling the combustor down during the night with air.

The probes were taken out carefully one by one and placed on a desk (Figure 5-26). First of all, the thickness of the deposit (especially on the upstream) was evaluated roughly with a ruler. Moreover, ash was brushed off from the upstream, left and right sides and downstream whose surface areas were calculated previously (Table 5-4) and collected into plastic bags (of known weight). Ash from different sides of the probes was then weighed to calculate the deposition flux [$\text{mg}/(\text{cm}^2 \text{ hr})$] according to Equation (5-4) and the results are reported in Chapter 6.

$$\text{deposition flux} \left[\frac{\text{mg}}{\text{cm}^2 \text{ hr}} \right] = \frac{\text{mass of deposit}}{(\text{surface area} \cdot \text{exposure time})} \quad (5-4)$$

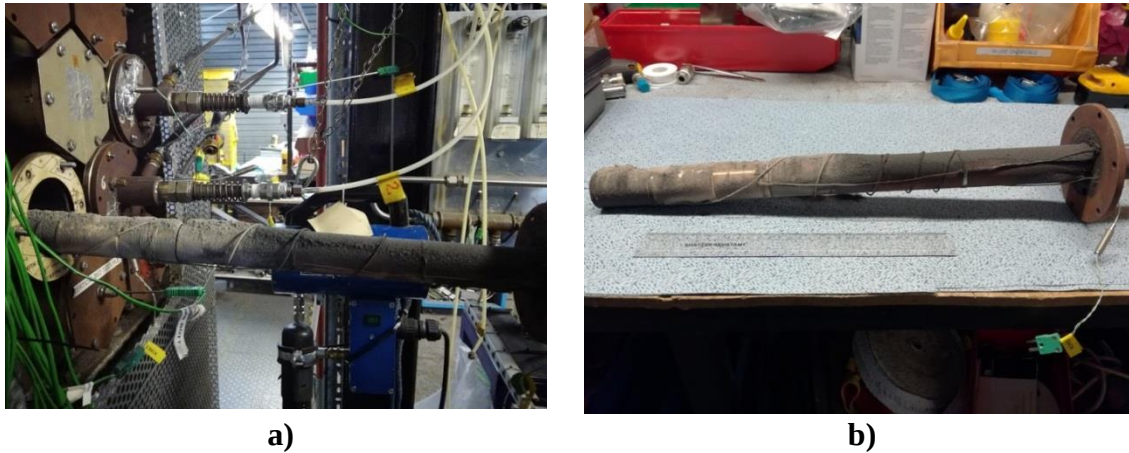


Figure 5-26: a) Extraction of probe from the combustion chamber; b) probe on a work desk for ash collection.

Apart for deposition flux calculations, the samples were also used for ash characterisation. The main types of analysis done in this work and the methodology used to get the required information for the CFD model are listed below. However, a detailed description of the results is given in Chapter 6:

- SEM/EDX: Scanning Electron Microscope and Energy Dispersive X-ray Spectroscopy.

The SEM allowed the identification of the ash microstructure, while the EDX was used to get the corresponding chemical compositions (Figure 5-27).

In this work, the elements were identified from different parts of the same sample and an average value was calculated to get the composition (in terms of highest element oxides) which was used later for the model validation (Chapter 7). This type of technique was used for all the fly ash and deposit samples.

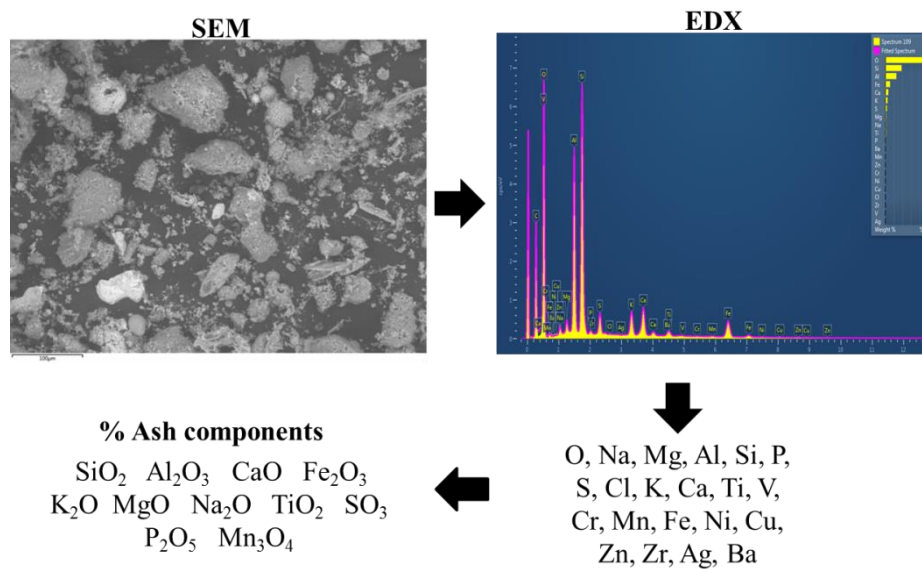


Figure 5-27: SEM/EDX analysis for ash microstructure identification and ash chemical composition.

- XRD: X-ray diffraction.

This analysis gives information about the mineral phases in the deposits. However, a reasonable amount of deposit sample was necessary to fully cover the glass slide used for the analysis. Therefore, this technique was used only for the deposit collected from the upstream zones of the probes, where it was more abundant (Figure 5-28).

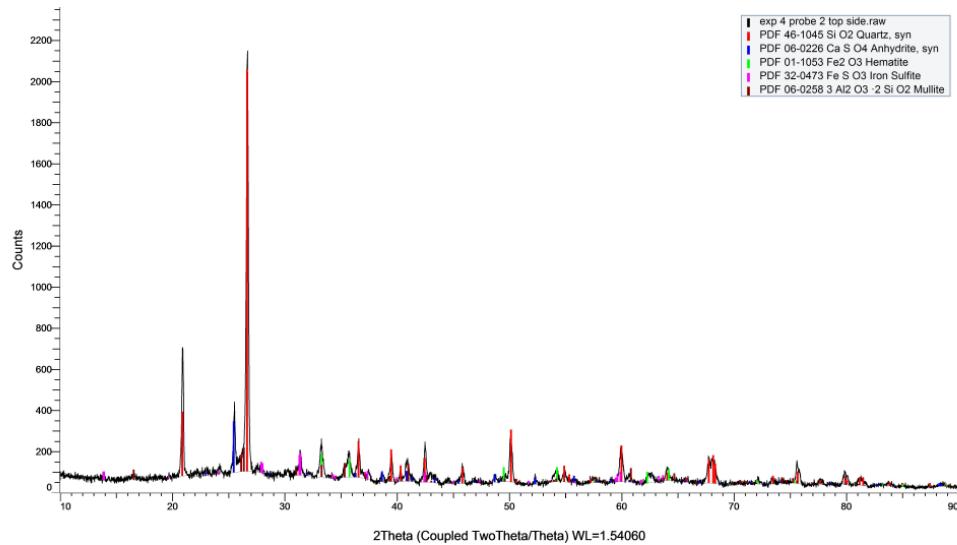


Figure 5-28: Example of XRD analysis for one of the deposits.

- Ash particle size distribution.

Ash was brushed from the ports along the vertical section of the combustion chamber where the probes were located (Figure 5-29). These samples were taken as the fly ash that caused deposition and a particle size distribution was necessary to provide the information required in Fluent[®] to define the DPM Injection properties (section 3.6).



Figure 5-29: Ash collection from one of the ports along the vertical section of the combustor used to place the probe.

The ash particle size distribution determinations were conducted by an Industrial Sponsor, Doosan Babcock, located at Renfrew (Scotland), using a laser diffraction particle size analyser (Malvern Mastersizer 2000) which provided the volumetric percentage of different particle diameters as in Figure 5-30 (a) and Table 5-8 (grey columns).

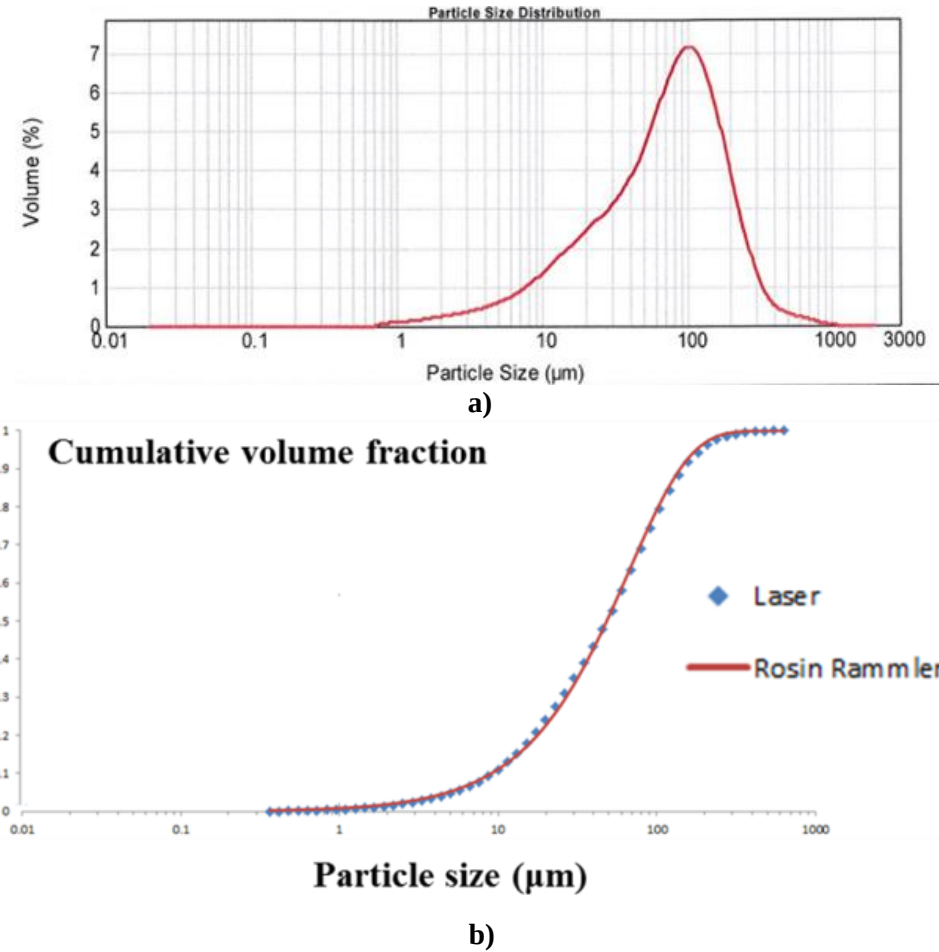


Figure 5-30: a) Volumetric ash particle size distribution provided by Doosan Babcock; b) cumulative volume fraction of ash particles ($1-Y_d$): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

The methodology followed to determine the parameters for the Rosin Rammler ash particle distribution required by the Fluent[®] model (d_{min} , d_{max} , d_{mean} , n) has been summarised in Table 5-8 and an example is shown in Figure 5-30 (b). This provided the parameters for the ash particle distribution used to validate the CFD model (Chapter 7).

Table 5-8: Simplification of the method used to fit the Rosin Rammler ash particle size distribution ($Y_d(RR)$) to the ash particle size distribution obtained using a Laser Diffraction Malvern Mastersizer 2000 ($Y_d(L)$) (Fluent, 2018).

Range [μm]	Volume [%]	d [μm]	Volume	$Y_d(L)$	$\ln Y_d(L)$	n Eq. (5-6)	$\bar{n}$	$Y_d(RR)$ Eq.(5-5)
0.01-50	20	50	0.20	1-0.20				
50-70	30	70	0.30	1-(0.20+0.30)				
70-150	50	150	0.50	1-(0.20-0.30- 0.50)				
TOT	100		1					

According to the Rosin-Rammler particle size distribution, the volumetric fraction of particles with diameter greater than d is given by Equation (5-5).

$$Y_d = e^{-(d/\bar{d})^n} \quad (5-5)$$

Where:

Y_d is the percentage of particles with diameters greater than d and the percentage is assumed to be exponential ($Y_d (RR)$ in Table 5-8)

d is the diameter representative of each range [μm] (Table 5-8)

$\bar{d}$ is the average size parameter (called d_{mean} in Fluent®) [μm]

n is the size distribution parameter, also called spread diameter, defined by Equation (5-6) for each line of Table 5-8. However its average, $\bar{n}$, was used in Equation (5-5) and in Equation (5-7)

$$n = \frac{\ln(-\ln Y_d)}{\ln(d/\bar{d})} \quad (5-6)$$

The distribution can be expressed also as a cumulative volume form defined in Equation (5-7) (Bailey *et al.*, 1983) and an example has been plotted in Figure 5-30 (b).

$$1 - Y_d = e^{-(d/\bar{d})^n} \quad (5-7)$$

The values of $\bar{d}$ and, as a consequence n , have to guarantee the fitting between the model (applying Equation (5-5) ($Y_d (RR)$) in Table 5-8) and the experimental Y_d

($Y_d(L)$). In particular, the correct $\bar{d}$ was obtained by identifying the value of $d = \bar{d}$, which implies $Y_d(L) = e^{-1} \approx 0.368$ (Fluent, 2018).

5.9 Deposition test matrix

The main parameters taken into account during the experiments are summarised as follows and the test matrix of the experiments carried out is given in Table 5-9.

- 1) Test duration
- 2) Probe temperature
- 3) Probe configuration (Figure 5-21)

Table 5-9: Matrix of experimental tests carried out at Cranfield combustion rig using pulverised Daw Mill-12 wt.% Miscanthus.

Test	Number of probes	Probe configuration	Probes' T [°C]	Test duration [hr]	[O ₂] _{vol}
1	3	1	500	2.5	~ 4%
2	3	1	500	5	~ 4%
3	3	2	500	5	~ 4%
4	3	2	600	5	~ 4%

Therefore, the main difference between test 1 and 2 was the exposure time which was double in the second test. Moreover, between test 2 and 3, the main difference was the probe configuration, while in test 4, the temperature of the probes was increased but the configuration was the same as in test 3.

5.10 Summary

In this chapter, the combustion rig operation has been explained in detail and the fuel properties have been reported for a Daw Mill coal-12 wt.% Miscanthus mixture which was used in the experiments. The fuel ash and moisture contents were re-measured in Cranfield and compared with data available in the literature. In addition, a brief procedure of how to run the combustion rig and the main operating parameters has been reported.

A methodology was followed to get valid results for the model set-up and boundary conditions (geometry, gas velocity and temperature, ash particle size distribution and

chemical composition) and its validation (deposition flux, shape, location and thickness) (Chapters 6 and 7).

6 EXPERIMENTAL RESULTS AND DISCUSSIONS

6.1 Introduction

This chapter shows the results obtained during the experiments using pulverised Daw Mill-12 wt.% Miscanthus in the combustion rig at Cranfield University. The main focus was on the gas composition, deposition flux, deposit and ash chemical composition and ash particle size distribution. The methodology outlined in Chapter 5 was applied in all the experiments in order to allow a comparison of the results and get reliable information for use in the model boundary conditions and model validation (Chapter 7).

The main parameters varied during the experiments are reported as in Table 6-1 and the configurations used for the air cooled ceramic probes are illustrated in Figure 6-1.

Table 6-1: Matrix of experimental tests carried out in Cranfield's combustion rig using pulverised Daw Mill-12 wt.% Miscanthus.

Test	Number of probes	Probe configuration	Probes' T [°C]	Test duration [hr]	[O ₂] _{vol}
1	3	1	500	2.5	~ 4%
2	3	1	500	5	~ 4%
3	3	2	500	5	~ 4%
4	3	2	600	5	~ 4%



Figure 6-1: Configuration of the air cooled ceramic probes during combustion of pulverised Daw Mill-12 wt.% Miscanthus in Cranfield's combustion rig: a) first configuration; b) second configuration.

6.2 Gas composition

The tests were all carried out following the procedure described in section 5.7, using the same fuel (Daw Mill-12 wt.% Miscanthus) and operating conditions. In fact, the main differences between the experiments were the exposure time, the probes' configuration and their temperature. These parameters did not affect the flue gas composition, therefore only one example is reported in this section to show the main species detected by the FTIR gas analyser which represents the real gas composition (not dry).

The major and minor gas components produced during almost 5 hours of the test n°3 (Table 6-1) are shown in Figure 6-2 and Figure 6-3 respectively. In these graphs, the time zero represents the switch from natural gas to solid fuel which caused instability in the gas composition; therefore the first 15 minutes were omitted.

The main species were CO₂, H₂O and O₂ and their average concentrations were ~ 10% ± 6.5%, 6% ± 16% and 4% ± 19% respectively. In fact, during the tests, the fuel feed rate was adjusted to keep the oxygen concentration ~ 4%vol which is a common value in coal-fired boilers.

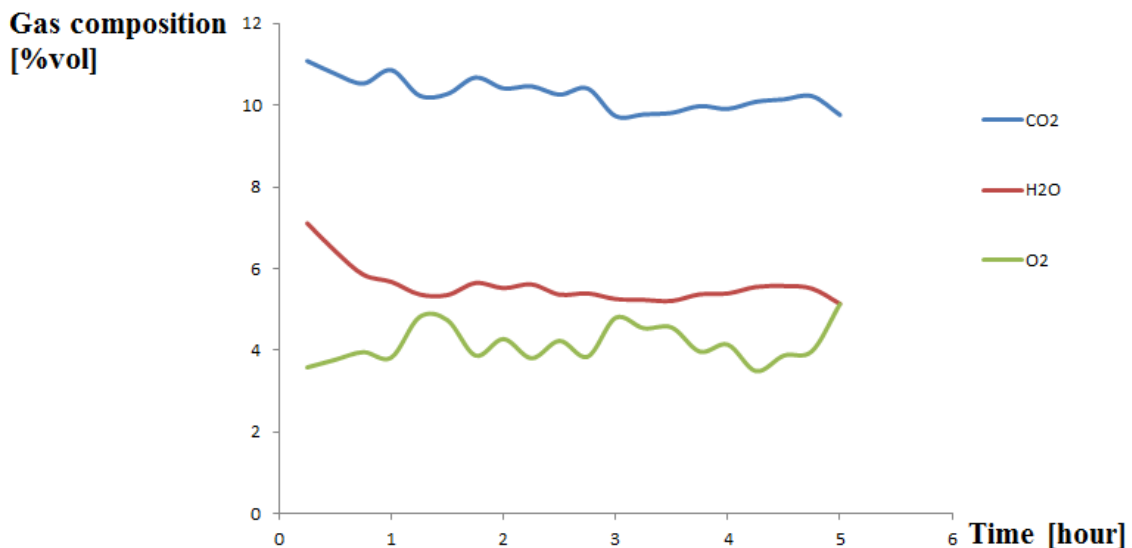


Figure 6-2: Major gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus.

The minor species for the same test are shown in Figure 6-3 and the average concentrations were: CO $\sim 680 \text{ ppm} \pm 74\%$, indicative of complete combustion, NO $\sim 370 \text{ ppm} \pm 13.6\%$, NO₂ $\sim 2.4 \text{ ppm} \pm 17.3\%$, N₂O $\sim 4 \text{ ppm} \pm 36\%$, SO₂ $\sim 810 \text{ ppm} \pm 7\%$ and HCl $\sim 60 \text{ ppm} \pm 75.6\%$. The gas compositions for the other tests are reported in Appendix C.

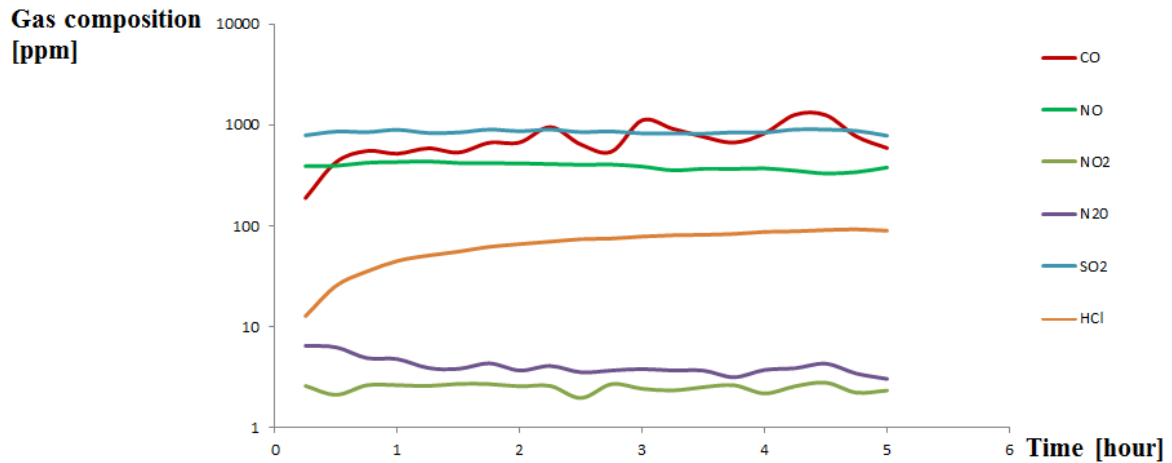


Figure 6-3: Minor gas components from combustion of pulverised Daw Mill-12 wt. % Miscanthus.

6.3 Deposit and fly ash collection, deposition flux and analysis

At the end of each test, once the combustor had cooled down, the probes were carefully extracted for deposit collection as explained in section 5.8. First of all, pictures of the different surfaces (upstream, sides and downstream) of each probe were taken. Deposit was collected in plastic bags and was weighed to calculate the deposition flux knowing the ceramic probe surface area and the exposure time. Moreover, the deposits were analysed with SEM/EDX to obtain the microstructures and the chemical compositions (which were also used for the model validation (Chapter 7)). For the deposit samples in bigger amounts, such as those deposited on the upstream surfaces, XRD analysis was carried out.

Finally, ash was collected from the ports where the probes were placed. This was taken to represent the fly ash that caused deposition; it was used for SEM/EDX analysis and to get the ash particle size distribution (provided by the Industrial Sponsor, Doosan

Babcock), using a laser diffraction particle size analyser (Malvern Mastersizer 2000). The results are shown in the following sections for each experiment and a comparison between them is given in section 6.5.

6.3.1 Test n°1

This test was run using Daw Mill-12 wt.% Miscanthus for 2.5 hours and deposition was studied on three air-cooled ceramic probes ($\sim 500^{\circ}\text{C}$ surface temperatures) located as in the first configuration (Figure 6-1 (a)).

One of the view ports along the vertical section of the chamber was used to take pictures during combustion of the pulverised fuel. Generally, it was possible to appreciate the rain of incandescent ash moving from the top of the rig, where combustion took place, down towards the ceramic probes (Figure 6-4).

In some of the tests, this view port allowed the observation of deposit building up on probe 1, the top of which was just below the level of the view port. However, during this test, the deposit thickness was very thin and could not be seen.

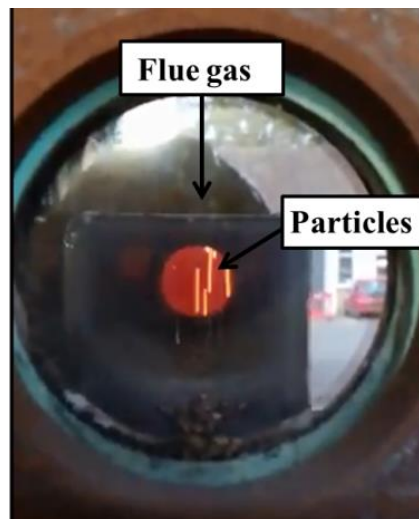


Figure 6-4: Ash particles seen from a view port during combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Once the combustor had been switched off and cooled down, pictures of the deposits were taken for the three probes as shown in Figure 6-5, Figure 6-7 and Figure 6-8. The deposits were generally quite powdery and sand colour, but with some darker areas,

especially on the back of the probe, probably because of an inefficient combustion and a blockage of the fuel feeding system that occurred during the test. Moreover, the deposits on the sides and downstream surfaces were generally stickier, typical of vapour condensation deposition mechanism, and, as a consequence, it was slightly more difficult to brush the deposits off these sides, which remained quite dark also after cleaning (Figure 6-6).

The thickness of the deposits on the top of each probe was irregular along the probe length. Moreover, it was thicker on the upstream than the side and downstream surfaces which confirmed what is stated in the literature (Baxter, 1993; Tomeczek *et al.*, 2004). The maximum deposit thickness on the top was estimated to be ~ 0.5 cm for probe 1, slightly thicker than probes 3 and 2. Moreover, in Figure 6-9, the shape of the deposit for the three probes was captured.



Figure 6-5: Deposit formed on probe 1 ($\sim 500^{\circ}\text{C}$, tube diameter, $d_t = 39$ mm) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.



Figure 6-6: Downstream of the ceramic probe 1 ($\sim 500^{\circ}\text{C}$, $d_t = 39$ mm) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.



Left side



Right side

Figure 6-7: Deposit formed on probe 2 ($\sim 500^{\circ}\text{C}$, $d_t = 39\text{ mm}$) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.



Left side



Right side

Figure 6-8: Deposit formed on probe 3 ($\sim 500^{\circ}\text{C}$, $d_t = 39\text{ mm}$) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.



Probe 1



Probe 2



Probe 3

Figure 6-9: Deposit shape on probes 1, 2 and 3 ($\sim 500^{\circ}\text{C}$, $d_t = 39\text{ mm}$) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Deposits were collected and weighed from the different sides of the probes to calculate the deposition flux knowing the area of each probe side and the test duration (Table 6-2, Table 6-3 and Figure 6-10).

Table 6-2: Deposit weights from the probes (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Side	Area [cm ²]	Deposit weight [g]		
		Probe 1	Probe 2	Probe 3*
Upstream	30.5	0.58	0.54	0.57
Left side	11.59	0.08	0.04	0.05
Right side	11.59	0.12	0.19	0.08
Downstream	21.02	0.04	0.07	0.05
Total	74.70	0.83	0.84	0.76

*Deposit loss during handling.

The results show that the deposition flux was always higher on the top than the sides and downstream for all the probes which confirms what already observed by Ala Khodier using a similar blend of Daw Mill and Miscanthus (Khodier, 2011). It is important to note that the deposition flux on the left and right sides were summed up in Table 6-3 and identified as from the side surfaces. However, in this test, some deposit was lost from probe 3 as the deposit was quite powdery and it fell easily while it was extracted from the combustor or placed on the desk for deposit collection (e.g. Figure 6-9). Therefore, some of the results may be affected by such deposit loss.

Table 6-3: Deposition fluxes on probes 1, 2 and 3 (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Side	Deposition flux [mg/(cm ² hr)]		
	Probe 1	Probe 2	Probe 3*
Upstream	7.63	7.06	7.46
Side (Left + Right)	3.47	4.03	2.35
Downstream	0.82	1.29	0.97
Total	4.42	4.50	4.05

*Deposit loss during handling.

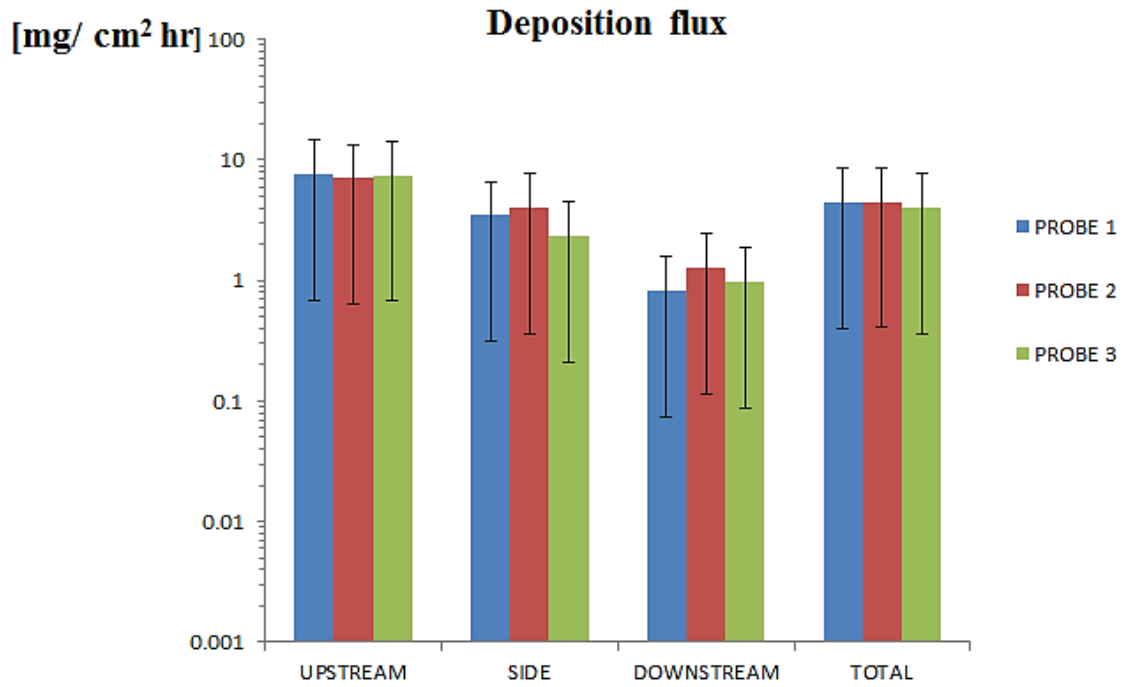


Figure 6-10: Deposition fluxes on different sides of probes ($\sim 500^\circ\text{C}$) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Once the deposition flux was calculated, the deposits were analysed with SEM to collect images and study its microstructure. The SEM images in Figure 6-11, Figure 6-12 and Figure 6-13 were all taken at a similar magnification on the upstream surfaces and a bigger one on the sides and downstream surface ($100\text{ }\mu\text{m}$ scale bar). It can be noticed that bigger particles deposited on the upstream surface and there was a higher concentration of smaller particles on the sides and downstream. This behaviour is in line with the literature (Chapter 2), in fact particles with diameter $d_p > 10\text{ }\mu\text{m}$ have more inertia to overcome the drag force and have their own trajectories, while smaller particles ($d_p < 10\text{ }\mu\text{m}$) are more likely to follow the flue gas streamlines and hit the rear side of the tubes (Lee *et al.*, 2014). However, especially on the downstream of probe 1 and the right and left sides of all the probes, bigger particles were found and this may be due to the rebound of big particles from one tube to the other.

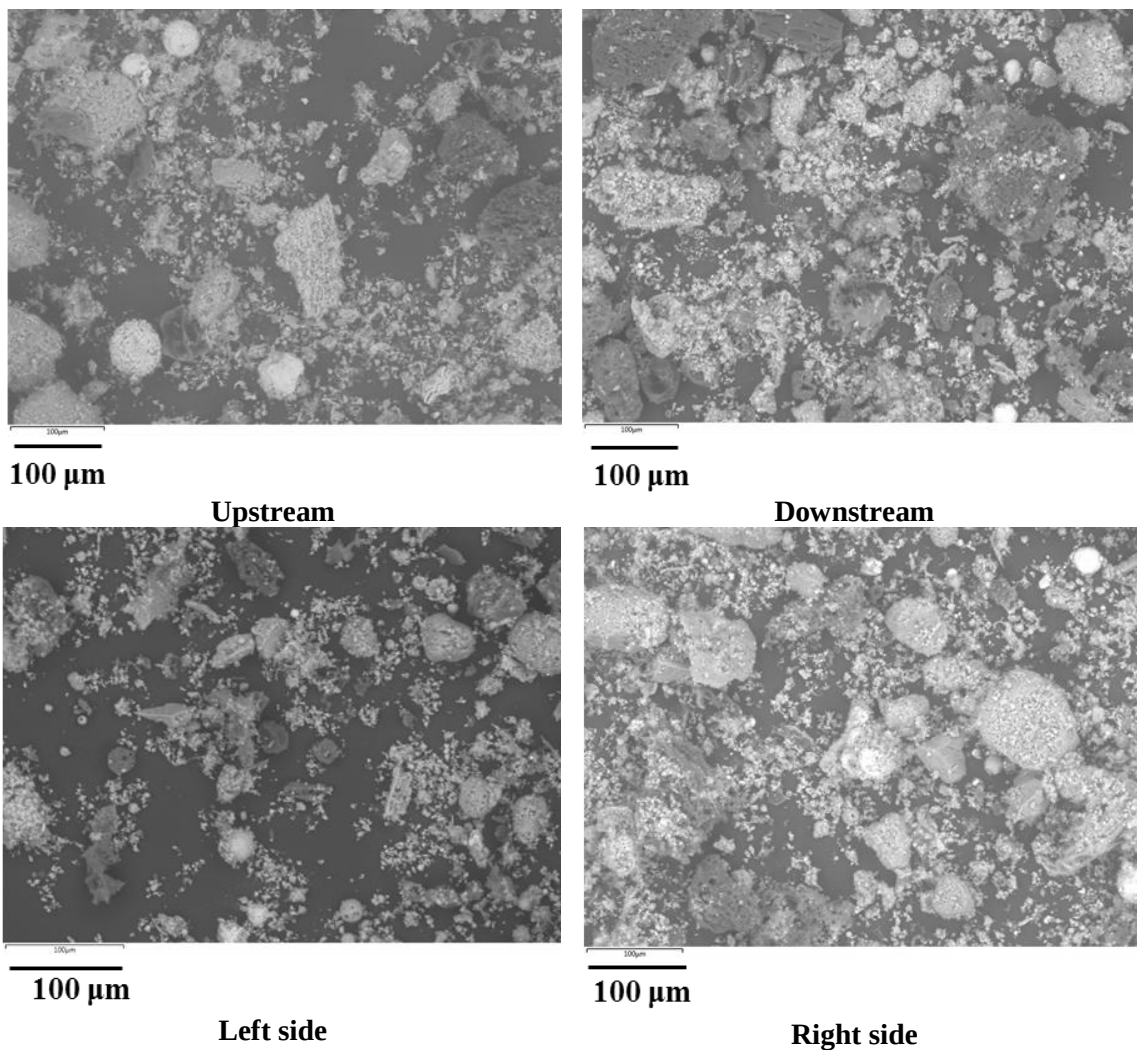


Figure 6-11: SEM images of deposit formed on different t sides of probe 1 (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

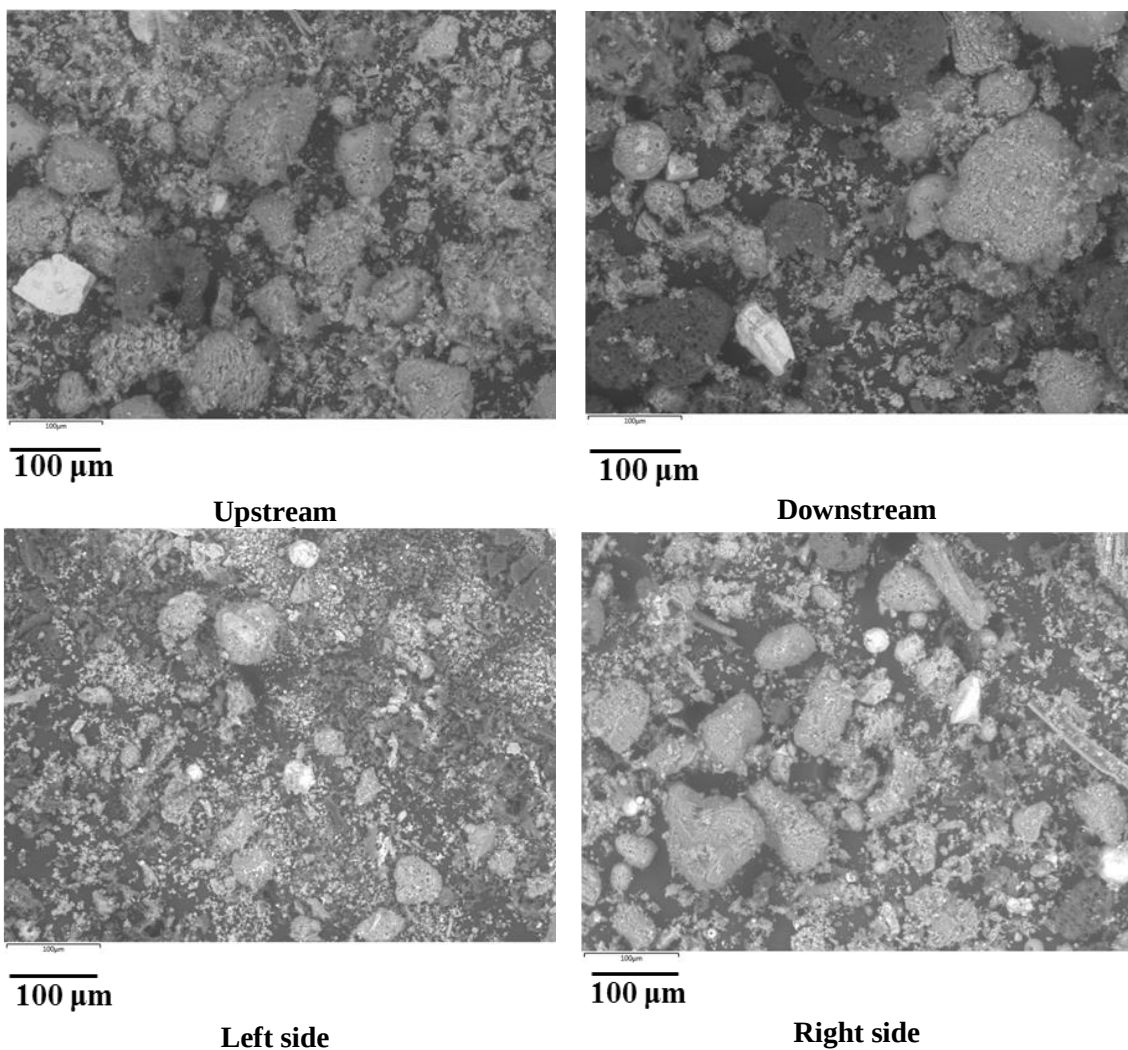


Figure 6-12: SEM images of deposit formed on different sides of probe 2 (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

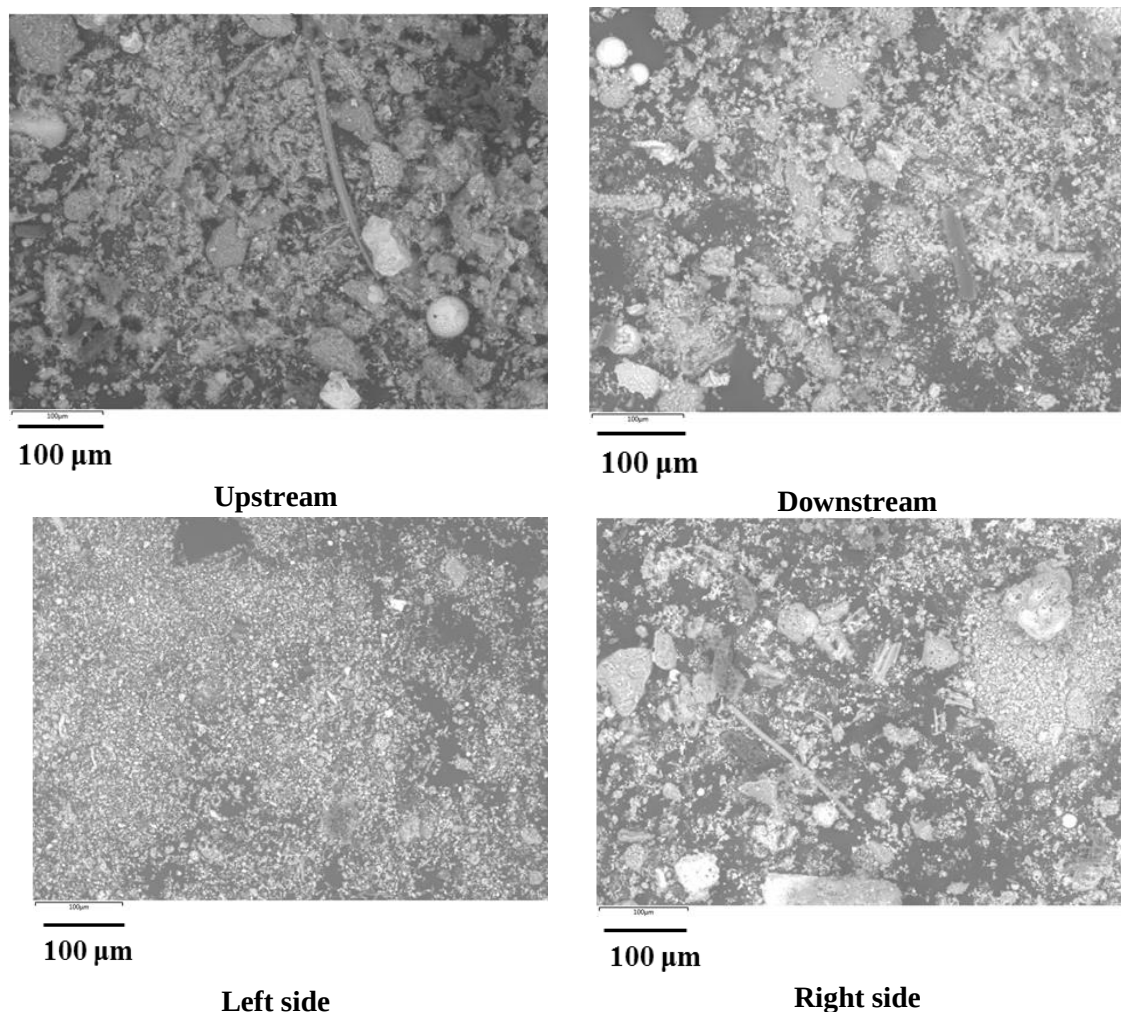


Figure 6-13: SEM images of deposit formed on different sides of probe 3 (~ 500°C) after. 2.5 hours from combustion of Daw Mill-12 wt. % Miscanthus using the 1st probes' configuration.

The EDX analyses were done to find the deposit chemical composition on each probe side. The weight percentage of the main elements present in the ash was measured from different locations on the same stub and an average was calculated in order to find the deposit composition in terms of the % by weight in the form of their highest oxides (Simms, 2011b). The results are given in Figure 6-14, Figure 6-15 and Figure 6-16 and the main species found were: SiO_2 , Al_2O_3 , CaO , Fe_2O_3 , K_2O , MgO , Na_2O , TiO_2 , SO_3 , P_2O_5 , Mn_3O_4 , whose percentages were comparable among the probes and their different sides. However, these oxides do not represent the real chemical compounds in the deposits which are characterised by a more complicated structure (mainly aluminosilicate) therefore care is needed in the data analysis (Simms, 2011b).

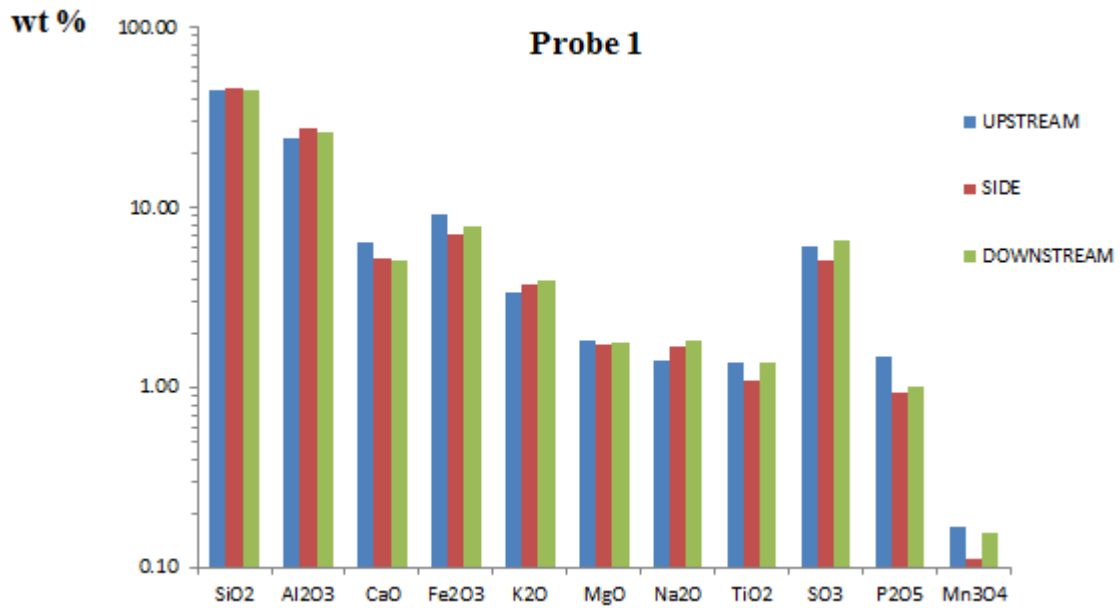


Figure 6-14: Deposit chemical composition on probe 1 (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration (in terms of highest oxides of elements).

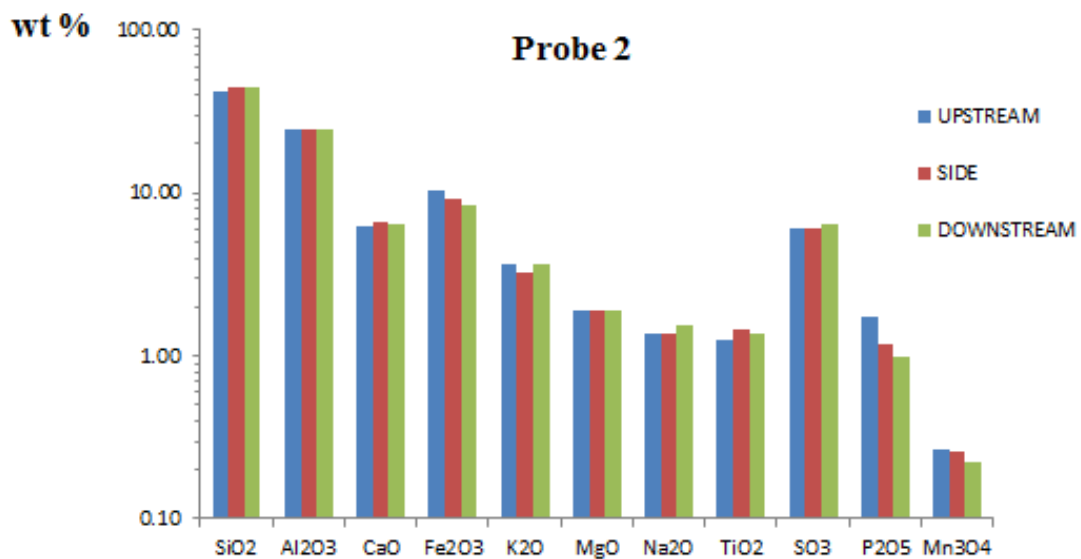


Figure 6-15: Deposit chemical composition on probe 2 (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration (in terms of highest oxides of elements).

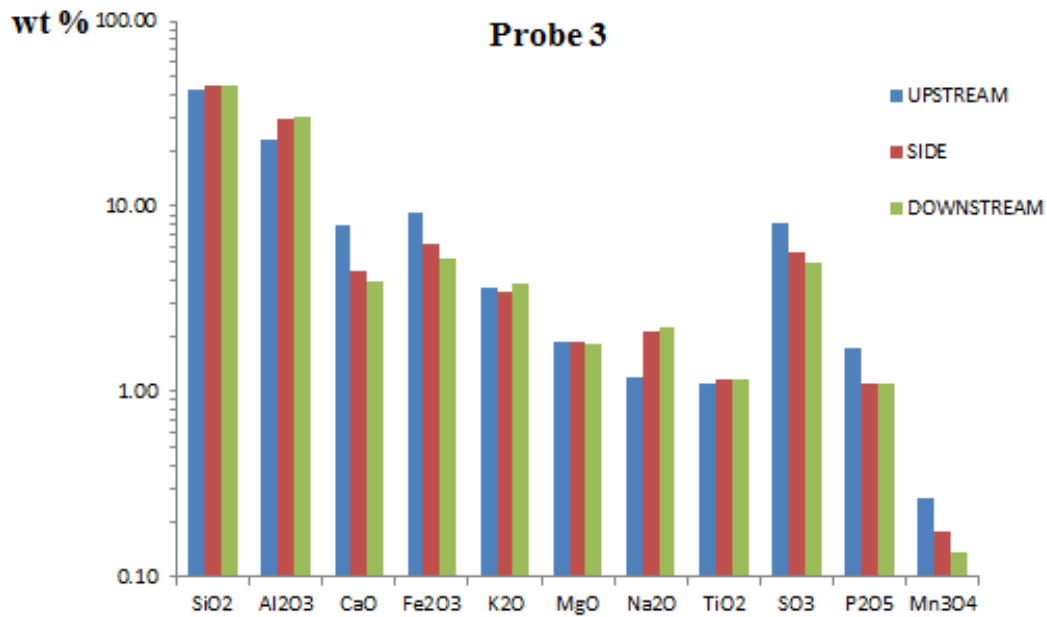


Figure 6-16: Deposit chemical composition on probe 3 (~ 500°C) after 2.5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration (in terms of highest oxides of elements).

For this test, XRD analysis was not carried out as the amount of deposit on the upstream surface was not enough.

6.3.2 Test n°2

This test can be considered a repetition of test n°1 with duration of 5 instead of 2.5 hours. Therefore, a longer exposure time allowed more ash to accumulate and the deposit formation on probe 1 could be observed from the view port during the experiment as in Figure 6-17.

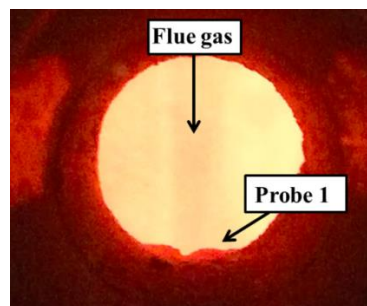


Figure 6-17: Deposit formation on probe 1 seen from a view port during combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Figure 6-18, Figure 6-19 and Figure 6-20 show the pictures of the deposits accumulated on the three probes after combustion of Daw Mill-12 wt.% Miscanthus for 5 hours using the first probe configuration.



Left side



Right side

Figure 6-18: Deposit formed on probe 1 ($\sim 500^{\circ}\text{C}$, $d_t = 39\text{ mm}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.



Left side



Right side

Figure 6-19: Deposit formed on probe 2 ($\sim 500^{\circ}\text{C}$, $d_t = 39\text{ mm}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.



Figure 6-20: Deposit formed on probe 3 ($\sim 500^{\circ}\text{C}$, $d_t = 39\text{ mm}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

As already mentioned in section 6.3.1, the deposits were thicker on the upstream than right/left sides and downstream. However, it can be noticed from the pictures that the thickness was not constant along the upstream and the maximum value was $\sim 1\text{-}1.1\text{ cm}$, higher than the one measured in section 6.3.1 as the probes were exposed for a longer time which allowed more deposition. Moreover, the deposits were quite powdery on the top of the probes and stickier on the sides and back of the ceramic.

Some deposit was lost from the right side of probe 1 while the deposit from the top was being brushed. Therefore, only for this test and this probe, the results were indicated as upstream + right side. Deposit was weighed from the different sides of the probes and the results in Table 6-4 were then used to calculate the deposition flux (Table 6-5 and Figure 6-21).

Table 6-4: Deposit weights from probes ($\sim 500^{\circ}\text{C}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Side	Area [cm^2]	Deposit weight [g]		
		Probe 1*	Probe 2	Probe 3
Upstream	30.5	0.85	1.34	1.40
Left side	11.59	0.10	0.10	0.11
Right side	11.59	-	0.16	0.16
Downstream	21.02	0.02	0.16	0.11
Total	74.70	0.97	1.76	1.78

*Deposit loss during handling.

Table 6-5: Deposition fluxes on probes 1, 2 and 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Side	Deposition flux [mg/(cm ² hr)]		
	Probe 1*	Probe 2	Probe 3
Upstream	5.59	8.77	9.18
Side (Left + Right)	0.85	2.24	2.36
Downstream	0.24	1.55	1.06
Total	2.61	4.71	4.78

*Deposit loss during handling.

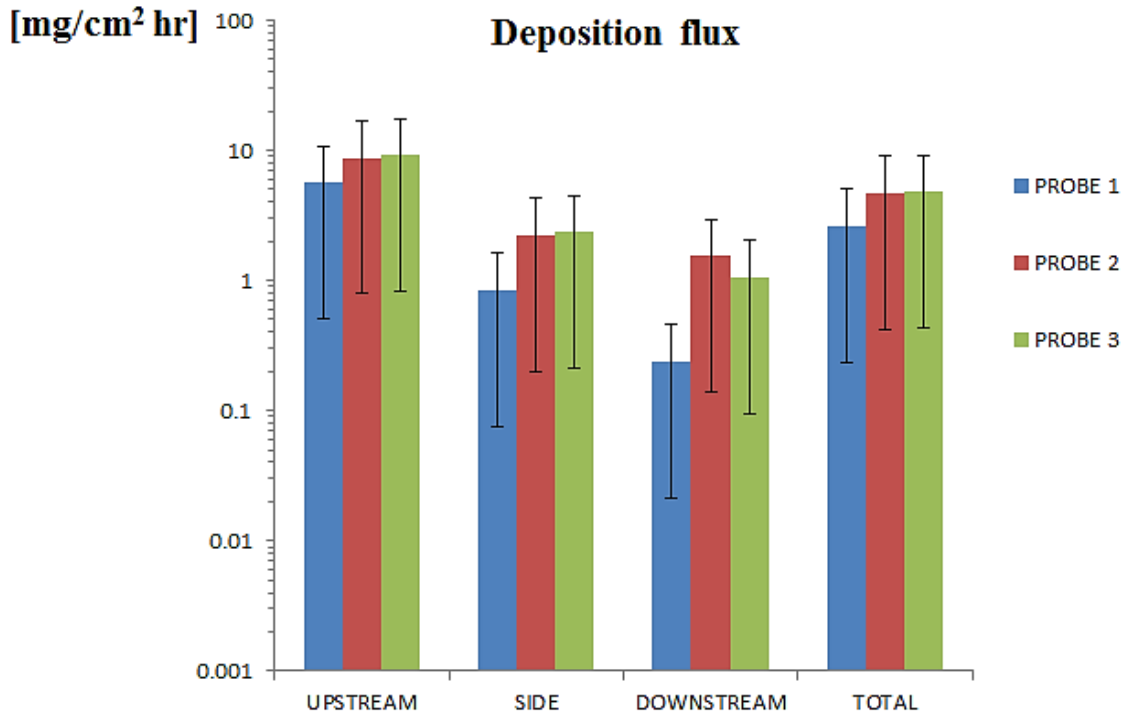


Figure 6-21: Deposition fluxes on different sides of probes (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

The values in Figure 6-10 and Figure 6-21 show that, despite the deposit loss from probes 3 and 1 respectively, the deposition fluxes have the same order of magnitude since a bigger amount of ash deposited on the same surface area in a longer (double) time. Moreover, as noticed before, in test n°2, the maximum deposit thickness was almost double if compared with test n°1.

The SEM analyses for the deposit all around the probes are in Figure 6-22, Figure 6-23 and Figure 6-24. These show that bigger particles tend to deposit on the upstream

surface and the smaller ones on the sides and downstream surfaces. However, in particular for probe 1, the downstream and the left side were characterised by the presence of bigger particles which may be due to the rebound of this type of particles from the top side of probe 2.

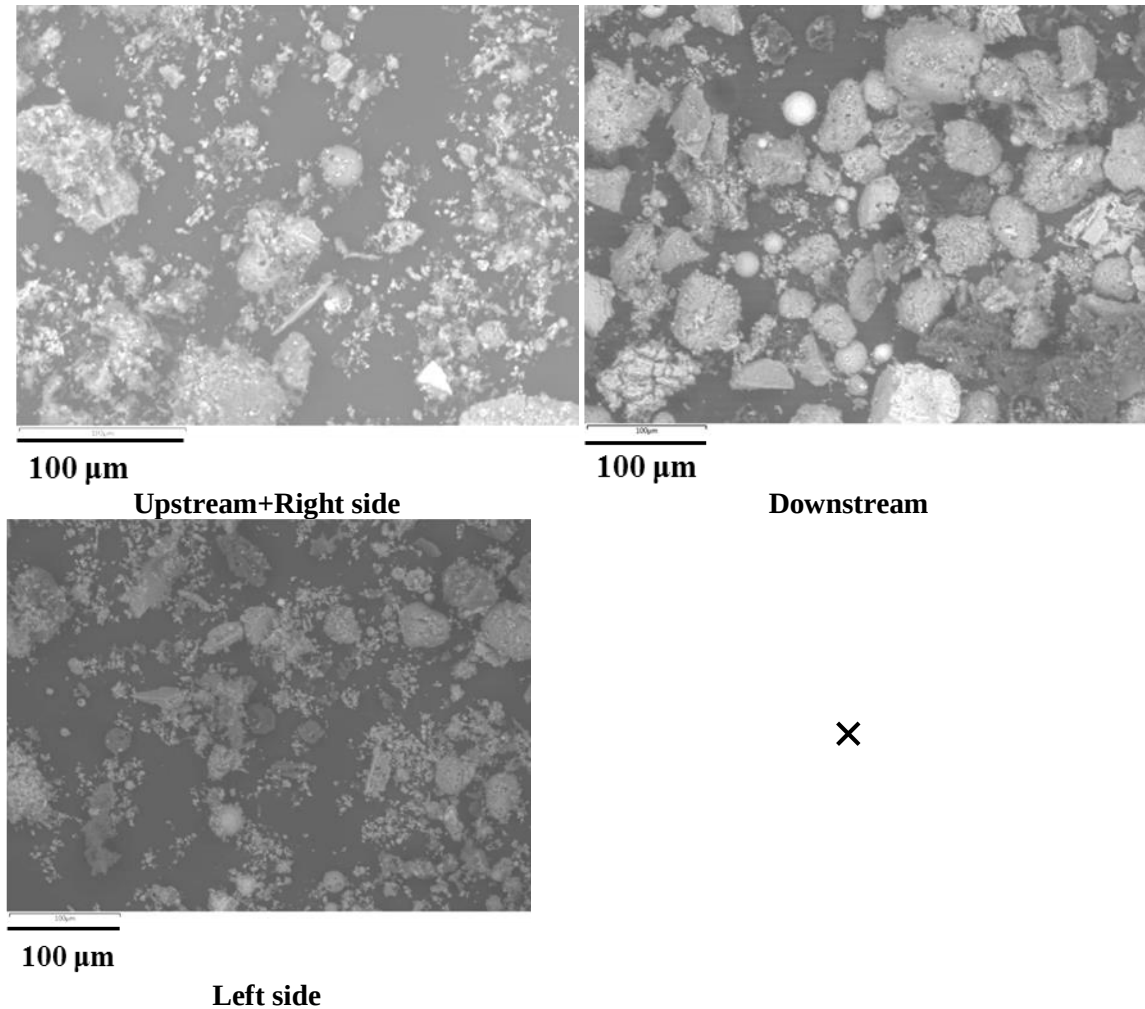


Figure 6-22: SEM images of deposit formed on different sides of probe 1 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

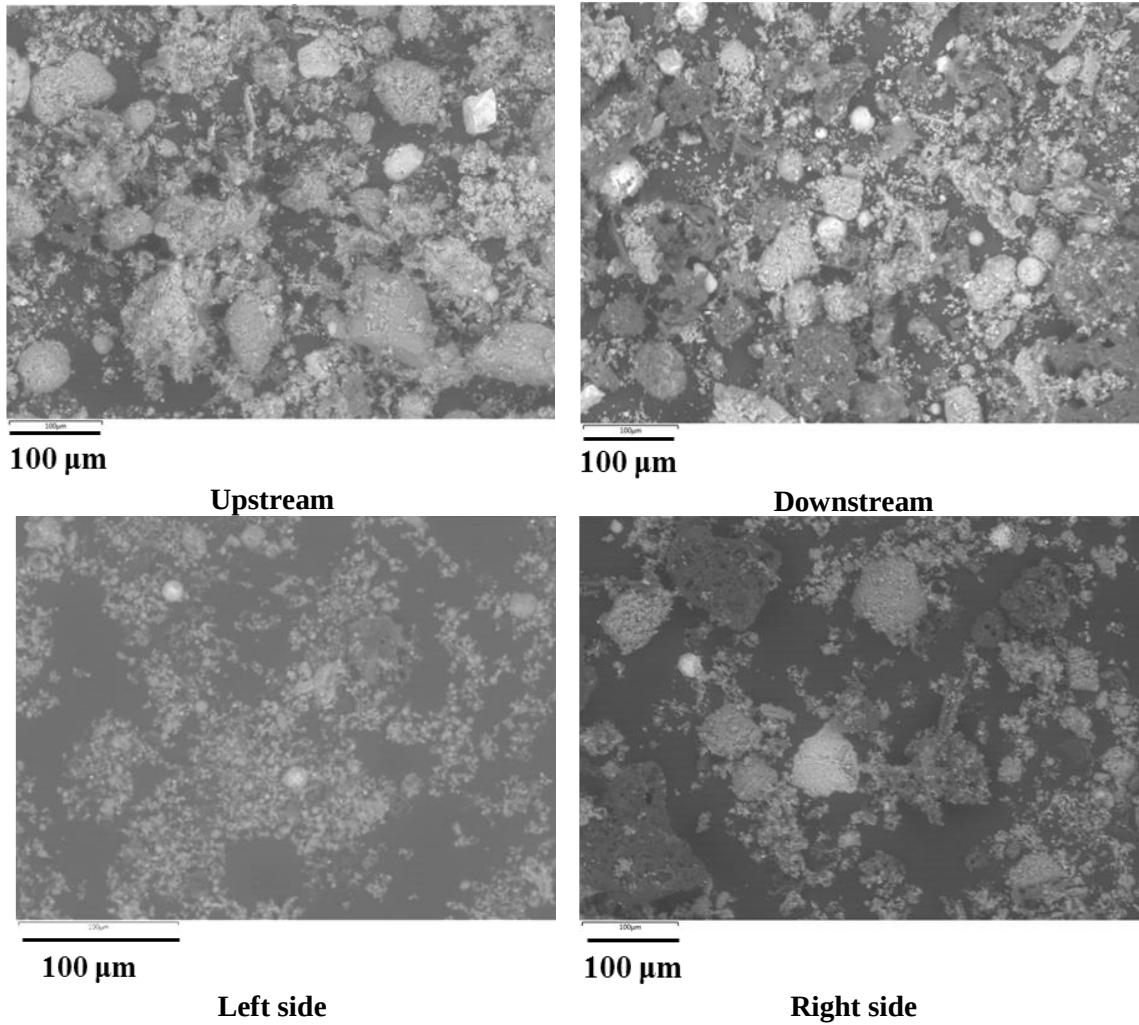


Figure 6-23: SEM images of deposit formed on different sides of probe 2 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

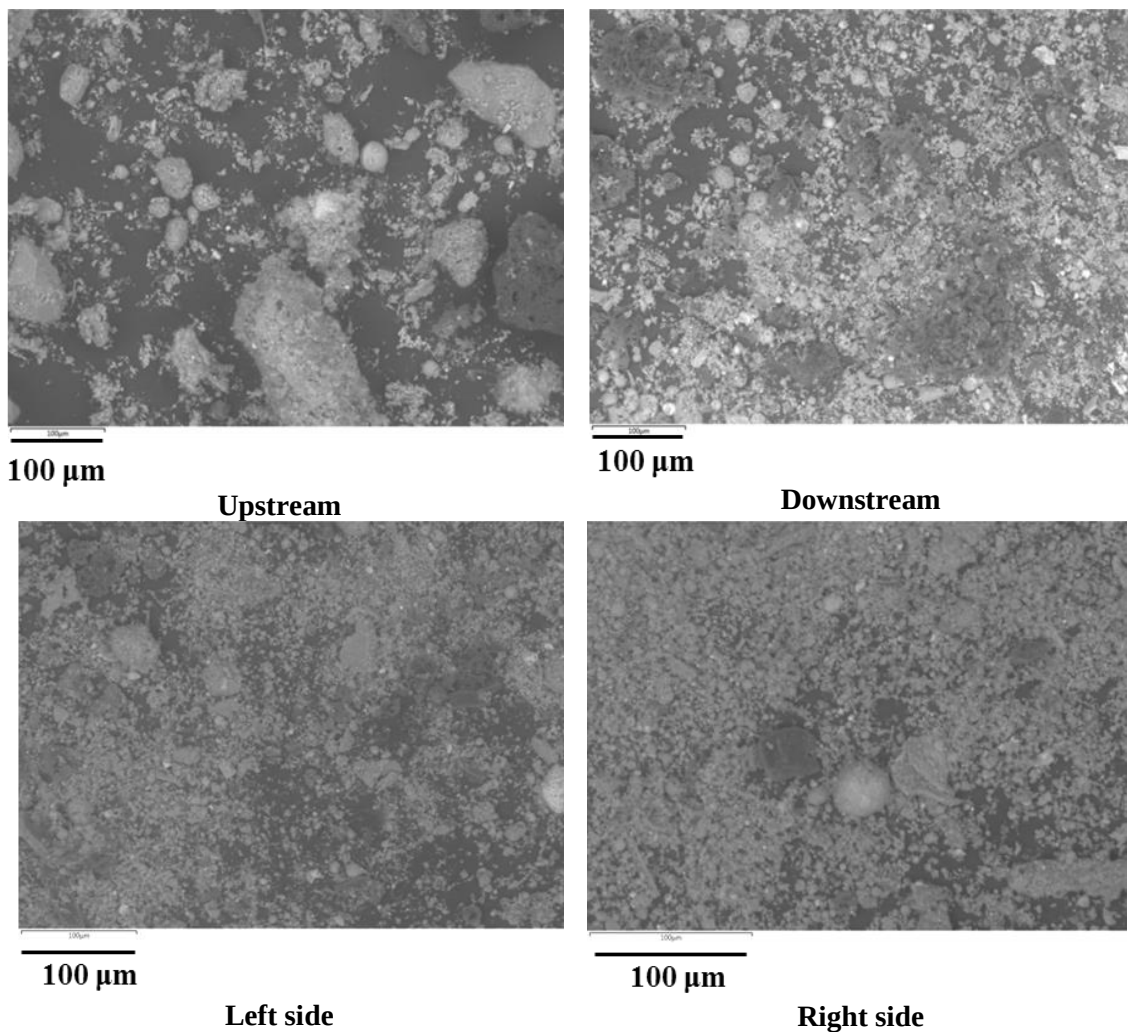


Figure 6-24: SEM images of deposit formed on different sides of probe 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

The deposit chemical composition obtained with the SEM/EDX analyses for the probes 1, 2 and 3 are in Figure 6-25, Figure 6-26 and Figure 6-27 respectively (in terms of the highest oxides of elements). These results have the same trend and comparable percentages as the deposits from test n°1 which means that a longer exposure time did not affect the deposit composition.

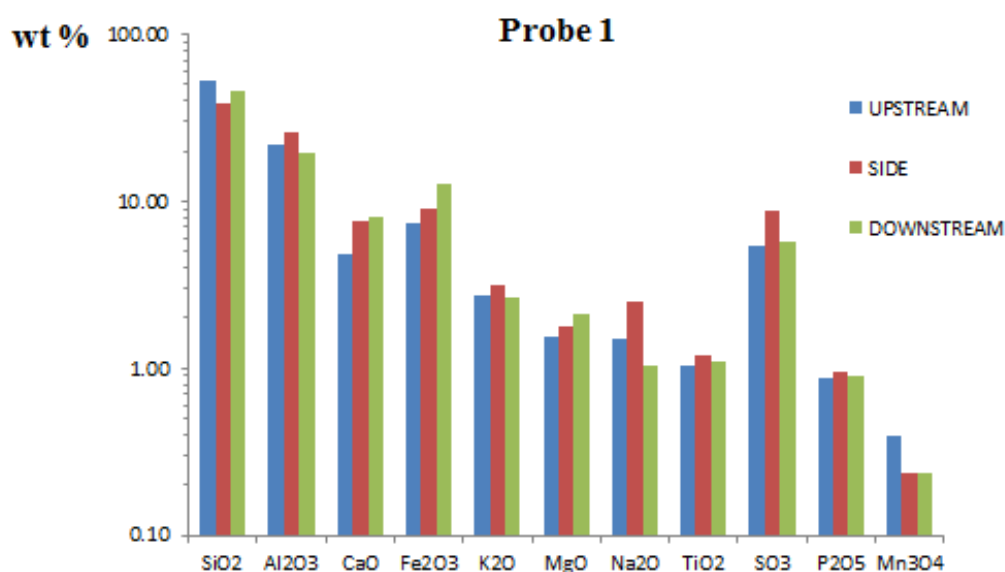


Figure 6-25: Deposit chemical composition on probe 1 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration (in terms of highest oxides of elements).

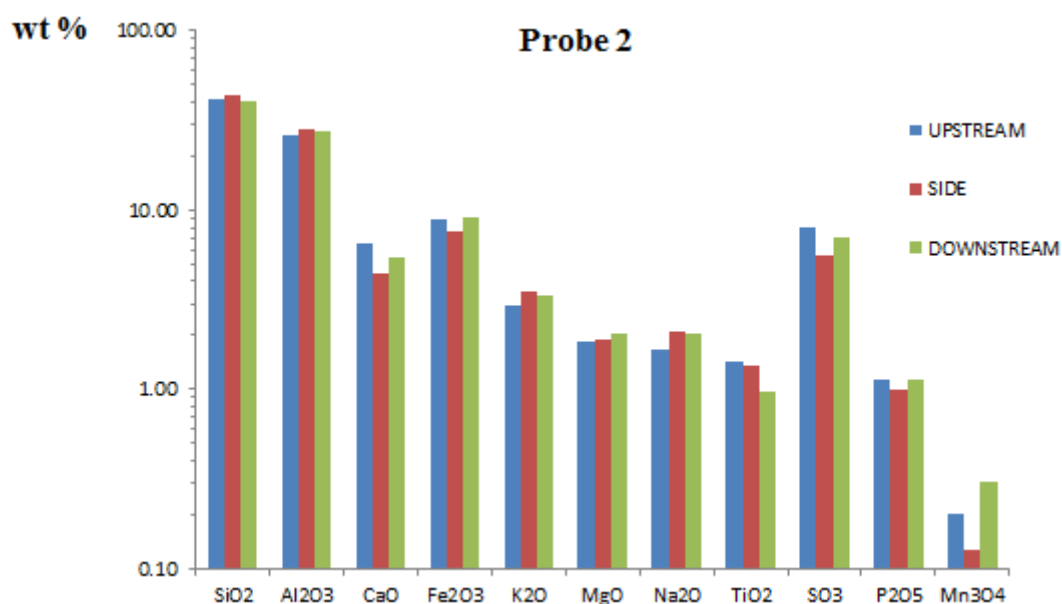


Figure 6-26: Deposit chemical composition on probe 2 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration (in terms of highest oxides of elements).

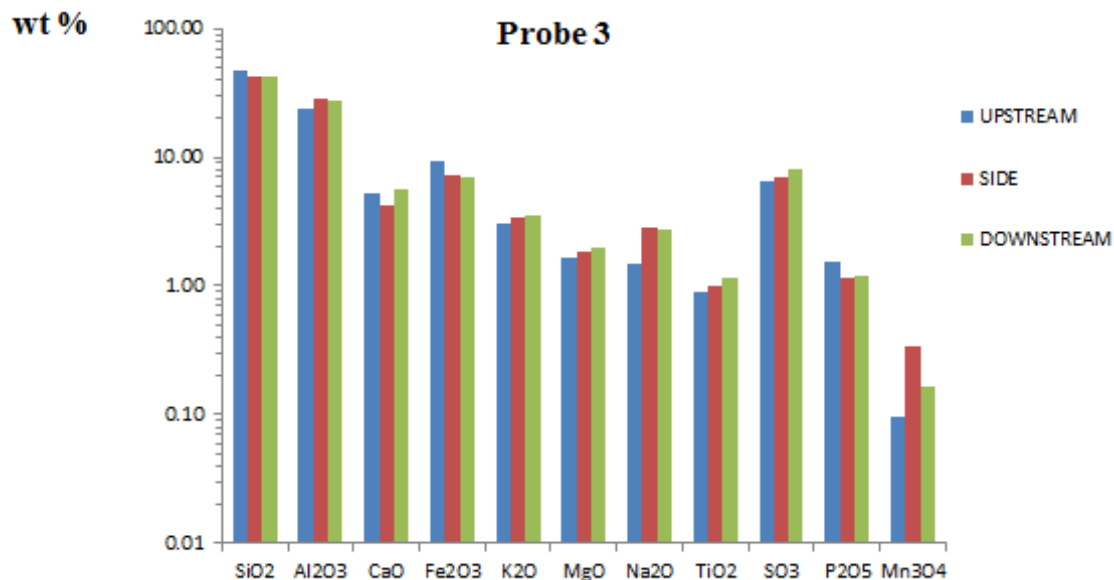


Figure 6-27: Deposit chemical composition on probe 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration (in terms of highest oxides of elements).

Moreover, XRD analysis was carried out for the deposits on the upstream surfaces of probes 1, 2 and 3 as these were more abundant. The results are summarised in Figure 6-28 where the spectra for the top of each probe were overlapped and shifted upwards in order to compare the peaks.

The main species were identified and highlighted with different symbols. These were Quartz (SiO_2), Hematite (Fe_2O_3), Magnetite (Fe_3O_4), Anhydrite (CaSO_4), Alumina Silicate ($\text{SiO}_2 \cdot \text{Al}_2\text{O}_3$) and Aluminium Oxide (Al_2O_3).

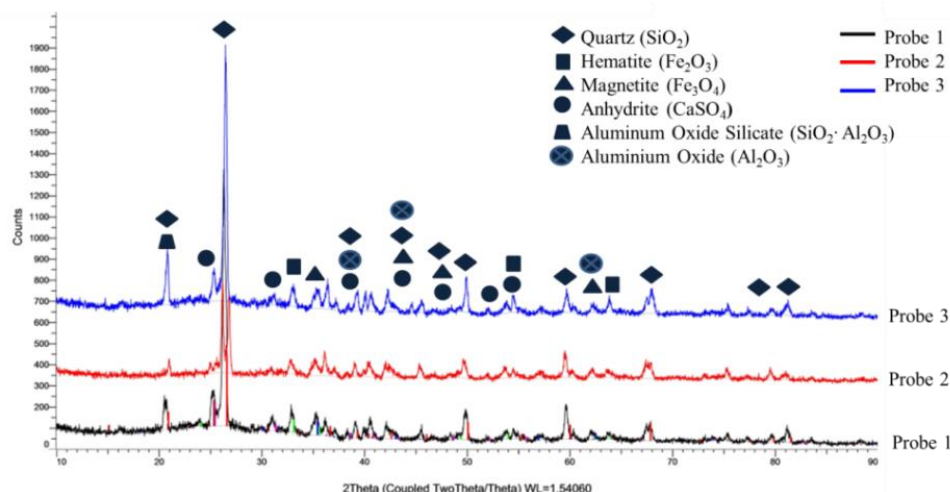


Figure 6-28: XRD analysis of the deposits on the top of probes 1, 2 and 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

After the first test, it was decided to collect ash from the ports where the probes were located (Figure 5-29) and assume that this ash represented the fly ash that caused particle deposition. These samples were analysed with SEM/EDX and the average composition among the three ports was calculated and reported in Figure 6-29. These values were similar to the chemical composition in the deposits and to data from all the experiments, summarised in section 6.5 (Figure 6-75).



Figure 6-29: Average chemical composition of fly ash collected from the ports 1, 2 and 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration at ~ 500°C (in terms of highest oxides of elements).

These samples were also used to get an ash particle size distribution and the volumetric percentage of different ash particle diameters, provided by Doosan Babcock for the three ports, were overlapped and reported in Figure 6-30. These results were then fit to the Rosin Rammler model applying the procedure explained in section 5.8 in order to get d_{min} , d_{max} , d_{mean} and n for the model validation (Chapter 7) (Figure 6-31, Figure 6-32, Figure 6-33).

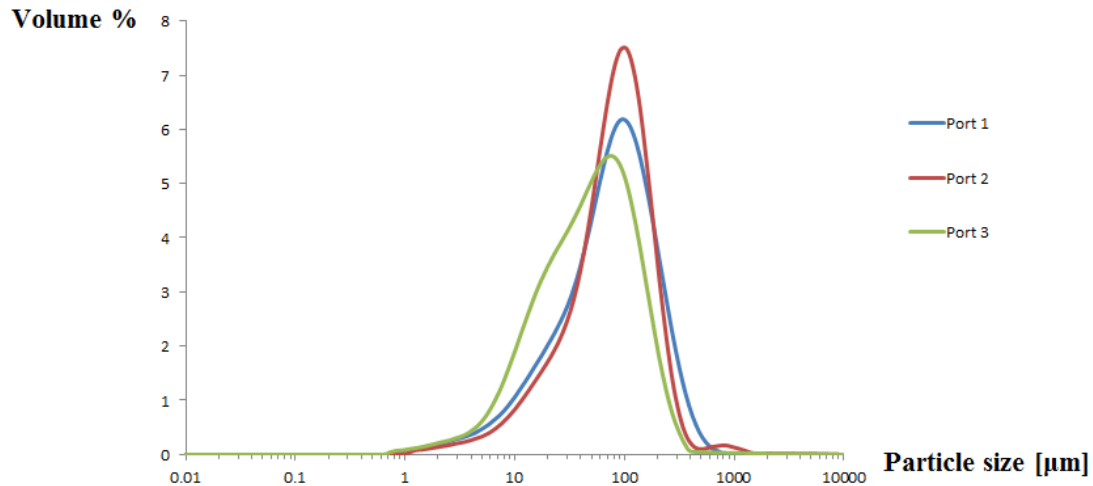


Figure 6-30: Volumetric ash particle size distribution for fly ash collected from the ports 1, 2 and 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

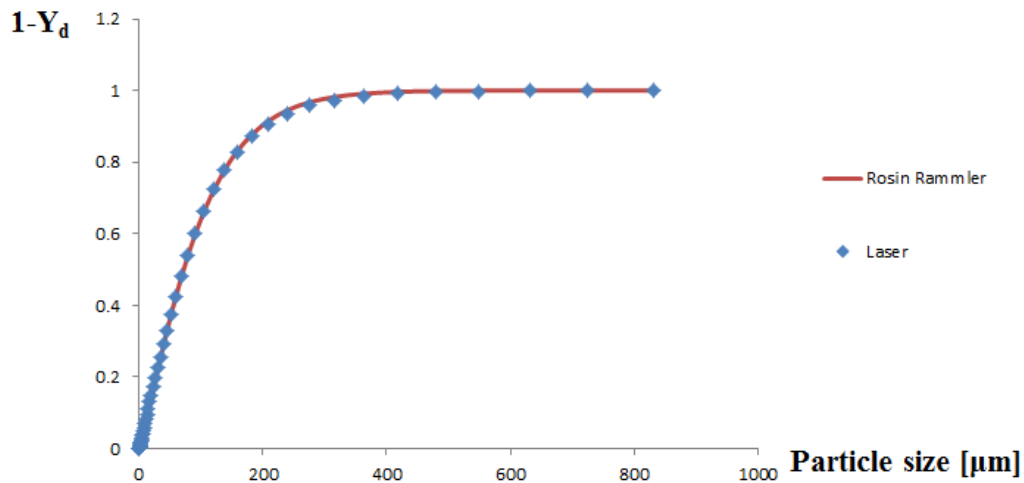


Figure 6-31: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 1 (test n°2): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

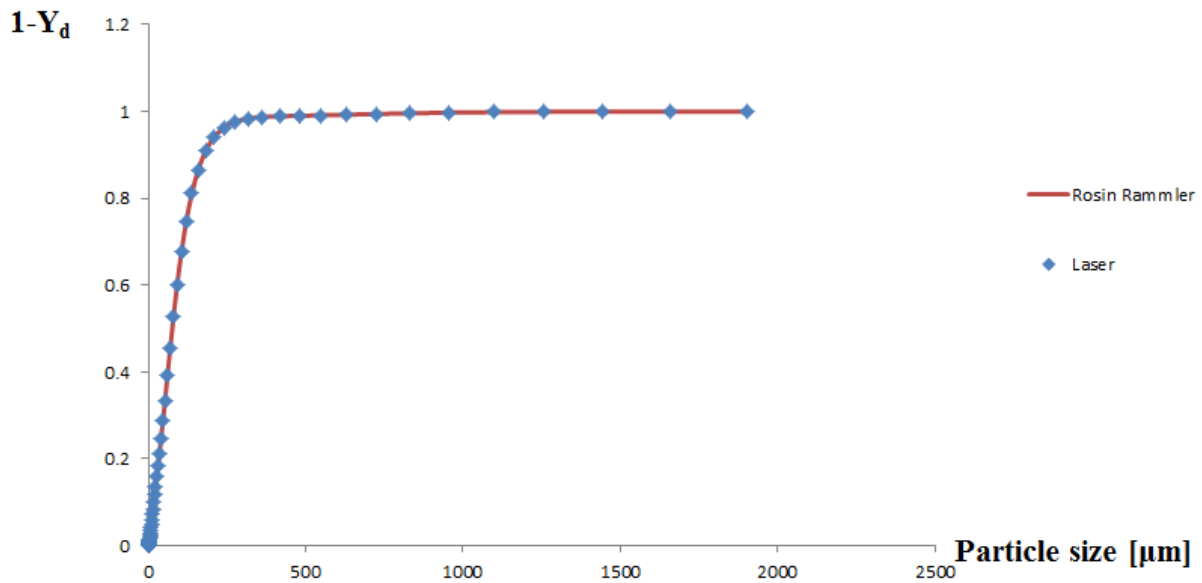


Figure 6-32: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 2 (test n°2): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

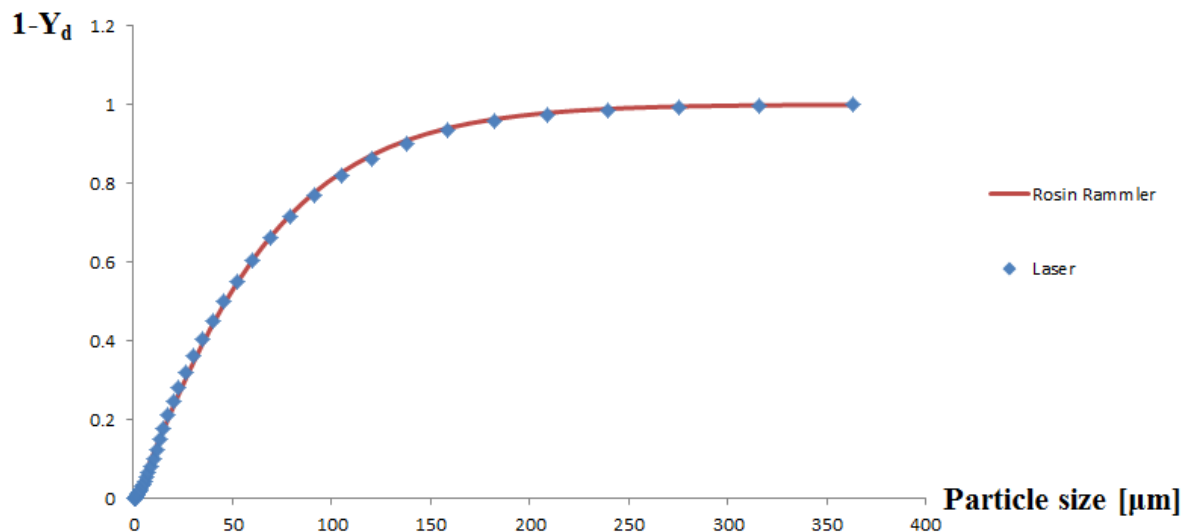


Figure 6-33: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 3 (test n°2): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

The results obtained from the fittings between the ash particle size distribution using a Laser Diffraction and the Rosin Rammler model for the three ports have been summarised in Table 6-6. This confirms the presence of a wide range of particles in the

flue gas, from very small to bigger diameters which justifies the ash particles' behaviour and their tendency to deposit on different sides of the probes as detected in the SEM images. In fact, small particles ($d_p < 10 \mu\text{m}$) follow the flue gas and deposit mainly on the downstream and sides of the probes. Bigger particles ($d_p > 10 \mu\text{m}$) instead tend to bound and rebound on the upstream of the tubes. These are more likely to deposit in the presence of an initial sticky layer from vapour condensation or a previous deposit. Very big particles (e.g. $d_p \gg 100 \mu\text{m}$) were not even found on the probes since they have enough inertia to hit the top of the probe and rebound.

Table 6-6: Main Rosin Rammler parameters obtained from the fitting between the experimental results and the model after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

Port	$d_{min} [\mu\text{m}]$	$d_{max} [\mu\text{m}]$	$d_{mean} [\mu\text{m}]$	n
1	0.724	831.76	98.30	1.16
2	0.955	1905.46	97.23	1.37
3	0.631	416.87	64.03	1.14

For this test, several SEM images of deposits around the ceramic probes were taken with different magnifications (Appendix D) and the software Image J was used to measure the ash particle diameters and study their distribution around the probe. The results for probes 1, 2 and 3 are given in Figure 6-34, Figure 6-35 and Figure 6-36 respectively, where each ring represents one side of the probe with a different percentage of particle diameters.

The results show that particles with diameter bigger than $100 \mu\text{m}$ tend to deposit on the front and, only for probe 1, some of them were found on the left side, possibly because of their rebound from the top of probe 2. Particles with diameter $10 \mu\text{m} < d_p < 100 \mu\text{m}$ were found all around the probes, whereas particles with diameter smaller than $10 \mu\text{m}$ deposited on the sides and downstream. Finally, particles with $d_p < 1 \mu\text{m}$ were mainly on the downstream and, in smaller amount, on the sides. This confirms the ash particle behaviour explained in the literature (section 2.8.1) and predicted by the CFD model in section 4.2.3.

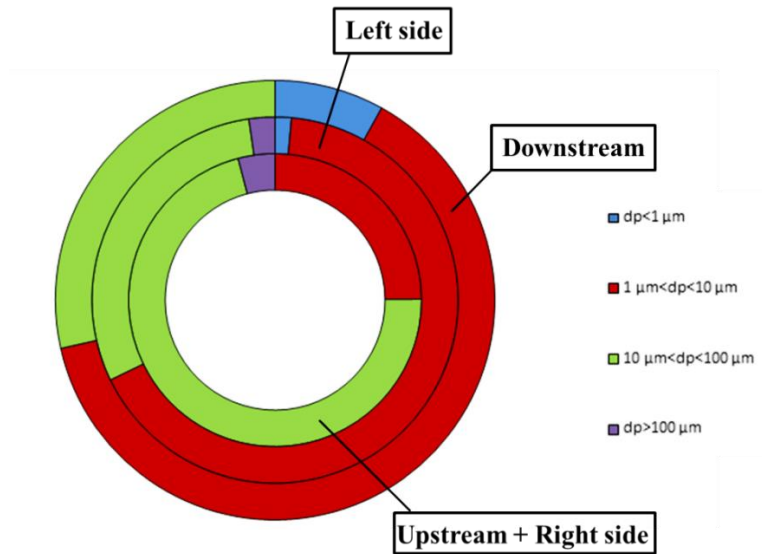


Figure 6-34: Dimensions of ash particles deposited around probe 1 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

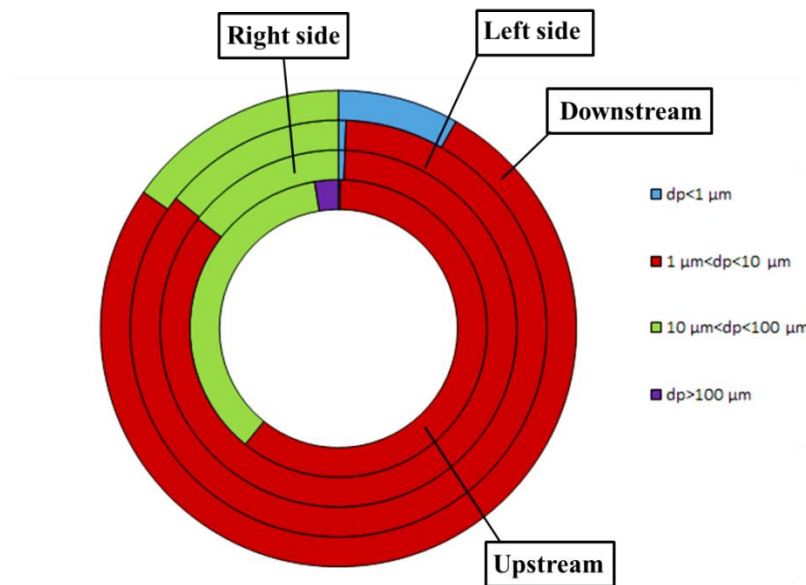


Figure 6-35: Dimensions of ash particles deposited around probe 2 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

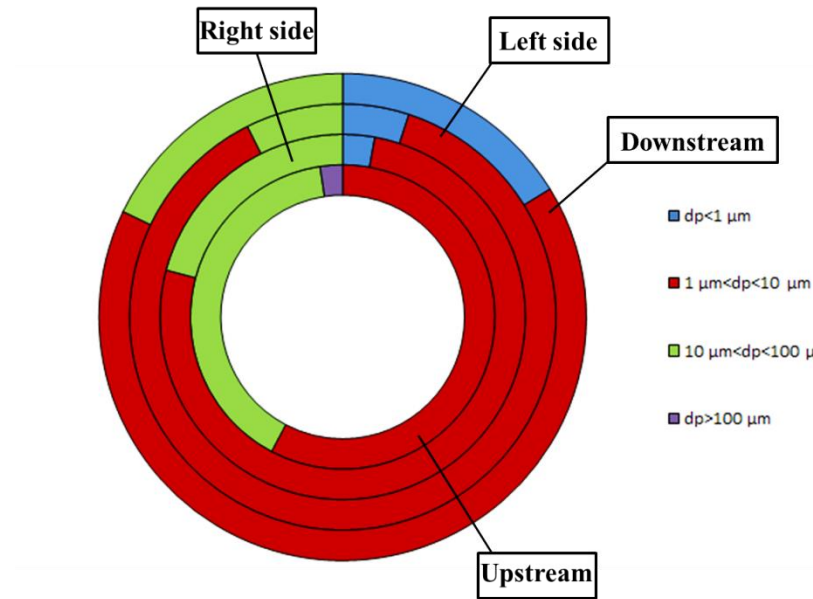


Figure 6-36: Dimensions of ash particles deposited around probe 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 1st probes' configuration.

6.3.3 Test n°3

In this test, the same conditions as in the previous experiments were applied and the only difference was the position of probe 1 (Figure 6-1 (b)). This configuration allowed a better view of the probe from the view port and several pictures were taken during the experiment to monitor the increase in deposit thickness over time (Figure 6-37). Figure 6-37, after 4 hours, shows the presence of incandescent ash particles while they were hitting and settling on the surface of the deposit.

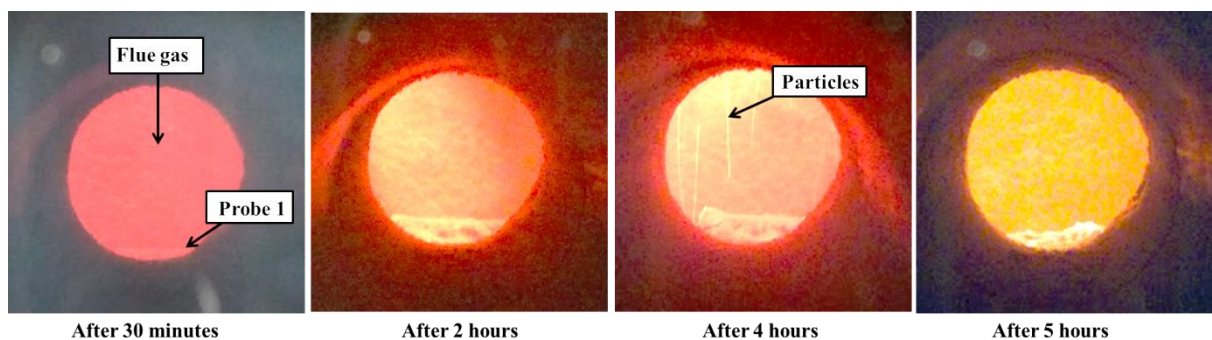


Figure 6-37: Deposit formation on probe 1 seen from a view port during combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Pictures given in Figure 6-38, Figure 6-39 and Figure 6-40 show the appearance of probes 1, 2 and 3 respectively. It is evident that the deposits were quite powdery and of a lighter colour, which means that the combustion was more efficient in this run. In fact there were less problems with blockages in the fuel feeding system in this test, which was also confirmed by a more stable flue gas composition when compared with the other tests (Appendix C). The deposit was thicker on the upstream surfaces for all the probes with a maximum thickness of ~ 1 - 1.1 cm which varied along the probe length. Moreover, for probe 1 the deposit resulted quite thick also on the right side and the shape of the deposit is shown in Figure 6-41.



Figure 6-38: Deposit formed on probe 1 ($\sim 500^{\circ}\text{C}$, $d_t = 39$ mm) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.



Figure 6-39: Deposit formed on probe 2 ($\sim 500^{\circ}\text{C}$, $d_t = 39$ mm) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

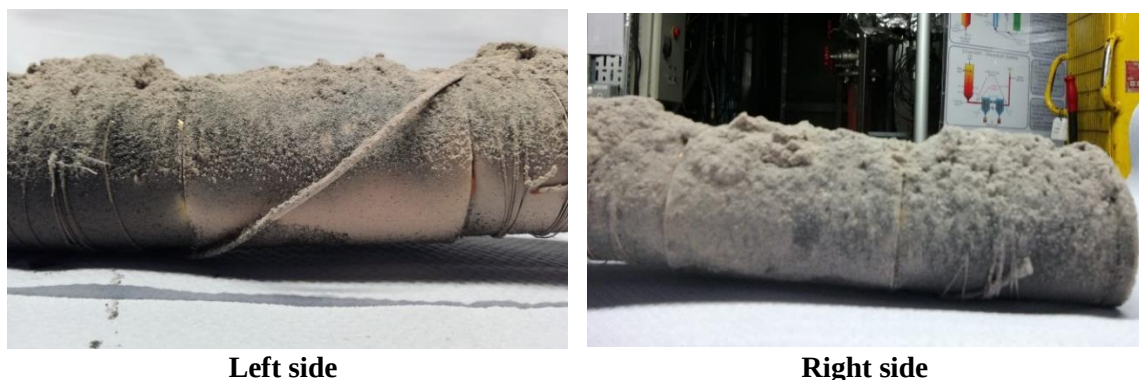


Figure 6-40: Deposit formed on probe 3 ($\sim 500^\circ\text{C}$, $d_t = 39\text{ mm}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

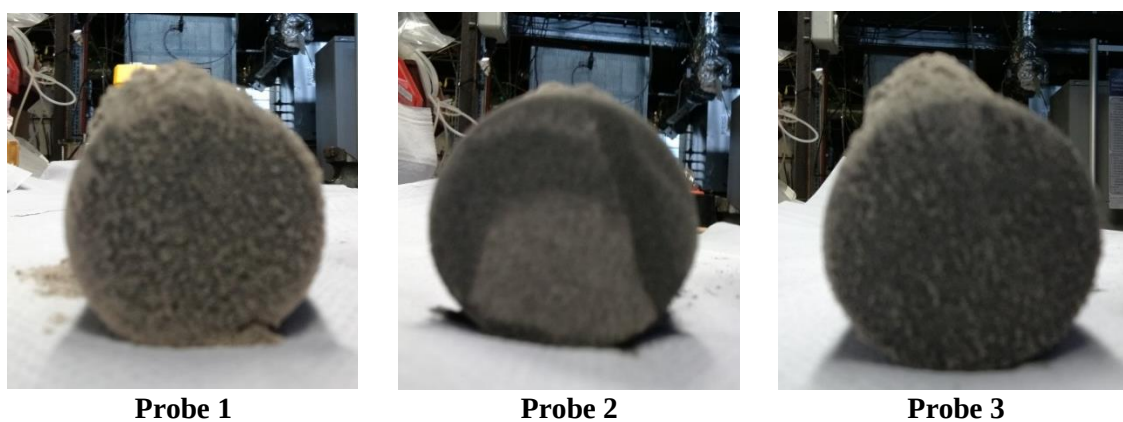


Figure 6-41: Deposit shape on probes 1, 2 and 3 ($\sim 500^\circ\text{C}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration ($d_t = 39\text{ mm}$).

Deposits were collected from different sides of the probes and their weights are given in Table 6-7, which were used to calculate the deposition fluxes in Table 6-8 and Figure 6-42.

Table 6-7: Deposit weights from probes ($\sim 500^\circ\text{C}$) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Side	Area [cm^2]	Deposit weight [g]		
		Probe 1	Probe 2	Probe 3
Upstream	30.5	1.26	1.74	1.99
Left side	11.59	0.09	0.21	0.09
Right side	11.59	0.40	0.43	0.47
Downstream	21.02	0.13	0.21	0.08
Total	74.70	1.89	2.59	2.64

Table 6-8: Deposition fluxes on probes 1, 2 and 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Side	Deposition flux [mg/(cm ² hr)]		
	Probe 1	Probe 2	Probe 3
Upstream	8.27	11.40	13.07
Side (Left + Right)	4.26	5.54	4.84
Downstream	1.29	2.03	0.81
Total	5.06	6.94	7.06

In this case, the deposition fluxes showed a different trend compared to the previous tests. First of all, the values of deposition flux were slightly higher and this may be due to a more regular combustion which did not require any stops for blockages in the fuel feeding system. Moreover, a comparison with the previous two experiments shows that the deposition fluxes on probe 1 were lower than the other probes. This may be because of its position, which is still leading but further from the chamber wall and, as a consequence, less subject to particles' rebound from the wall. This implies that big particles were more likely to rebound from the top of probe 1 and hit probes 2 and 3 resulting in a lower deposition flux on probe 1. Another possible explanation is that deposit was lost from the top of this probe inside the combustor.

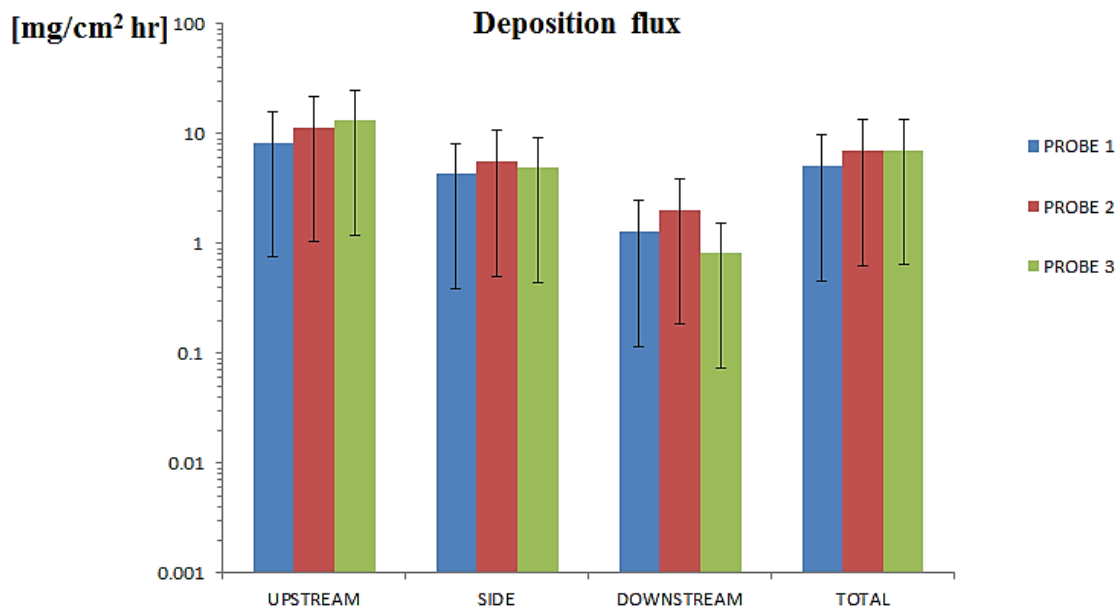


Figure 6-42: Deposition fluxes on different sides of probes (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Examples of SEM images taken from the different sides of each probes are given in Figure 6-43, Figure 6-44 and Figure 6-45. Bigger particles were found on the upstream surface for all the probes and smaller particles on the sides and downstream. However, for probe 1 it can be noticed that bigger particles were on the back and on the sides which can be due to their rebound from the top of probes 2 and 3. Some bigger particles were also found on the left and right sides of probes 2 and 3 because of the rebound of particles from the adjacent probes.

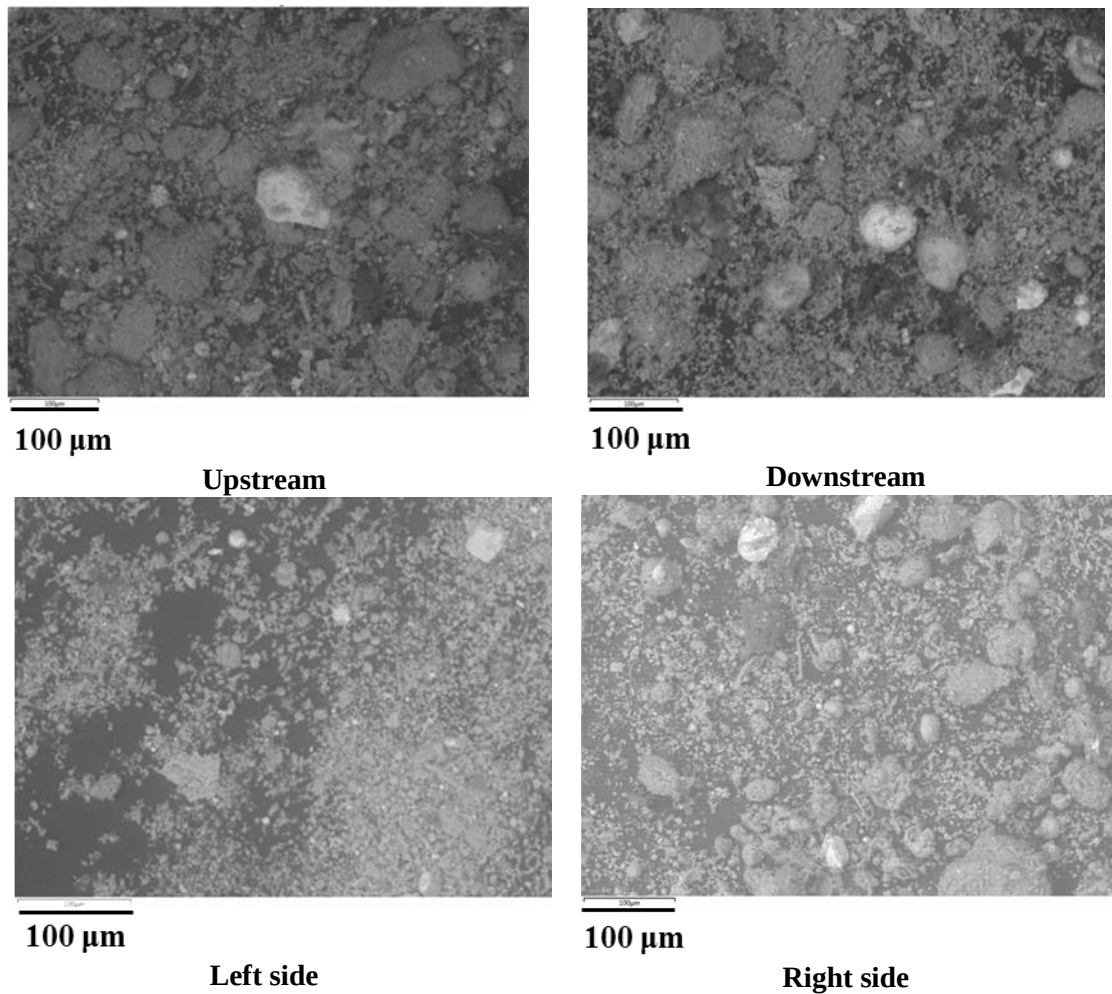
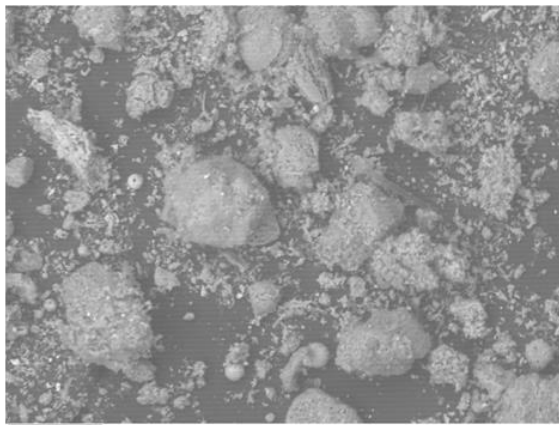
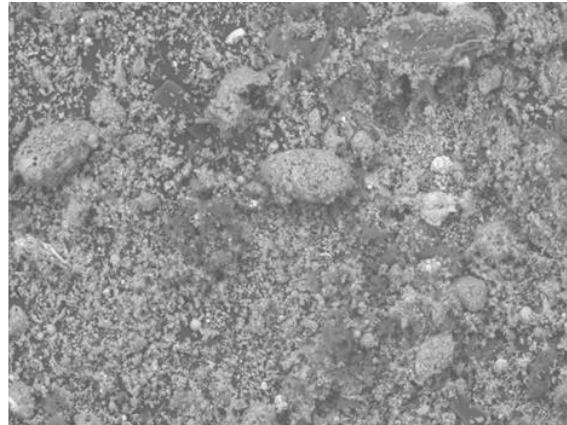


Figure 6-43: SEM images of deposit formed on different sides of probe 1 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.



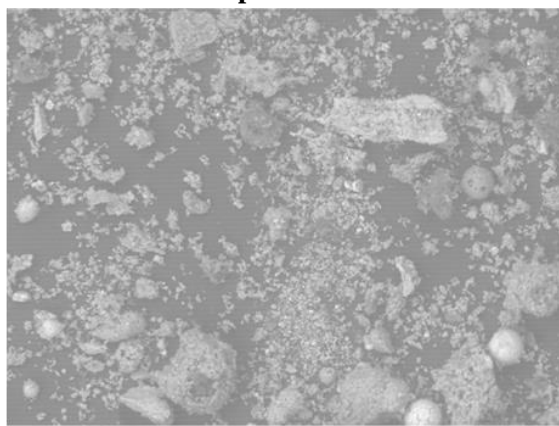
100 μm

Upstream



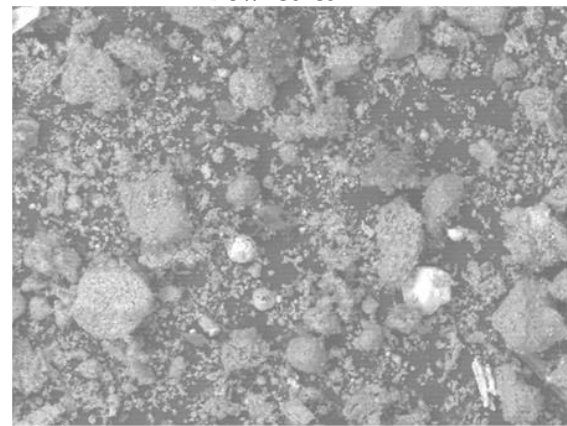
100 μm

Downstream



100 μm

Left side



100 μm

Right side

Figure 6-44: SEM images of deposit formed on different sides of probe 2 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

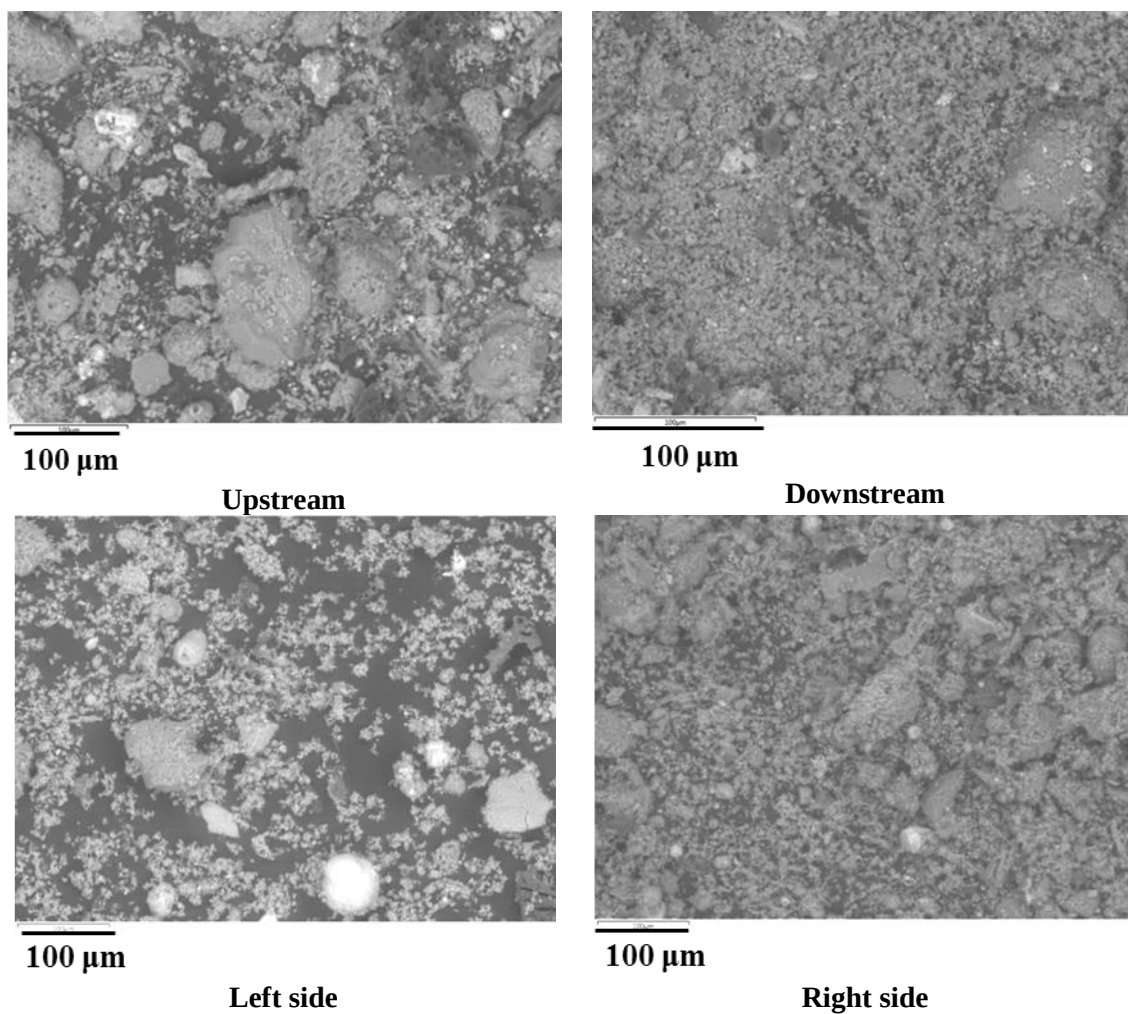


Figure 6-45: SEM images of deposit formed on different sides of probe 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

The chemical compositions for the deposits on probes 1, 2 and 3 were calculated as explained in section 5.8 and are shown in Figure 6-46, Figure 6-47 and Figure 6-48.

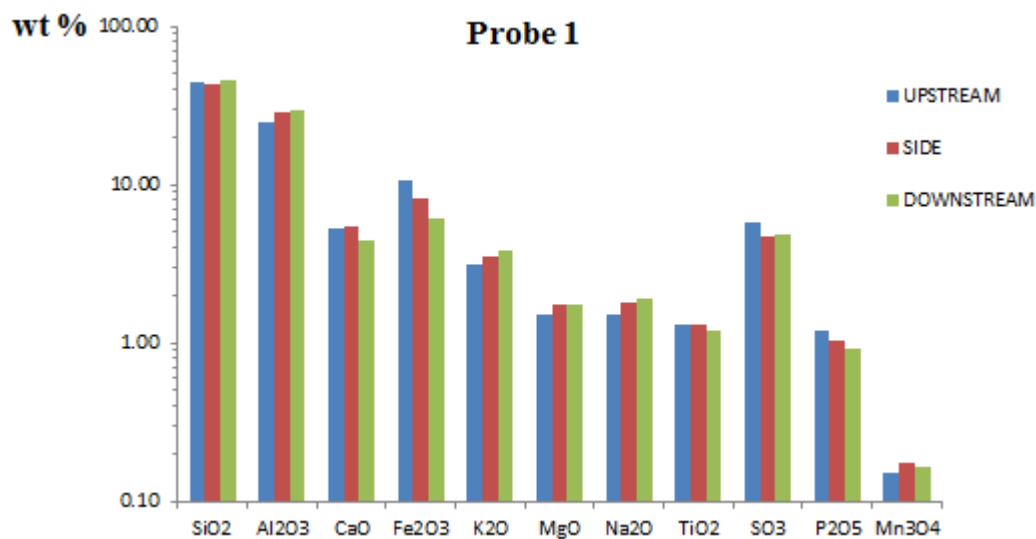


Figure 6-46: Deposit chemical composition on probe 1 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration (in terms of highest oxides of elements).

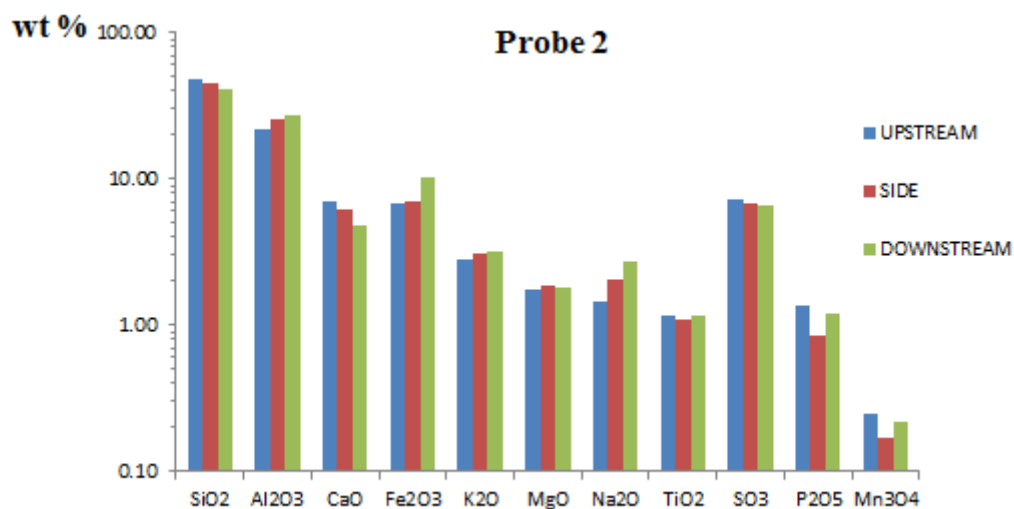


Figure 6-47: Deposit chemical composition on probe 2 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration (in terms of highest oxides of elements).

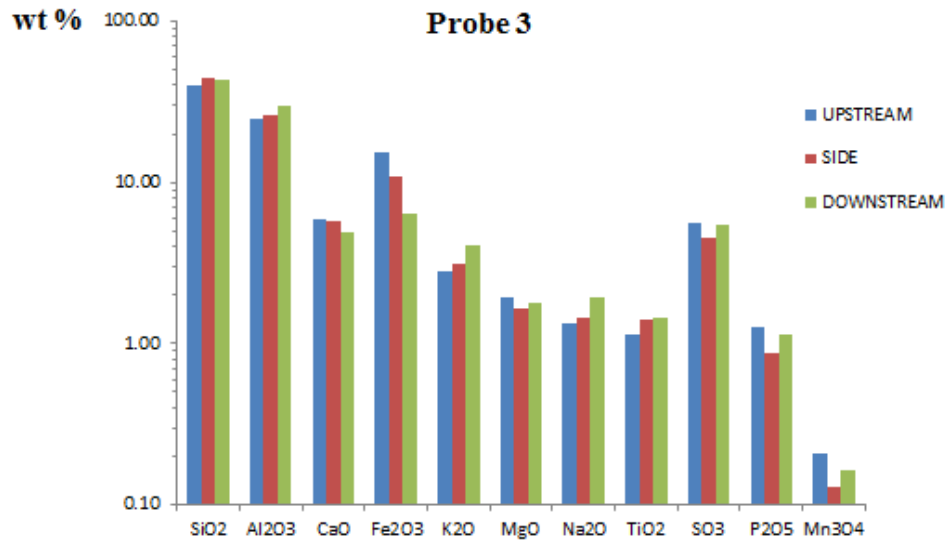


Figure 6-48: Deposit chemical composition on probe 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration (in terms of highest oxides of elements).

The main elements were identified and their oxide percentages were of the same order of magnitude as for the previous tests.

XRD analyses were carried out for the deposits collected from the upstream of probes 1, 2 and 3 and the results are given in Figure 6-49. The main species were identified and highlighted with different symbols: Quartz (SiO_2), Hematite (Fe_2O_3); Magnetite (Fe_3O_4), Anhydrite (CaSO_4) and Iron Sulphite (FeSO_4); no Alumina Silicate ($\text{SiO}_2 \cdot \text{Al}_2\text{O}_3$) was identified in this case.

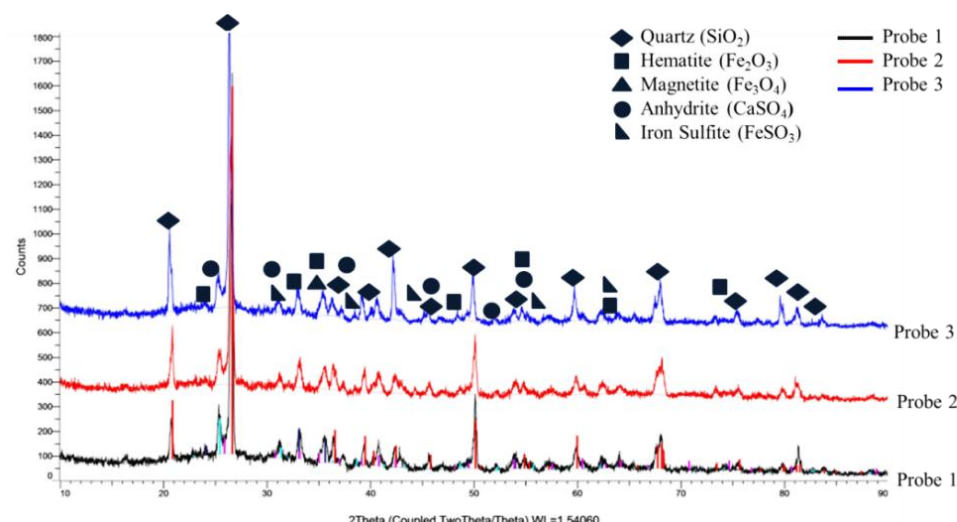


Figure 6-49: XRD analyses of deposits on the top of probes 1, 2 and 3 (~ 500°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Moreover, ash was collected from the ports where the three probes were placed, these were analysed with SEM/EDX and an average chemical composition was calculated in terms of highest oxides of elements (Figure 6-50). The result was similar to the deposits on the probes as shown in Figure 6-75.

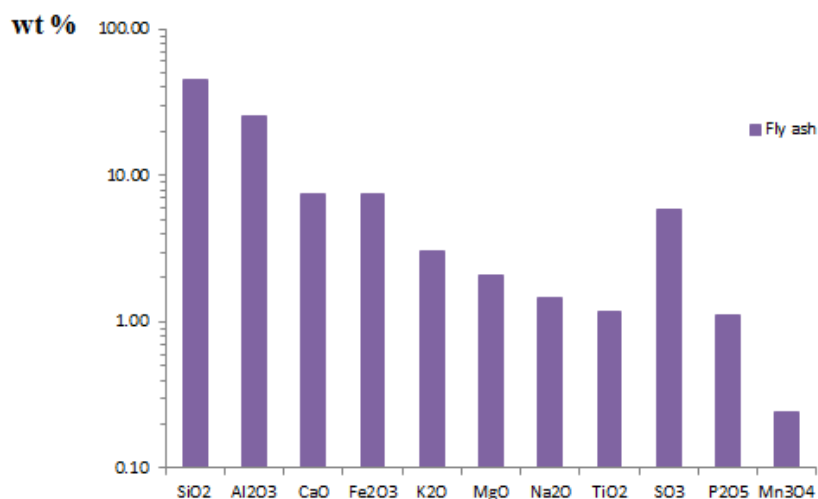


Figure 6-50: Average chemical composition from fly ash collected from the ports 1, 2 and 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration at ~ 500°C (in terms of highest oxides of elements).

These ash samples were also analysed (by Doosan Babcock) using a laser diffraction particle sizer to get the volumetric ash particle distribution whose values were illustrated for all the ports in Figure 6-51.

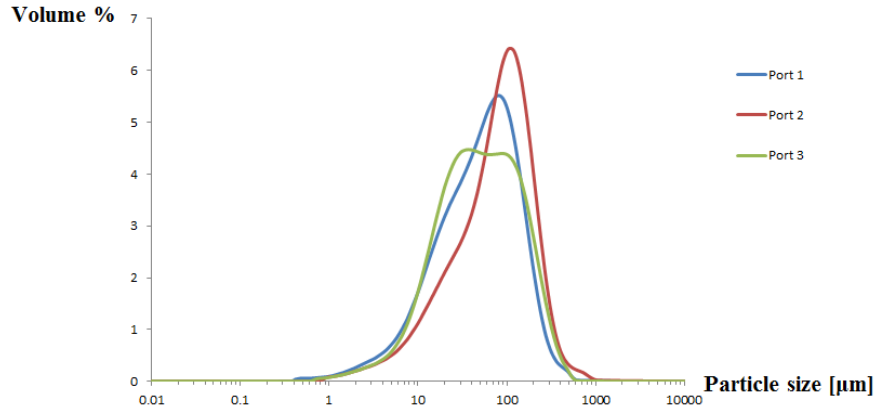


Figure 6-51: Volumetric ash particle size distribution for fly ash collected from the ports 1, 2 and 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

These percentages were used to fit the Rosin Rammler model and get the main parameters for the ash particle size distribution used in Fluent[®]. The main results are given in Figure 6-52, Figure 6-53, Figure 6-54 and summarised in Table 6-9.

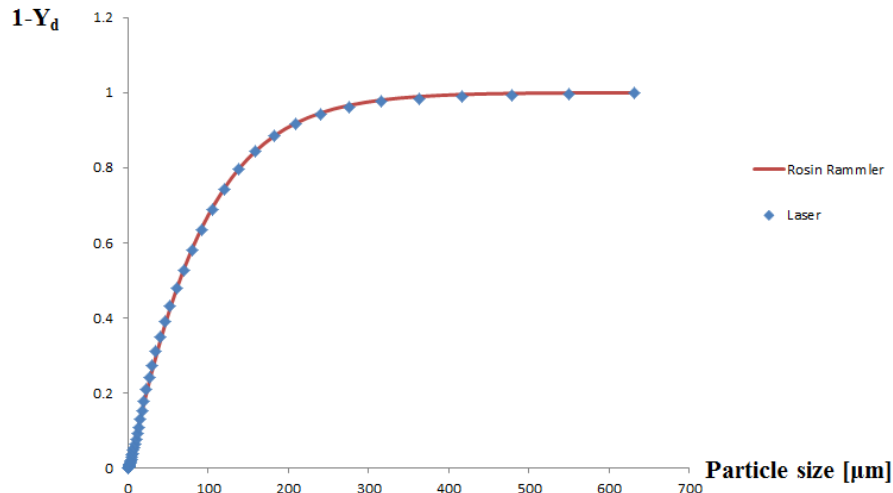


Figure 6-52: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 1 (test n°3): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

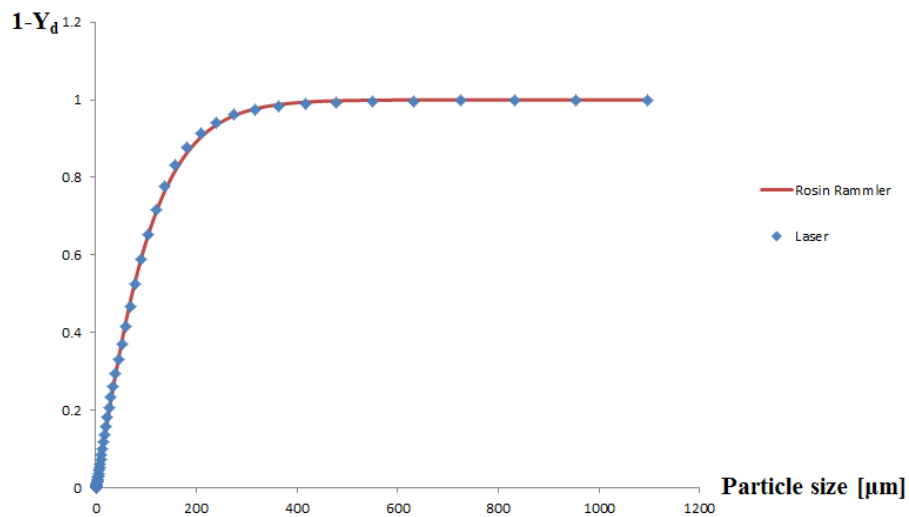


Figure 6-53: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 2 (test n°3): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

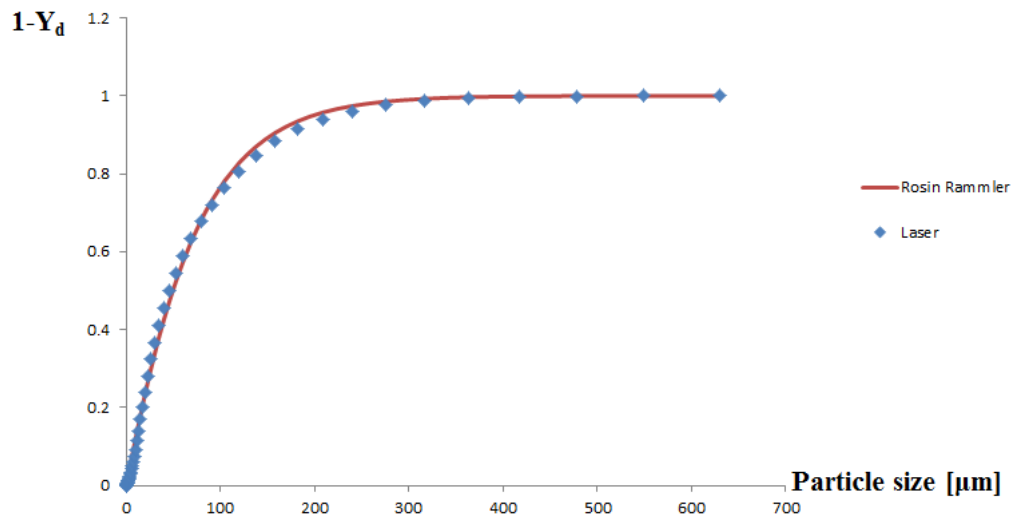


Figure 6-54: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 3 (test n°3): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

Table 6-9: Main Rosin Rammler parameters obtained from the fitting between the experimental results and the model after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Port	$d_{min}[\mu\text{m}]$	$d_{max}[\mu\text{m}]$	$d_{mean}[\mu\text{m}]$	n
1	0.363	639.96	68.10	1.09
2	0.724	1096.48	99.24	1.14
3	0.55	630.96	70.18	1.05

The ash particle size distribution included very small particles ($<1 \mu\text{m}$) and bigger particle ($>> 10 \mu\text{m}$) which justifies their tendency to deposit around the probes according to the different deposition mechanisms as explained in section 2.7 and from the previous experiments.

During the tests, the temperature of the probes was kept almost constant (~ 500 and 600°C) by adjusting the compressed air-cooling flow rate. In Figure 5-23 it was shown that two thermocouples, placed on the metal rings (i.e. front and back), were used to control the ceramic probe temperature which tended to increase during combustion. The temperature profile of the probes is reported only for this experiment (Figure 6-55); however, the same approach was applied during all the others. The air flow rate values used in this test are given in Figure 6-56 which shows that, in order to keep the probes at $\sim 500^\circ\text{C}$, the air flow rate needed to be increased in particular for probe 1, followed by probes 2 and 3.

Probe 1 needed the highest air flow rate to cool it to the target temperature. This could be due to its leading position, which implied that the probe was exposed to a higher gas temperature (and more radiation), but also to the presence of a thinner deposit, compared to probes 2 and 3. This increased the heat transfer through the deposit and towards the probe surface; therefore more air flow was needed to keep the surface temperature constant. Probes 2 and 3 showed higher deposition fluxes and, as a consequence, thicker deposits, which could exert more heat transfer resistance between the hot flue gas and the cooling air. However, this is only one possible explanation since the temperature of the probes were not significantly different ($500^\circ\text{C} \pm 19\%$).

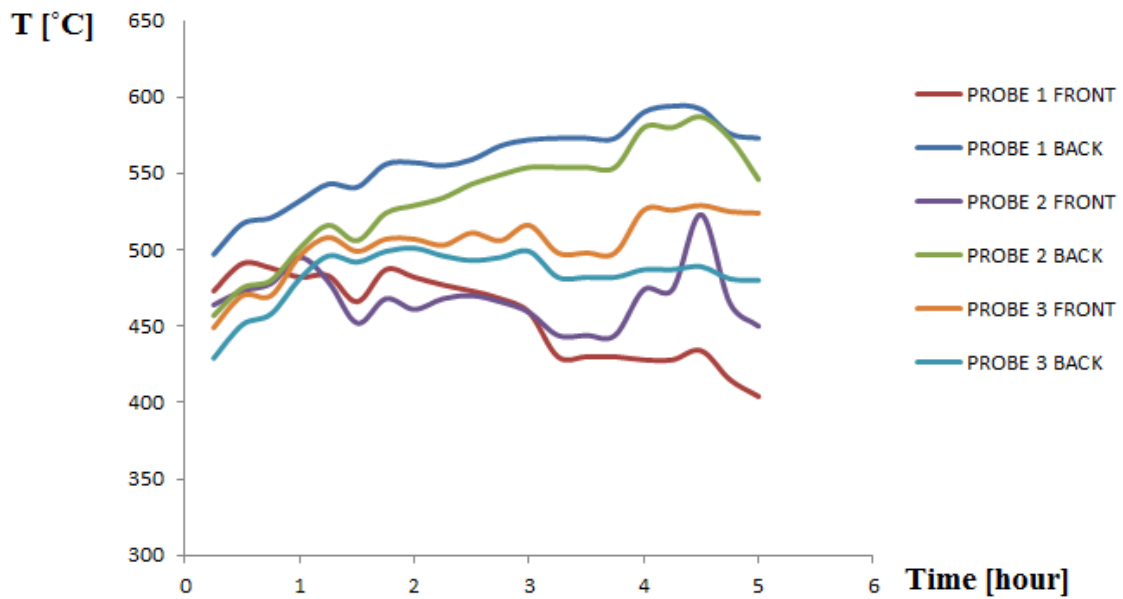


Figure 6-55: Probes' temperature (~ 500 °C) during the experiment with Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

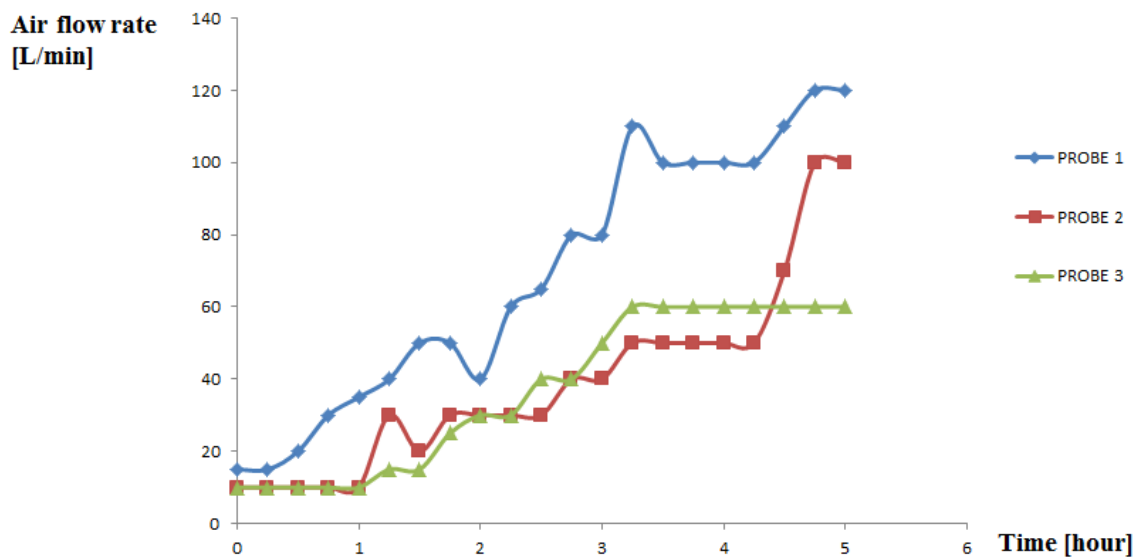


Figure 6-56: Air flow rate used during the experiment with Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration to keep the probes' temperature ~ 500 °C.

6.3.4 Test n°4

The last test was run in the same conditions as test n°3 but increased the probes' temperature up to 600 °C. The deposits were quite powdery and sand colour, thicker on

the top with a maximum thickness of ~ 1.1 cm, 0.8 cm and 1 cm on probes 1, 2 and 3 respectively (Figure 6-57, Figure 6-58 and Figure 6-59). Moreover, the downstream surface of these probes was less sticky and this may be due to the higher surface temperature which reduced the vapour condensation. An example of downstream surface after the experiment is given in Figure 6-60.



Left side



Right side

Figure 6-57: Deposit formed on probe 1 ($\sim 600^\circ\text{C}$, $d_t = 39$ mm) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.



Left side



Right side

Figure 6-58: Deposit formed on probe 2 ($\sim 600^\circ\text{C}$, $d_t = 39$ mm) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.



Left side



Right side

Figure 6-59: Deposit formed on probe 3 ($\sim 600^\circ\text{C}$, $d_t = 39$ mm) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.



Figure 6-60: Downstream of the ceramic probe n°3 (~ 600°C, d_t = 39 mm) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

At the end of this test, quite a lot of deposit was lost from the probe 2 and this affected the deposition flux calculations, summarised in Table 6-10, Table 6-11 and in Figure 6-61.

Table 6-10: Deposit weights from probes (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Side	Area [cm ²]	Deposit weight [g]		
		Probe 1	Probe 2*	Probe 3
Upstream	30.5	2.08	1.34	1.74
Left side	11.59	0.03	0.07	0.05
Right side	11.59	0.23	0.02	0.08
Downstream	21.02	0.14	0.03	0.001
Total	74.70	2.49	1.46	1.87

*Deposit loss during handling.

Table 6-11: Deposition fluxes on probes 1, 2 and 3 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Side	Deposition flux [mg/(cm ² hr)]		
	Probe 1	Probe 2*	Probe 3
Upstream	13.63	8.78	11.40
Side (Left + Right)	2.32	0.83	1.17
Downstream	1.38	0.29	0.01
Total	6.67	3.92	5.02

*Deposit loss during handling.

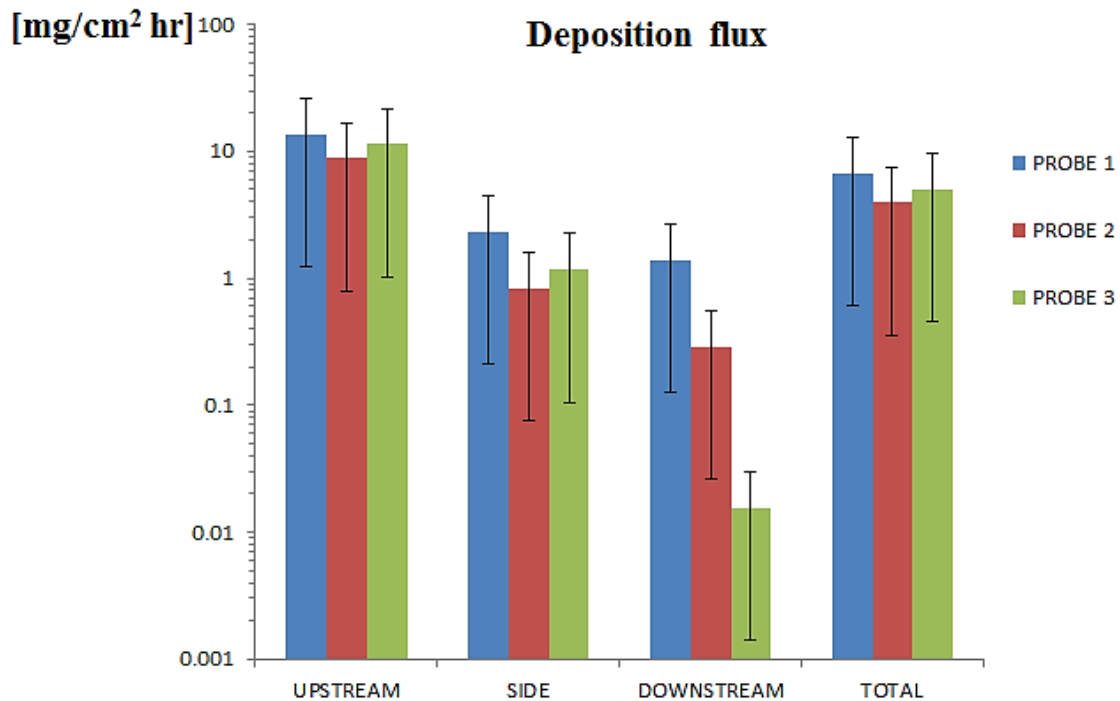


Figure 6-61: Deposition fluxes on different sides of probes (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

The SEM analysis results are summarised for all the probes in Figure 6-62, Figure 6-63 and Figure 6-64 which confirmed the same trends in behaviour observed in the previous experiments.

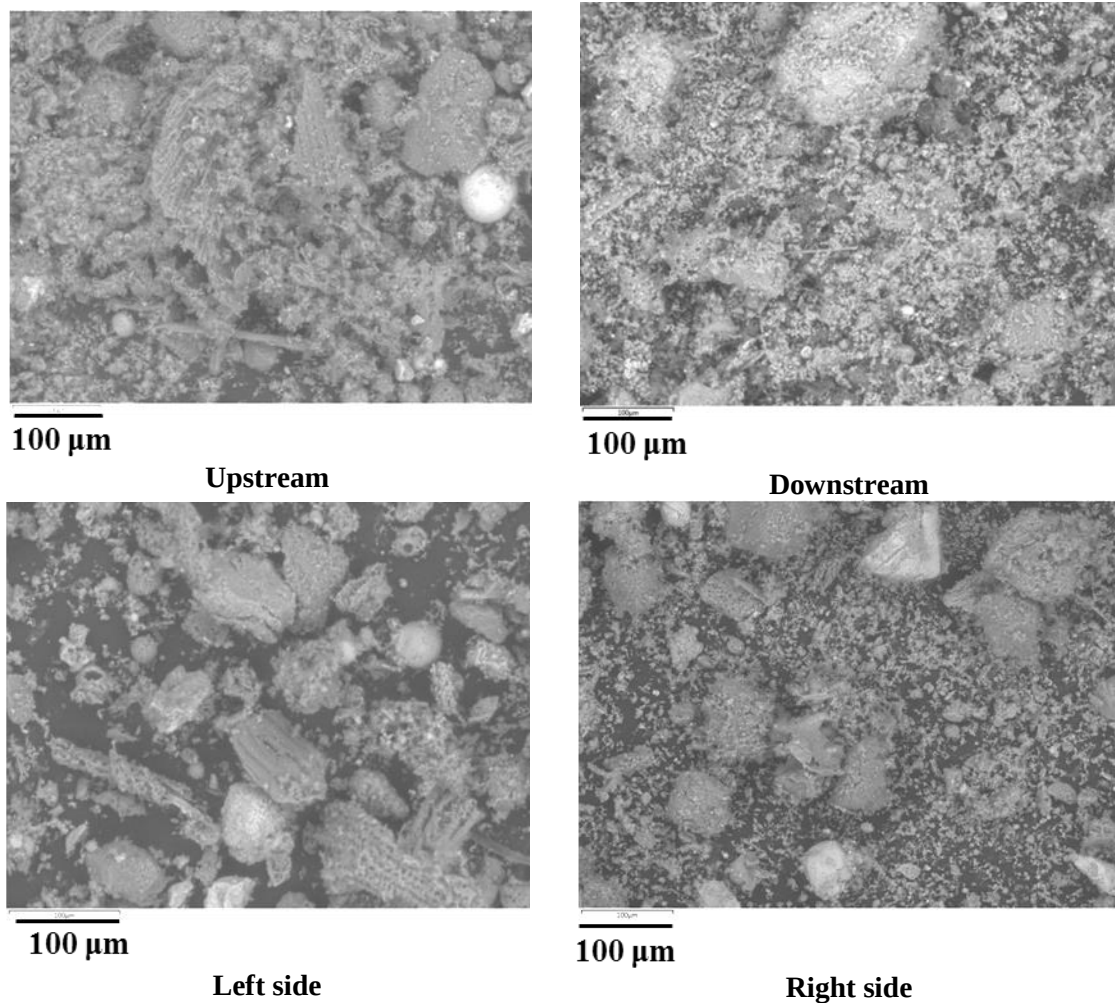


Figure 6-62: SEM images of deposit formed on different sides of probe 1 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

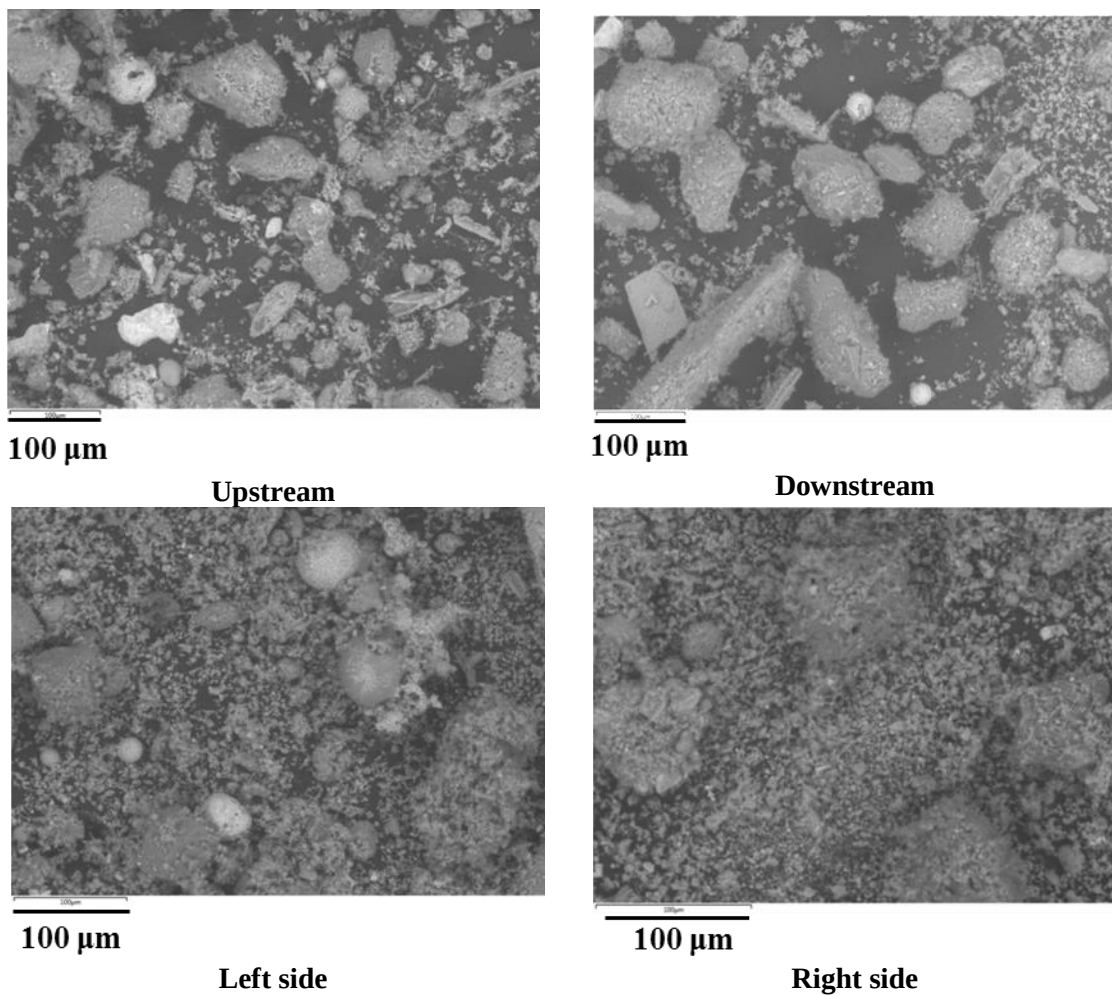


Figure 6-63: SEM images of deposit formed on different sides of probe 2 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

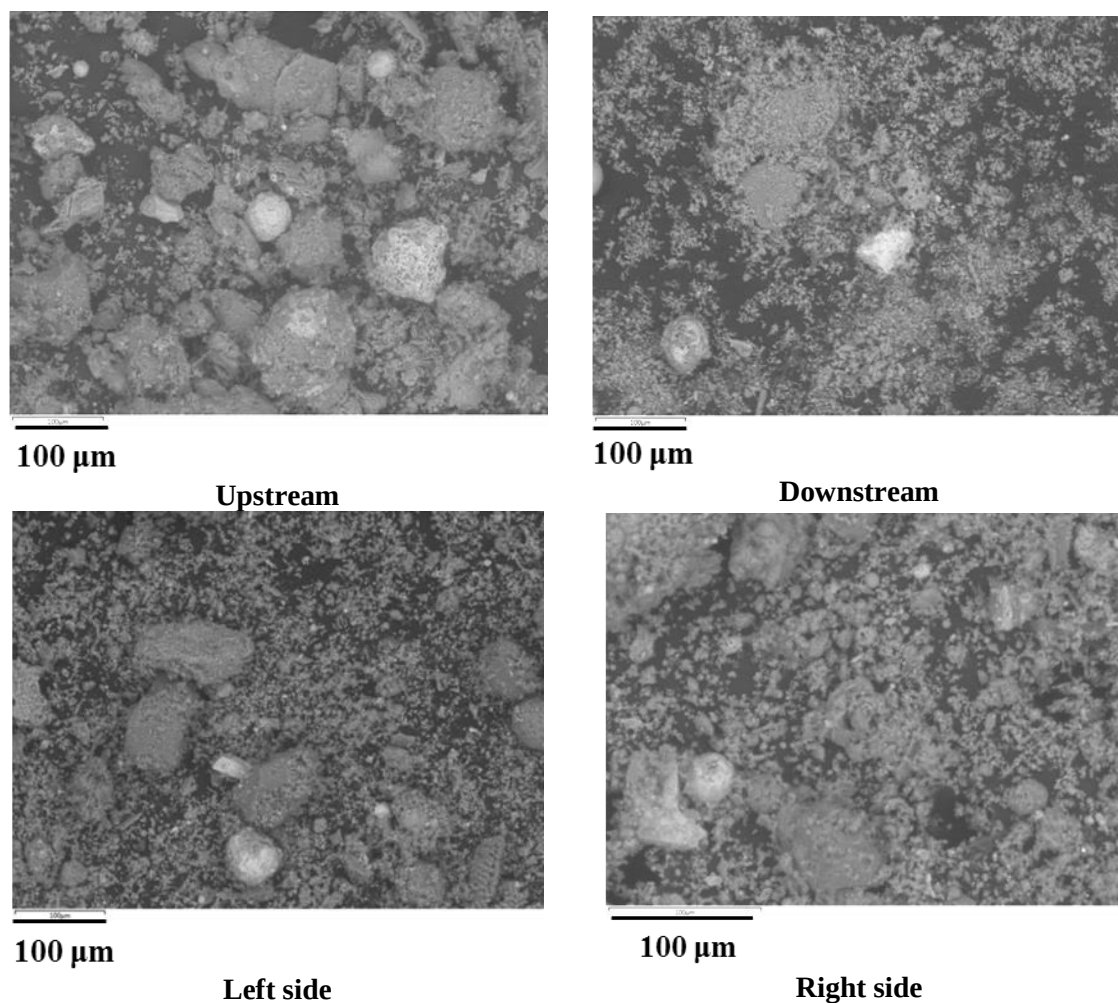


Figure 6-64: SEM images of deposit formed on different sides of probe 3 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

The EDX analysis allowed the calculation of the deposit chemical composition, and the main species are given in Figure 6-65, Figure 6-66 and Figure 6-67.

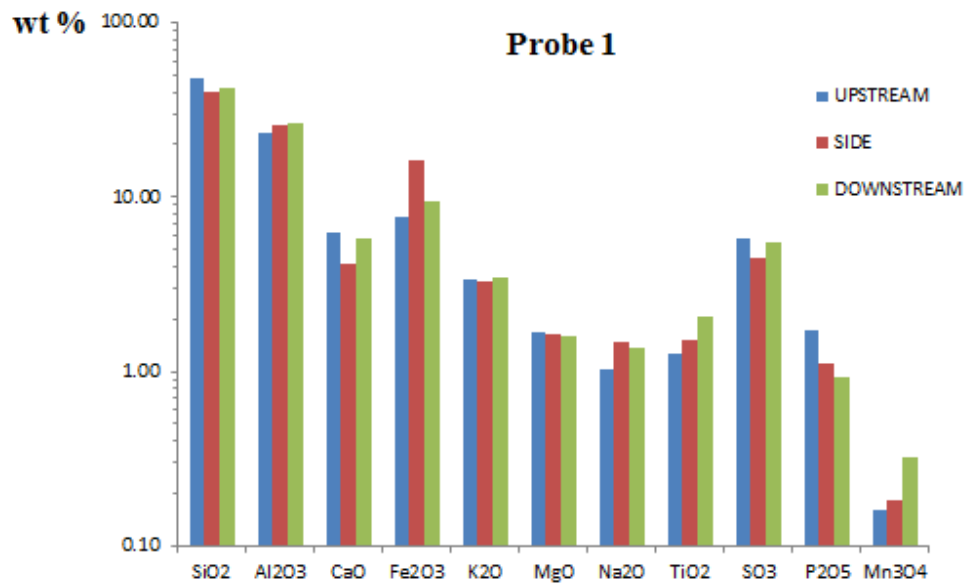


Figure 6-65: Deposit chemical composition on probe 1 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration (in terms of highest oxides of elements).

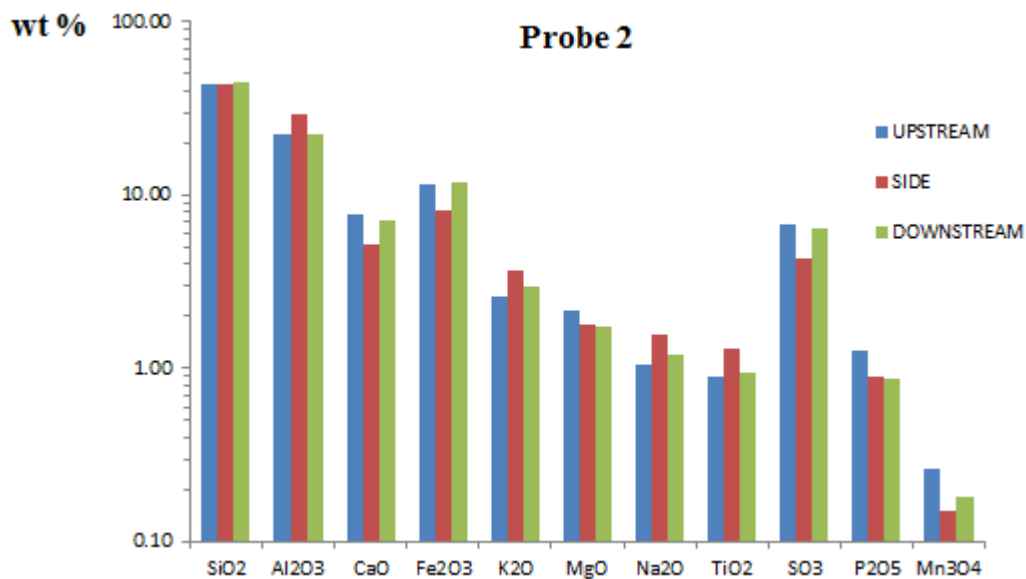


Figure 6-66: Deposit chemical composition on probe 2 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration (in terms of highest oxides of elements).

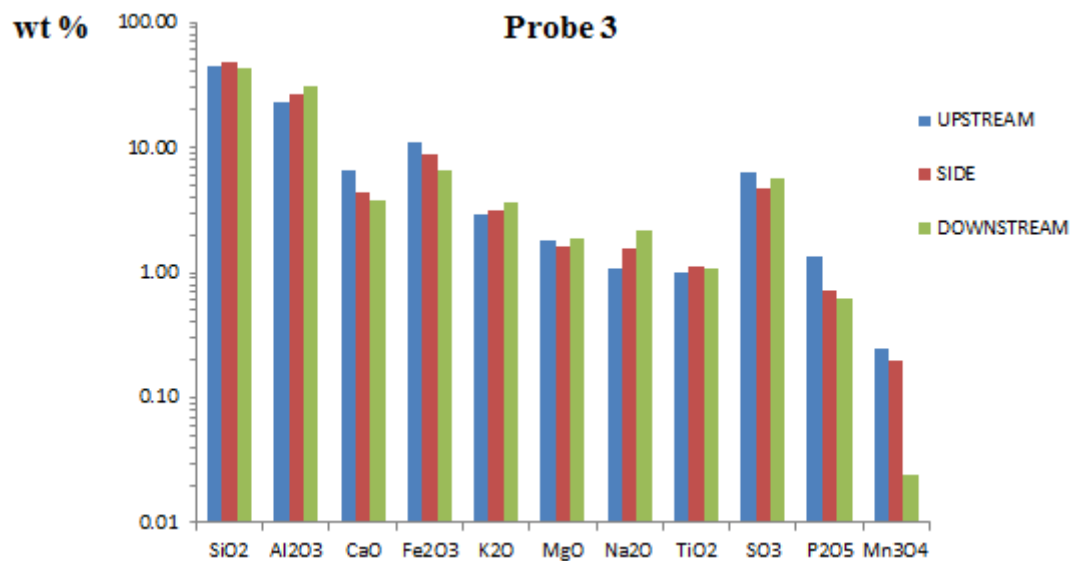


Figure 6-67: Deposit chemical composition on probe 3 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration (in terms of highest oxides of elements).

Moreover, the XRD analysis for the deposit formed on the upstream surfaces of each probe is in Figure 6-68; and the main species were Quartz (SiO_2), Hematite (Fe_2O_3), Magnetite (Fe_3O_4), Anhydrite (CaSO_4), Iron Sulphite (FeSO_4). Iron Silicate ($\text{Fe}_2\cdot\text{SiO}_4$) and Millosevichite ($\text{Al}_2(\text{SO}_4)_3$) were also identified.

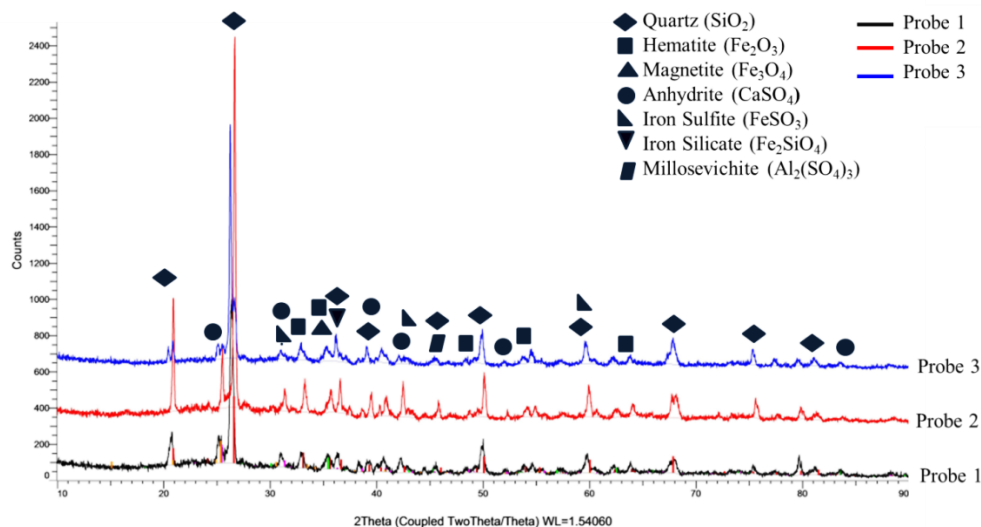


Figure 6-68: XRD analyses of the deposits on the top of probes 1, 2 and 3 (~ 600°C) after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

In addition, as for the other tests, ash from the ports was collected and analysed to get the ash chemical composition whose average was plotted in Figure 6-69.



Figure 6-69: Average chemical composition from fly ash collected from the ports 1, 2 and 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration at ~ 600°C (in terms of highest oxides of elements).

The ash particle size distribution results provided by Doosan Babcock were overlapped for the three ports as in Figure 6-70.

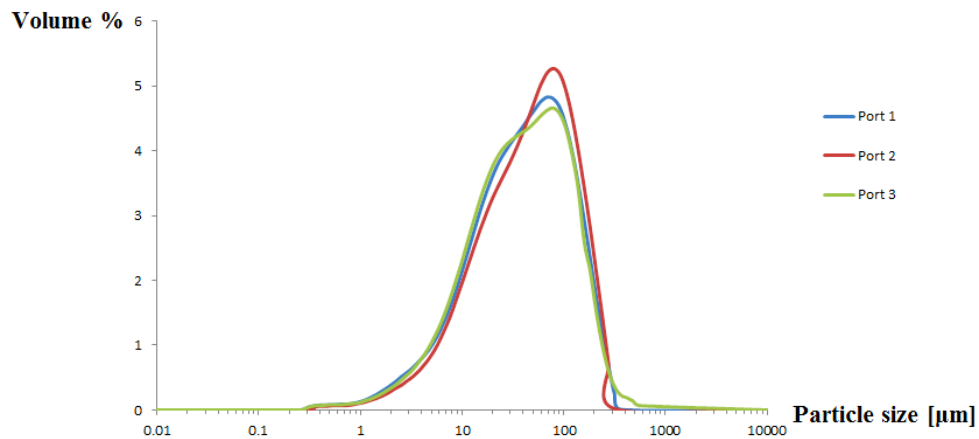


Figure 6-70: Volumetric ash particle size distribution for fly ash collected from the ports 1, 2 and 3 after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

These results were fit to the Rosin Rammler model as shown in Figure 6-71, Figure 6-72 and Figure 6-73 and the main parameters for the Rosin Rammler ash particle size distribution are given in Table 6-12.

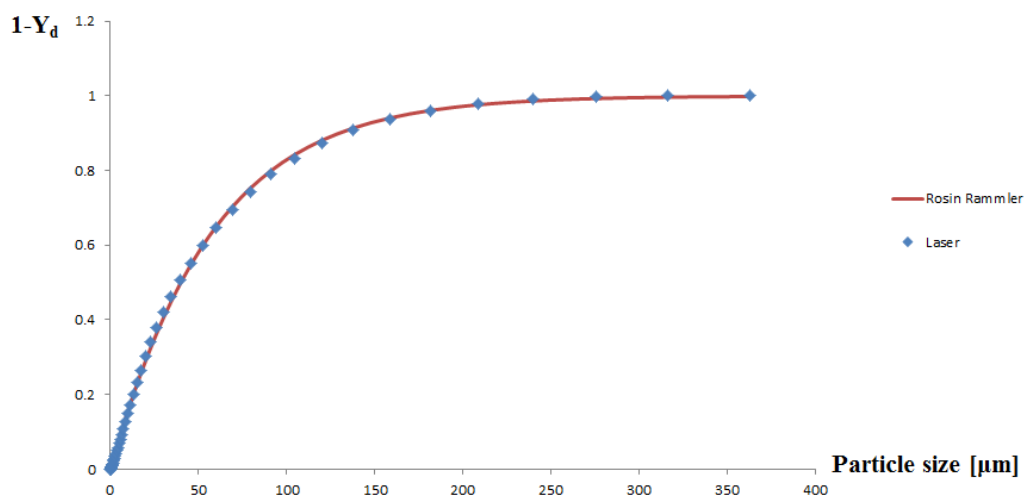


Figure 6-71: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 1 (test n°4): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

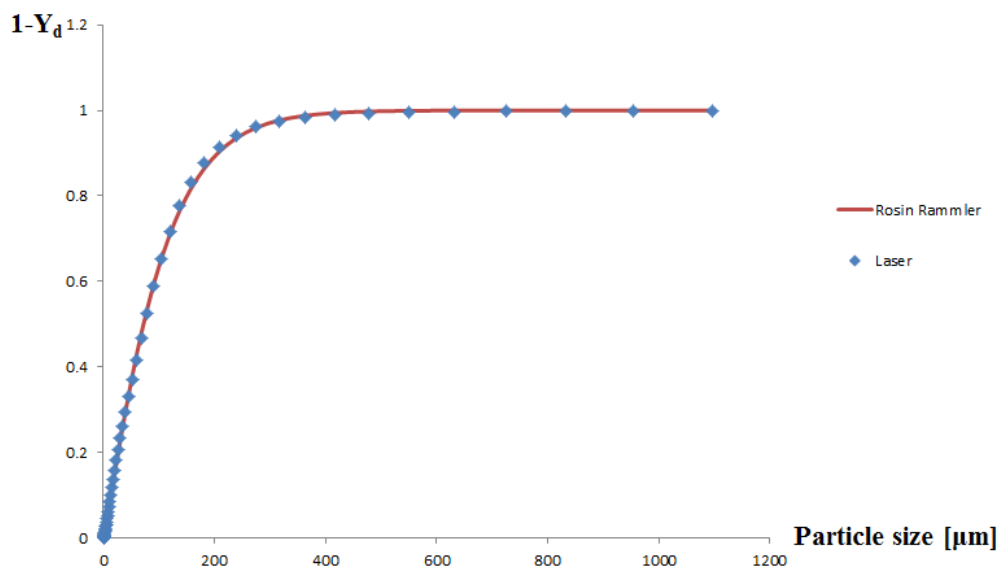


Figure 6-72: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 2 (test n°4): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

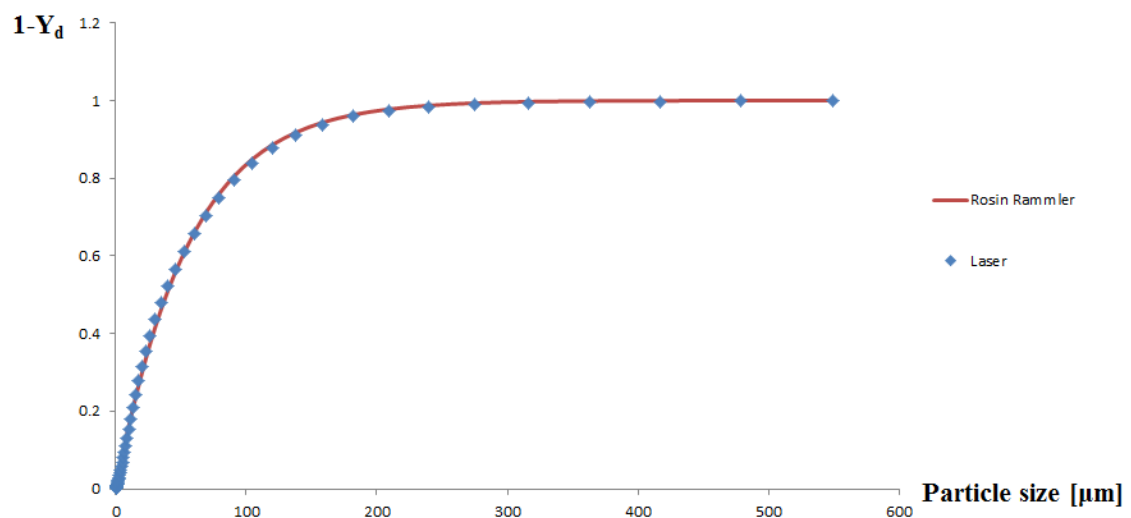


Figure 6-73: Cumulative volume fraction of ash particles ($1-Y_d$) collected from port 3 (test n°4): fitting of the Rosin Rammler model to the experimental data (analysed with a Laser Diffraction Malvern Mastersizer 2000).

Table 6-12: Main Rosin Rammler parameters obtained from the fitting between the experimental results and the model after 5 hours from combustion of Daw Mill-12 wt.% Miscanthus using the 2nd probes' configuration.

Port	d_{min} [μm]	d_{max} [μm]	d_{mean} [μm]	n
1	0.24	363.08	57.28	1.02
2	0.316	316.23	63.87	1.06
3	0.24	549.54	55.69	1.01

The ash particle size distribution obtained from this test confirmed what already found from the previous experiments.

6.4 Experimental uncertainty

In the previous paragraphs (6.3.1-6.3.4), deposition flux calculations have been carried out measuring the deposit weights around different sides of the probes, the exposure time and the area. The experiments were run in the same experimental rig with the same fuel and operating conditions. Some parameters were varied (probe location and temperature, exposure time); however, the depositon flux measurements had the same order of magnitude (Figure 6-10, Figure 6-21, Figure 6-42 and Figure 6-61). This means that the aforementioned parameters did not have a significant impact on the deposition mechanisms and that the error trend was almost constant. Some possible reasons of errors and uncertainty have been identified as follows:

- 1) Deposit loss inside the combustor and/or during the probe extraction and collection (especially if the deposit was powdery).
- 2) Deposit collection technique: a brush was used to collect deposit ash from the different sides of the probe. This method is not rigorous but it represented the best available way to carry the work out.
- 3) Deposit thickness measurements: a ruler was used to estimate the deposit thickness. However, it was not constant along the probe and it was difficult to measure.

All these factors may have influenced the measurements and the calculations of deposit thickness and deposition flux. Therefore, a minimum (0.05 cm) and a maximum (1.1 cm) thickness were identified and used to calculate the experimental error (as in Figure 6-10, Figure 6-21, Figure 6-42 and Figure 6-61).

6.5 Supporting ash analysis

In this section, some of the ash analysis results have been summarised and compared with available data from the literature. For example, Chapter 5, Table 5-1 indicated the ash content and the ash chemical composition of single fuels (Daw Mill and Miscanthus) and their blend calculated using data from the literature (BCURA, 2018; Phyllis, 2018b, 2018a). Section 5.4.1 illustrated the ash content tests that were carried out at Cranfield using two horizontal furnaces to measure the percentage of ash in the fuel blend. These samples were analysed with SEM/EDX and their chemical compositions calculated, averaged and compared with the one provided in the literature. The experimental results were comparable for almost all the species, except for K_2O and P_2O_5 whose experimental values were higher (Figure 6-74).

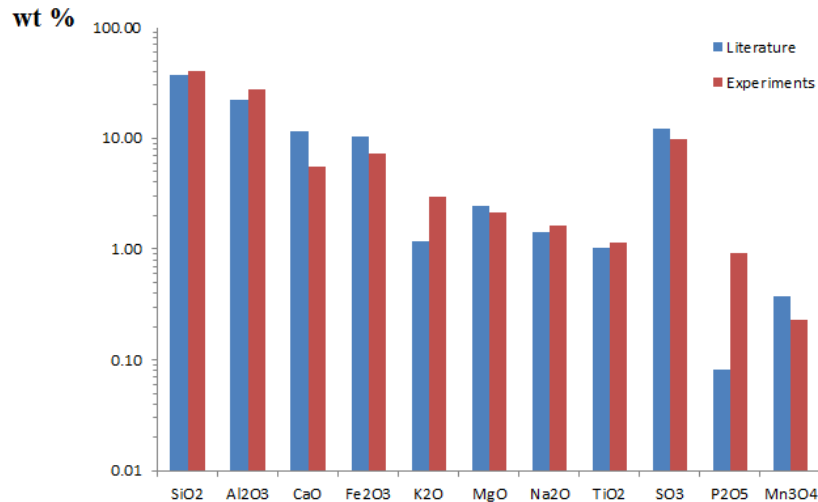


Figure 6-74: Fuel ash chemical composition obtained from the literature (BCURA, 2018; Phyllis, 2018b, 2018a) and the average value from the ash analysis tests in the horizontal furnaces at Cranfield.

In Figure 6-75, a comparison of the chemical composition for the probe deposits in all the experiments, the fly ash from the ports, the ashed fuel from the literature and the ash tests in the horizontal furnaces was illustrated. In particular, for the deposit formed on the different zones of the probes (upstream, sides and downstream), an average value was calculated in order to reduce the amount of data and make Figure 6-75 clearer.

The graph shows that the results from the experimental activity (deposition tests and ash content tests), obtained using the same methodology (section 5.8), were very similar while the ashed fuel chemical composition found in the databases was slightly different. However, this latter does not represent the real ash composition and it demonstrates that the ash analysis, for the same fuel, can vary significantly according to the part of the fuel that is used, its storage conditions etc. Moreover, the discrepancy in the ashed fuel composition from the databases can be attributed to the technique used for ash analysis (e.g. wet chemistry) which was different from the one applied in this work. Finally, the comparison demonstrated that deposition and accumulation on ceramic probes did not alter significantly the chemical composition of fly ash released during combustion.

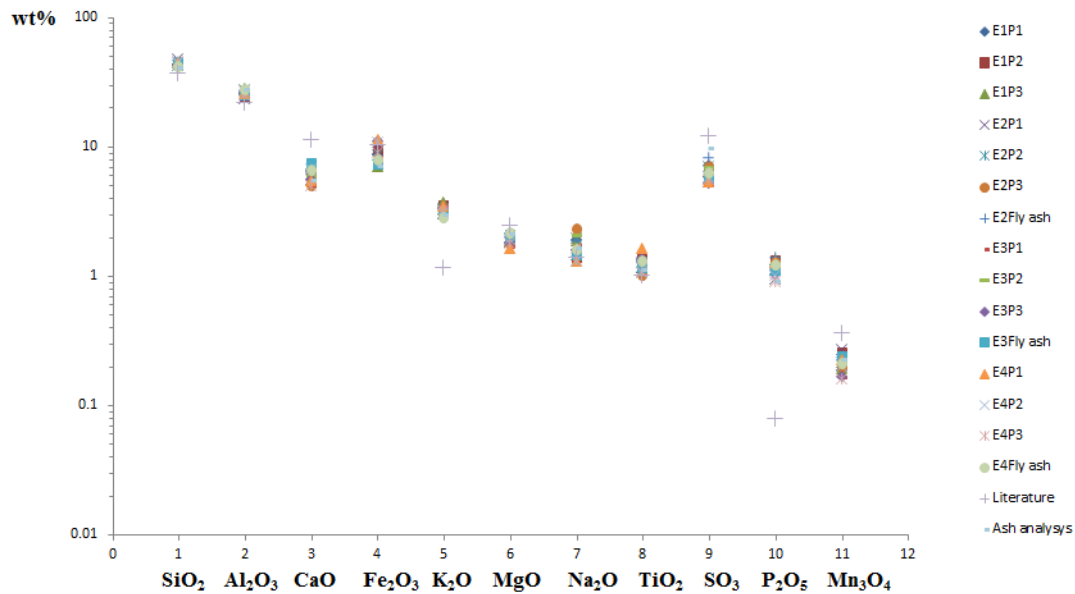


Figure 6-75: Comparison of the ash chemical composition from deposits on all the probes, fly ash from the ports, fuel ash composition found in the literature and obtained from the ash analyses at Cranfield. Abbreviations: E= experiment, P= probe (e.g. E1P1= experiment 1 probe 1).

Finally, an average of the Rosin Rammler parameters was calculated and is given in Table 6-13 that included the results obtained in the previous experimental sections (sections 6.3.1-6.3.4) and these values were used in the model validation (Chapter 7) for all the simulations. Only two series of data, with $d_{max} > 1000 \mu m$, were neglected as

considered out of the range of interest (particles with $d_p > 100 \mu\text{m}$ are already too big to deposit).

Table 6-13: Average of the Rosin Rammler parameters obtained from the fitting between the experimental results and the model after 5 hours from combustion of Daw Mill-12 wt.%Miscanthus.

$d_{min}[\mu\text{m}]$	$d_{max}[\mu\text{m}]$	$d_{mean}[\mu\text{m}]$	n
0.43	535	68	1.07

6.6 Summary of key findings

This chapter has provided an overview of the main experimental results obtained during combustion of pulverised Daw Mill-12wt.% Miscanthus in the combustion rig at Cranfield University. The experiments were all run in the same conditions, changing the test duration (2.5 and 5 hours), the probe configuration (1st and 2nd in Figure 6-1 varying the position of probe 1) and their temperatures (~ 500 and 600°C). These values were not supposed to influence the gas composition, therefore, only one example of the gas components was included (in section 6.2) and the major and minor species were identified. In particular, during the tests, the fuel feed rate was adjusted to keep an oxygen concentration $\sim 4\%_{\text{vol}}$.

The results were coherent with the literature and they showed that deposits were thicker and more powdery on the upstream surfaces than on the sides and downstream surfaces of the probes, where they were tackier and consisted in a very thin layer of deposit probably because of initial alkali vapour condensation. However, the deposition flux values were very similar in all the experimental tests, some differences were noticed but it was difficult to find a correlation between the deposition flux, the probe configurations and temperature because of the deposit loss and the measurement error that may have affected the results.

The deposits were analysed with SEM/EDX to capture images and to calculate the chemical compositions in terms of weight % of the highest oxides (SiO_2 , Al_2O_3 , CaO , Fe_2O_3 , K_2O , MgO , Na_2O , TiO_2 , SO_3 , P_2O_5 , SO_3 , P_2O_5 , Mn_3O_4). For one of the tests (test

n°2), SEM images were also used to evaluate the type of particles that deposited around the probes, according to their diameters, using the software Image J. The results showed that bigger particles deposited on the top of probes, while smaller and medium particles were located on the sides and rear side of probes. However, bigger particles were also found in the deposits on the sides of leading probes because of the rebounding effect in the presence of multiple tubes in the chamber.

Moreover, the compositions of the fly ash and deposits were compared with data previously found in some databases and obtained during the ash analysis tests conducted at Cranfield using the horizontal furnaces. They were all comparable except for the data found in the databases which were slightly different from the real ash composition. The consistency of the experimental results highlights that the chemical composition of fly ash released during combustion did not vary after deposition. For some of the samples, XRD analysis was carried out in order to identify the main phases (Quartz (SiO_2), Hematite (Fe_2O_3), Magnetite (Fe_3O_4), Anhydrite (CaSO_4), Aluminium Oxide Silicate ($\text{SiO}_2 \cdot \text{Al}_2\text{O}_3$)).

Ash samples were collected from the ports where the air-cooled probes were placed and assumed to behave as the fly ash that caused particle deposition. These samples were analysed with SEM/EDX and with a laser diffraction technique to get the ash particle size distributions using the Rosin Rammler model. This information was to be used for the model validation (Chapter 7); in fact it was important to know which type of particles were in the CFD domain in order to predict their tendency to deposit, as the deposition mechanisms are highly dependent on the particle diameters.

This modelling approach has helped improve the understanding of flue gas and particle behaviours that could not be directly observed during the combustion experiments. The experimental results and parameters illustrated in this Chapter have been used to develop a CFD based model for deposit formation on air-cooled ceramic probes in the combustion rig at Cranfield University (Chapter 7). Some of these data provided the model boundary conditions, while some others were used for its validation and they have been summarised as follows:

Model set-up and boundary conditions:

- Rig geometry (Figure 5-2)
- Probe configurations (Figure 5-21)
- Gas velocity and temperatures (2 m/s and 1273 K at inlet) (section 5.5)
- Probe temperature and material properties (mullite at 500, 600 and 700 °C)
- Fly ash particle size distribution ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $n=1.07$)
- Fly ash chemical composition (Table 6-14)

Table 6-14: Average chemical composition of fly ash collected from the ports after all the experiments of Daw Mill-12 wt.% Miscanthus combustion (in terms of highest oxides of elements).

Component	%wt _i
SiO ₂	42.57
Al ₂ O ₃	26.34
CaO	6.84
Fe ₂ O ₃	7.94
K ₂ O	3.08
MgO	2.09
Na ₂ O	1.65
TiO ₂	1.25
SO ₃	6.78
P ₂ O ₅	1.24
Mn ₃ O ₄	0.22

Model validation:

- Deposition flux results (Chapter 6)
- Deposit shape and thickness (Chapter 6)

7 MODEL VALIDATION

7.1 Introduction

This section describes improvements to the preliminary modelling results shown in Chapter 4. Existing models from the literature have been modified and combined to predict deposition on air-cooled ceramic probes during combustion of pulverised Daw Mill-12 wt.% Miscanthus in the pilot scale rig at Cranfield University. The methodology explained in Chapter 3 was applied to run all the simulations.

Some of the model boundary conditions and the information used for the refined model set up were obtained from the experimental results and operating conditions described in Chapter 6. Moreover, some of the experimental results were used to test the model and identify the main model limitations and areas of uncertainty.

Studying deposit formation on heat exchangers did not require the simulation of the entire combustion process. In fact, the definition of the area surrounding the ceramic probes (i.e. CFD domain) and the main inputs (i.e. flue gas, ash particles, etc.) were sufficient to develop a predictive model. This approach considerably reduced the computational costs.

The model took into account a variety of deposition mechanisms as well as the ash chemical composition and the vapour deposition effect. Moreover, a transient approach was enabled in order to include the effect of the deposit shape and temperature on the deposition processes.

In this Chapter, some of the results presented at the 12th ECCRIA - European Conference on Fuel and Energy Research and its Applications, Cardiff (September 2018) are reported.

7.2 Geometry and mesh

The geometries used for the model validation were obtained from the engineering drawings of the PF combustor at Cranfield University (as illustrated in Figure 5-2) with the same probe configurations adopted during the experiments (Figure 5-21). The real geometry was simplified to a 2D domain ($L = 2.45$ m; $H = 0.30$ m) with probe diameters

$d_t = 39$ mm and a 90° rotation anticlockwise (Figure 7-2 and Figure 7-4) and the bend ~ 0.5 m downstream from the probes being neglected (Figure 7-1) to reduce computational costs linked to the deposition flux calculations, the deposit shape and temperature predictions. In fact, it was demonstrated that the presence of the bend does not have a significant influence on the ash particle behaviour and deposition processes on the probes (section 7.7.1, Figure 7-24 and Figure 7-30). The results presented are for the straight configuration and more information about the simulations with the bend is in Appendix B (section B.2).

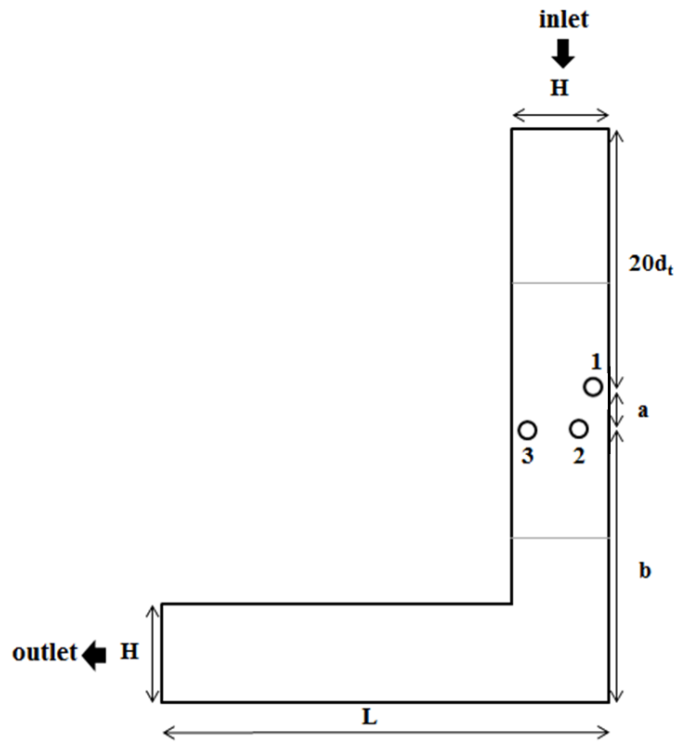


Figure 7-1: Example of geometry in the presence of the bend with the first probes' configuration ($L = 1407.527$ mm, $H = 305.054$ mm, $a = 113.538$ mm, $b = 837.22$ mm, $d_t = 39$ mm).

It is important to highlight that the expected vortex shedding has a 3D nature for Reynolds numbers > 200 and so the use of a 2D domain represents a simplification which could affect the particle behaviour in particular on the rear side of the tubes and, as a consequence, the deposit prediction results (Rahman *et al.*, 2008).

However, a 3D geometry would be very expensive computationally and a 2D domain allows the identification of the main areas where deposition takes place and represents a good starting point before further model improvements. In fact, this approach has already been widely used in the literature (e.g. Tomeczek and Waclawiak, 2009; Weber, Schaffe-Mancini, *et al.*, 2013; García Pérez *et al.*, 2014; Yang *et al.*, 2017) and it has been demonstrated to correctly identify the main areas where deposition takes place and to give a good prediction of the experimental results.

As in Chapter 4, the inlet was placed at $20d_t$ from the first tube and the outlet at $40d_t$ from the last tube to avoid the flow reflection (causing reversed flow) and to allow the vortex shedding to be developed enough (Dröge, 2007; Rahman *et al.*, 2007). Moreover, the boundary conditions were the same as in section 4.3.1 and in Figure 7-2 and Figure 7-4. Three vertical “interiors” (faces with fluid cells on both sides), which divide the domain in four blocks, were used to avoid the degeneration of the mesh and make the mesh finer around the probes as discussed in Chapter 4.

The software ANSYS Workbench was used to generate all the geometries and meshes, which were both unstructured in order to allow the dynamic mesh study as was mentioned in section 3.3. The meshes for the two configurations are illustrated in Figure 7-3 and Figure 7-5 respectively.

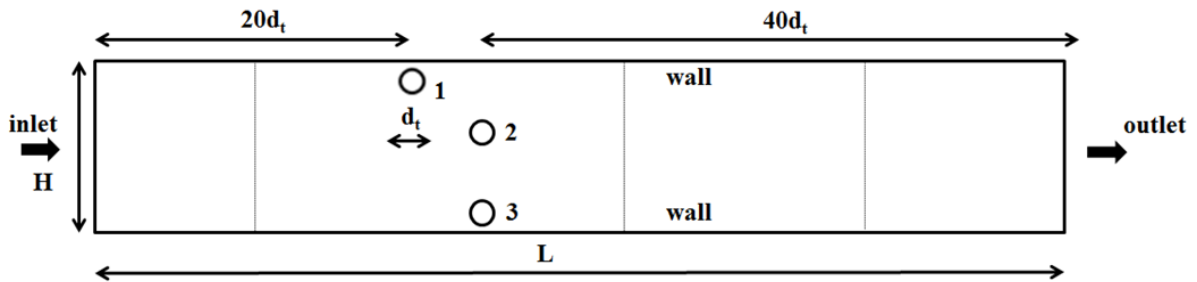


Figure 7-2: 2D geometry and boundary conditions (first probes' configuration, $d_t = 39$ mm).

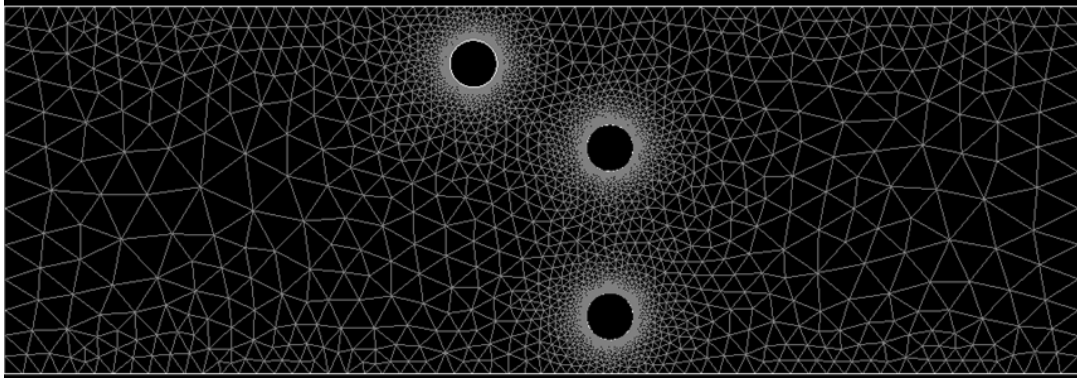


Figure 7-3: Unstructured mesh realised for the first probes' configuration (detail of the second block).

The estimated mesh quality is:

- Minimum Orthogonal Quality= $5.17 \cdot 10^{-1}$ (Orthogonal Quality ranges from 0 to 1, where values close to 0 correspond to low quality).
- Maximum Ortho Skew= $2.93 \cdot 10^{-1}$ (Ortho Skew ranges from 0 to 1, where values close to 1 correspond to low quality).
- Maximum Aspect Ratio= 4.56 (ideally equal to 1).

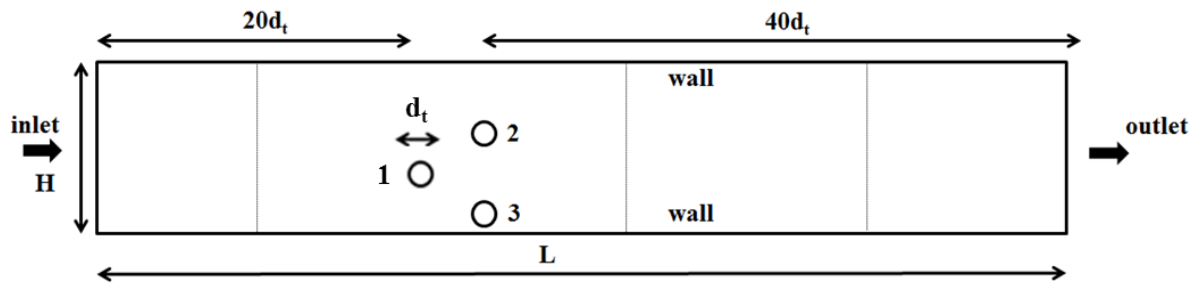


Figure 7-4: 2D geometry and boundary conditions (second probes' configuration, $d_t = 39$ mm).

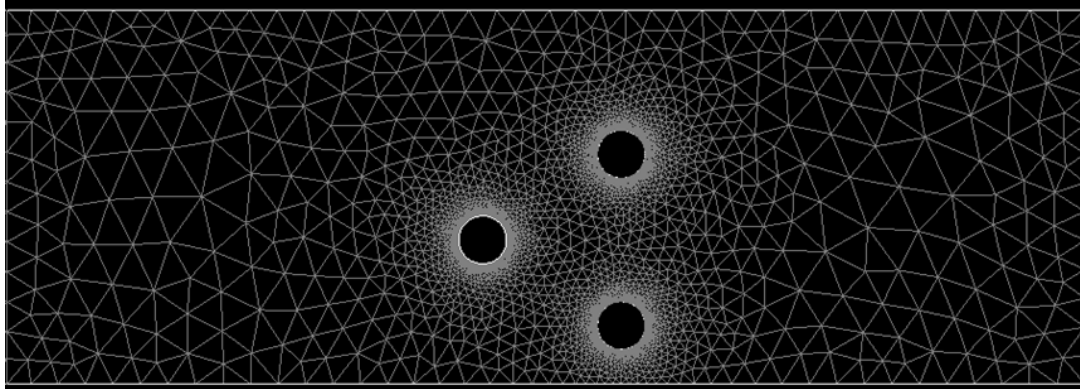


Figure 7-5: Unstructured mesh realised for the second probes' configuration (detail of the second block).

The estimated mesh quality is:

- Minimum Orthogonal Quality= $5.23 \cdot 10^{-1}$ (Orthogonal Quality ranges from 0 to 1, where values close to 0 correspond to low quality).
- Maximum Ortho Skew= $3.45 \cdot 10^{-1}$ (Ortho Skew ranges from 0 to 1, where values close to 1 correspond to low quality).
- Maximum Aspect Ratio= 5.09 (ideally equal to 1).

The main characteristics of the meshes are summarised in Table 7-1.

Table 7-1: Mesh features for the first and second configurations.

Mesh	Cylinder nodes	Nodes	Elements/Cells	Faces
1	150	5830	10804	16636
2	150	5706	10600	16308

The number of nodes around the cylinders was the same as in Chapter 4. This number represented a good compromise between the quality of results, convergence and computational costs in absence of particles. In fact, the grid convergence could not be carried out for all the geometries and models used in this thesis but, for the model presented in section 7.5, the adequacy of the grid has been verified (with 150 nodes on tube 2) and more details are in Appendix B (section B.1).

7.3 Model setup

The mesh was imported into Fluent[®] and the setup (explained in section 3.4) was followed to run all the simulations. The flue gas was approximated to be air entering the domain with a velocity (U_0) of 2 m/s, calculated in section 5.5.3 according to the air flow rate used in the experiments and the gas temperature (1273 K at the inlet). The tube surface temperatures were supposed to be constant (e.g. 773 K and 873 K) as well as in the experiments (500 and 600°C). The main properties for the gas and the cylinder walls are reported below and have been implemented in the Materials dialog box in Fluent[®].

Combusted gas properties (air):

Density $\rho_g = 0.345 \text{ kg/m}^3$ (*The Engineering ToolBox*, 2018)

Specific Heat $C_{p_g} = 1146 \text{ J/(kg K)}$ (*The Engineering ToolBox*, 2018)

Thermal Conductivity $k_g = 0.069 \text{ W/(m K)}$ (*The Engineering ToolBox*, 2018)

Viscosity $\mu_g = 44.07 \cdot 10^{-6} \text{ kg/(m s)}$ (*The Engineering ToolBox*, 2018)

Wall properties (mullite) (AZO Materials, 2018a):

Density $\rho_w = 2800 \text{ kg/m}^3$

Specific Heat $C_{p_w} = 1050 \text{ J/(kg K)}$

Thermal Conductivity $k_w = 6 \text{ W/(m K)}$

Using the gas properties, the Reynolds number (~ 610) was calculated with formula (3-1) and is in the range where the Von Karman vortex is turbulent (Haugen and Kragset, 2010). The Reynolds-Averaged Navier-Stokes (RANS) equations were used to determine the flow properties (Appendix A) with the $k-\omega$ SST turbulence model which is generally able to describe the boundary layer and the vortex shedding (García Pérez, 2016; Yang *et al.*, 2017) better than other turbulence models (Chapter 4). Transient simulations were run with time step size equal to 10^{-3} s which allowed a good description of the vortex formation and a Courant number ≤ 1 .

The DPM model was enabled and spherical inert ash particles were injected at the inlet (surface) with a Rosin Rammler size distribution and using the stochastic tracking model. The fitting between the experimental ash particle size distribution and the Rosin Rammler model obtained in Chapter 6 provided the parameters for the particle size distribution used in the model validation. During the experiments, the combustion conditions and the type of fuels did not change, therefore the ash particle size distribution released in the flue gas, and used for the model validation, was obtained as average of the parameters calculated in Chapter 6 and is summarised in Table 7-2.

Table 7-2: Average of the Rosin Rammler parameters obtained from the fitting between the experimental results and the model after 5 hours from combustion of Daw Mill-12 wt. % Miscanthus.

$d_{min}[\mu\text{m}]$	$d_{max}[\mu\text{m}]$	$d_{mean}[\mu\text{m}]$	n
0.43	535	68	1.07

The particle tracking was unsteady and the mass flow rate of ash particles ($\sim 10^{-4}$ kg/s) was calculated from the fuel feed rate and the ash percentage in the fuel.

The main properties for inert ash particles are summarised below:

Ash particle properties:

Density $\rho_p = 2200 \text{ kg/m}^3$ (Wacławiak and Kalisz, 2012)

Specific Heat $C_{p_p} = 923 \text{ J/(kg K)}$ (AZO Materials, 2018b)

Thermal Conductivity $k_p = 1.5 \text{ W/(m K)}$ (AZO Materials, 2018b)

Firstly, the flue gas was studied without particles until at least partial convergence; then particles were injected and allowed to flow around the probes before enabling the interactions between the two phases which allowed the deposition flux prediction. However, it is worth highlighting that studying the deposit accretion with a Rosin Rammler fly ash particle size distribution increases the computational costs compared to single particle size injections.

7.4 Ash particle trajectories

The main difference between the two geometries in Figure 7-2 and Figure 7-4 was the location of probe 1 which was closer to the upper wall in the first configuration (28.25 mm) and further in the second configuration (167.95 mm). This may have an effect on the particle trajectories and therefore on the deposition process. First of all, the gas velocity vectors were reported for the two configurations in Figure 7-6 and Figure 7-8 respectively. As expected, the gas velocities had their lowest values at the stagnation points, where the gas pressure was maximum. The gas velocities increased on the sides because of a reduction of the section available and of the gas pressure. Finally the gas velocities decreased again on the downstream surface when the separation of the boundary layers started.

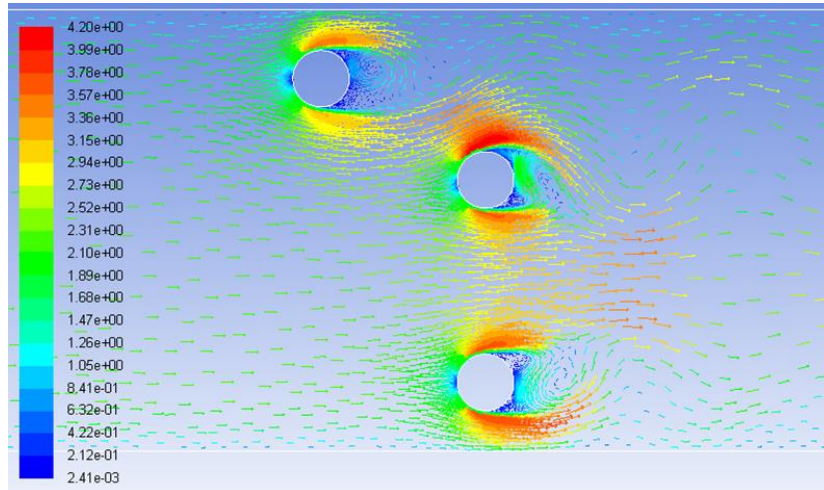


Figure 7-6: Gas velocity vectors around probes in the 1st configuration [m/s] ($U_0 = 2$ m/s, $d_i = 39$ mm).

Ash particle tracking for the two configurations is illustrated in Figure 7-7 and Figure 7-9 respectively. When the Rosin Rammler ash distribution was used, it became more difficult to identify the trajectory of the single particle (as was illustrated in Chapter 4). However, it can be seen that in both cases, probe 1 was characterised by the presence of bigger particles (red) on the downstream which could be due to the presence of the wall in the first configuration (Figure 7-7) and the rebound of particle from the top of probe 2. In the second configuration, the presence of bigger particles on the rear side of probe 1 was mainly due to the rebound from the top of probes 2 and 3 (Figure 7-9). Moreover,

in both configurations, on the rear sides of probes 2 and 3, there was a higher concentration of small particles (blue). In fact, small particles are more likely to follow the flue gas streamlines and deposit on the downstream surface because of their smaller inertia and eddy impaction. This confirms that the presence of other tubes can interfere with the ash particle trajectories and, as a consequence, the deposition process can be modified (as it was seen in the literature (e.g. Lee *et al.*, 2014) and in some preliminary results in Chapter 4).

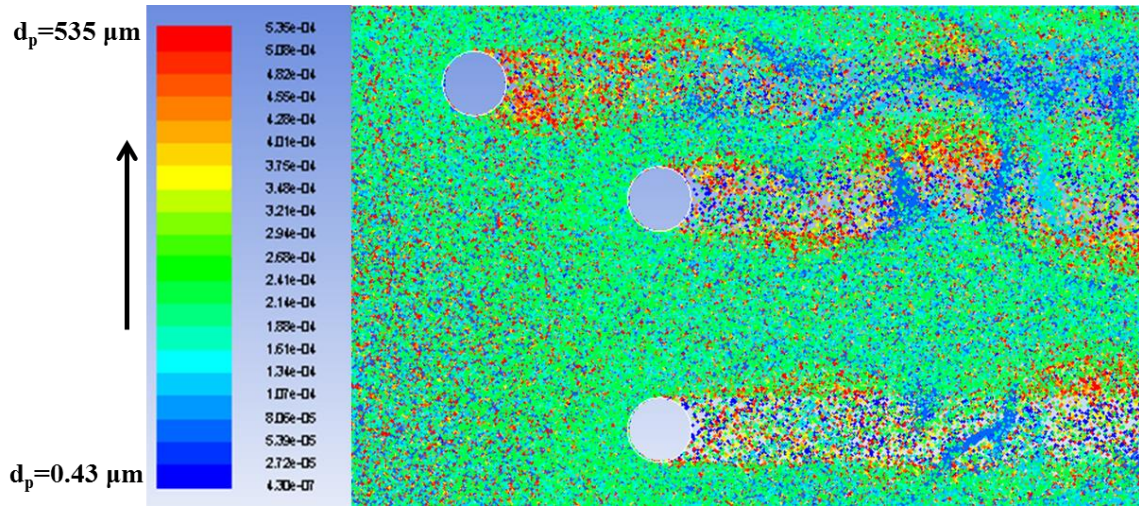


Figure 7-7: Tracking of ash particles around the probes ($d_t = 39 \text{ mm}$) in the 1st configuration ($d_{\min} = 0.43 \mu\text{m}$, $d_{\text{mean}} = 68 \mu\text{m}$, $d_{\max} = 535 \mu\text{m}$, polydispersion parameter $n = 1.07$, $U_0 = 2 \text{ m/s}$).

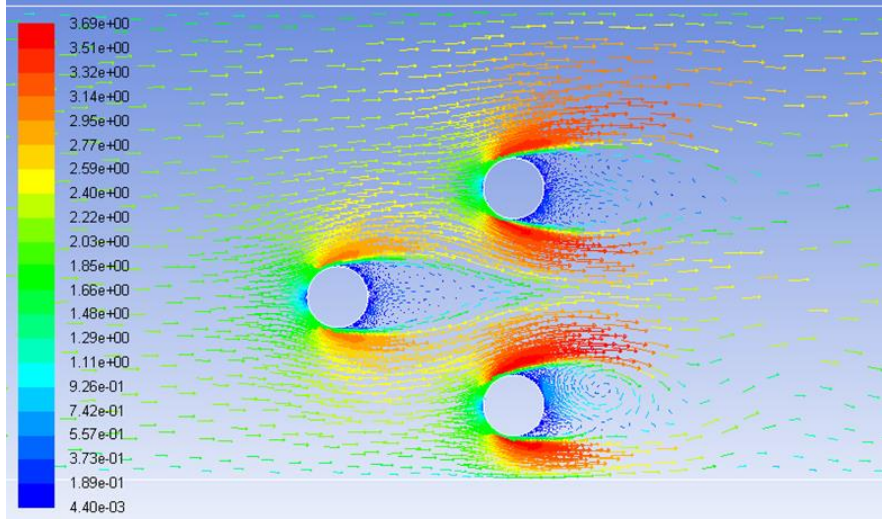


Figure 7-8: Gas velocity vectors around the probes in the 2nd configuration [m/s] ($U_0 = 2$ m/s, $d_t = 39$ mm).

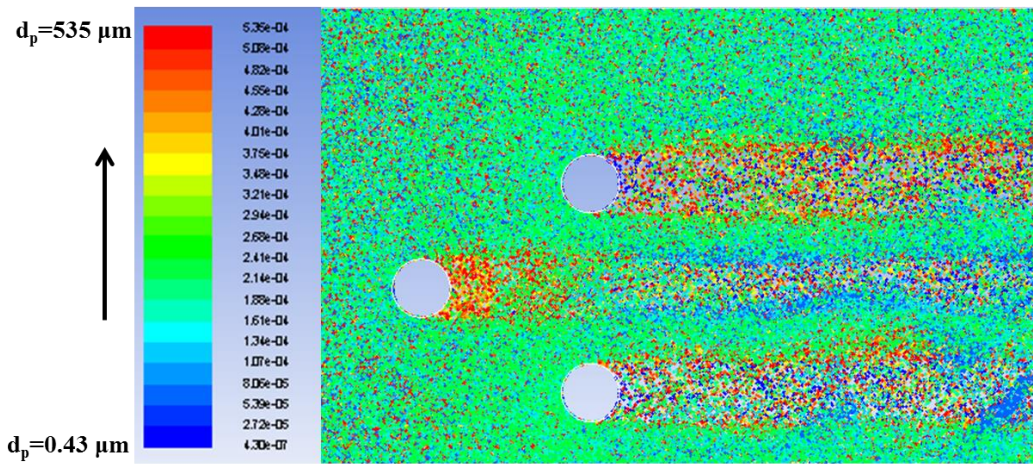


Figure 7-9: Tracking of ash particles around the probes ($d_t = 39$ mm) in the 2nd configuration ($d_{min} = 0.43$ μm, $d_{mean} = 68$ μm, $d_{max} = 535$ μm, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

Apart from calculating the deposition flux on the probes, the DEFINE_DPM_EROSION UDF allowed the calculation of the average diameter of particles that hit the cylinder walls. These values were saved in one of the UDMs (User Defined Memories) available and plotted in Figure 7-10 and Figure 7-11 where it is possible to identify the type of particles that hit the probes in the two configurations. However, the software could not highlight which particle sizes were more likely to

impact on a certain side of the probe (as had been experimentally observed in Chapter 6).

In both configurations (Figure 7-10 and Figure 7-11), bigger particles are more likely to hit the probe walls compared with small particles which generally follow the gas around the probes. Moreover, in configuration 2, a gap in particle sizes was identified between 53 μm and 214 μm (Figure 7-11).

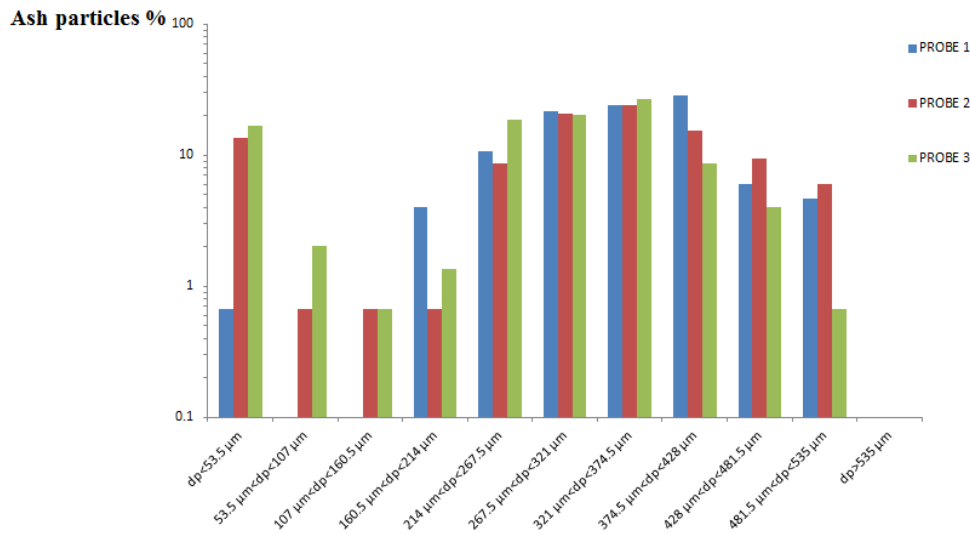


Figure 7-10: Prediction of average diameter of particles that hit the ceramic probes ($d_t = 39$ mm) in the 1st configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

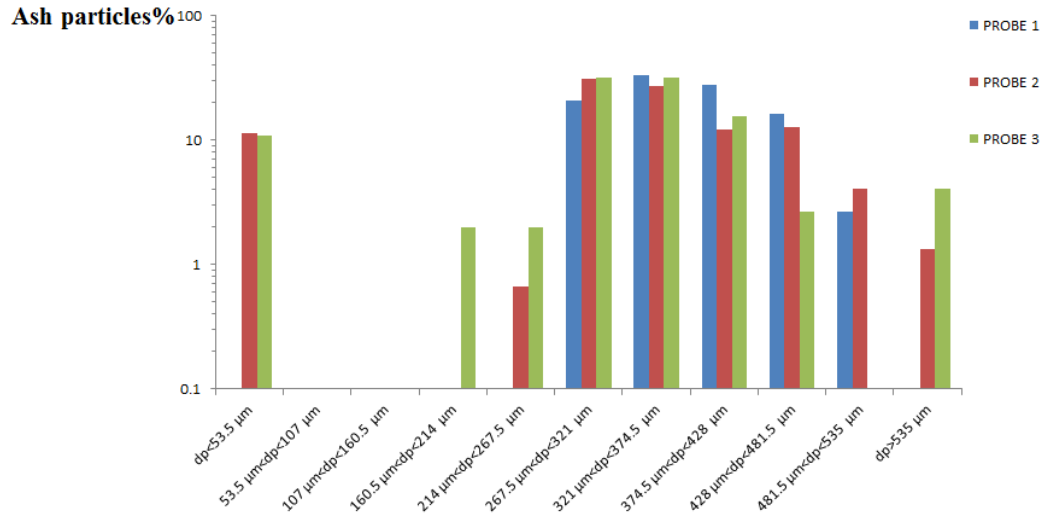


Figure 7-11: Prediction of average diameter of particles that hit the ceramic probes ($d_t = 39$ mm) in the 2nd configuration ($d_{min} = 0.43 \mu\text{m}$, $d_{mean} = 68 \mu\text{m}$, $d_{max} = 535 \mu\text{m}$, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

7.5 Sticking model

The path followed by the ash particles depends on their diameters, density, velocity, geometry, probe configuration, etc. Therefore, only a fraction of the particles injected into the domain hit the probe walls (i.e. injection efficiency) (Equation (2-2)). Moreover, depending on the condition of the particle and the surface, some of the particles that hit the probe deposit (i.e. sticking efficiency) while others rebound and leave the computational domain (Equation (2-3)). Consequently, the deposition efficiency can be calculated with Equation (2-4) or as the product between Equation (2-2) and Equation (2-3) (these situations are shown schematically in Figure 7-12).

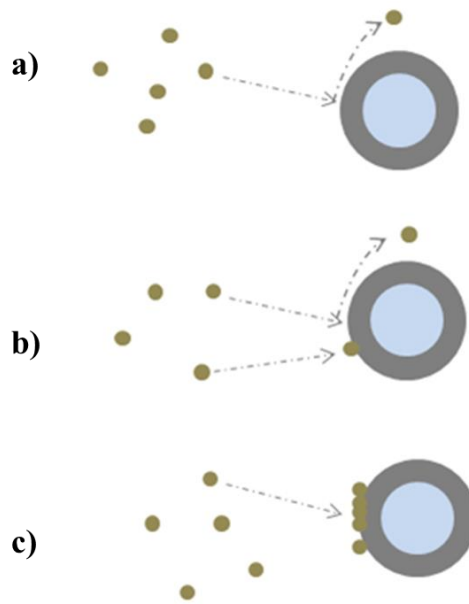


Figure 7-12: Representation of ash particle behaviour and deposition tendency on heat exchangers: a) impactation efficiency (Equation (2-2)); b) sticking efficiency (Equation (2-3)); c) deposition efficiency (Equation (2-4)).

The main deposition mechanisms were explained in detail in Chapter 2 and are summarised in Figure 7-13.

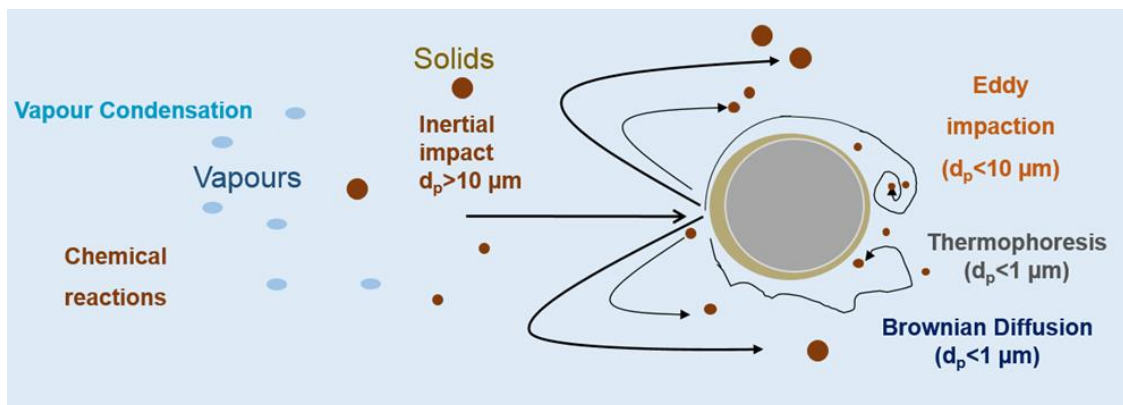


Figure 7-13: Representation of the main deposition mechanisms on heat exchangers (modified from (Simms, 2011)).

Figure 7-13 helps understanding how the particles and the vapour reach the surface of the tube and eventually deposit. Vapour condensation is particularly significant on a clean surface when its wall temperature is below the alkali species' dew point. Solid

particles reach the probe via inertial impaction, eddy impaction, Brownian diffusion and thermophoresis; however their probability of depositing depends on the condition of the particles and the wall surfaces. If particles are sticky, or molten/semi-molten from previous vapour heterogeneous condensation or chemical reactions, or if they hit a sticky surface where vapours have previously condensed, or there was a previous deposit layer, they tend to deposit (or stick) more easily compared to dry particles that hit a clean surface (Figure 7-14) (section 4.2.4, Figure 4-8).

In this thesis, the deposition routes that have been considered include inertial impaction (which is one of the main mechanisms for particles larger than 10 μm), vapour condensation, eddy impaction and thermophoresis. However, chemical reactions were not considered as they require a detailed knowledge of the chemical composition of the species released during the combustion as well as their temperature. Moreover, the Brownian diffusion was not included since it is not considered relevant for ash deposition (Zhou *et al.*, 2007).

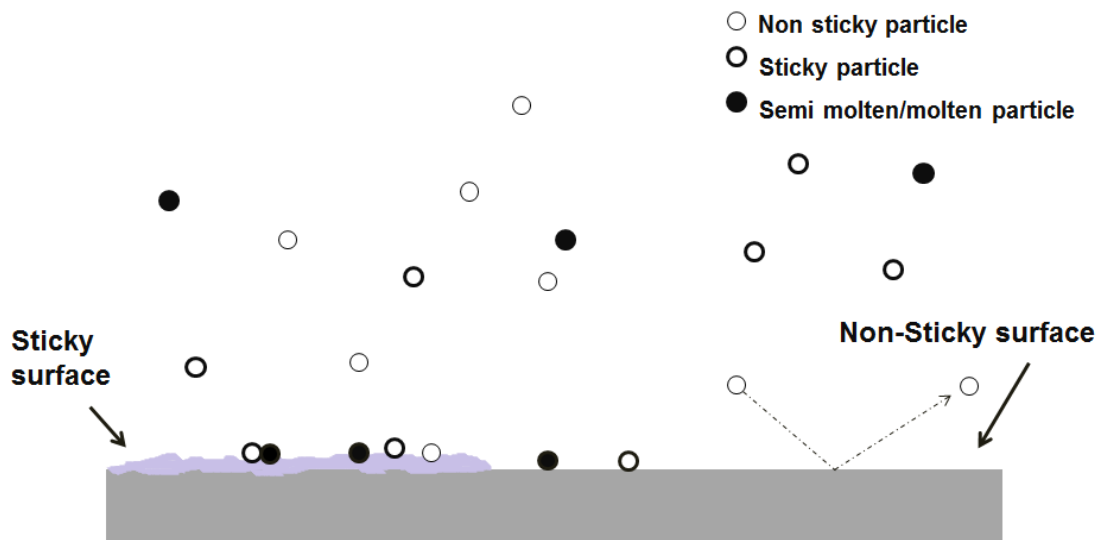


Figure 7-14: Schematic of particles in a hot gas stream sticking onto a cooled surface.

One of the objectives of this work was to develop a model to predict deposit formation on clean air cooled probes combining different deposition mechanisms. On a clean surface, the role of condensation is quite relevant to start the deposit build up. For this reason it has been taken into account and it was combined with the ash particle

stickiness calculated with the particle viscosity based on the real ash chemical composition.

The equation used to predict the total deposition flux is in Equation (7-1) which included the contribution of the particle deposition and the vapour condensation flux ($m_{c,A}$) on the ceramic probe.

$$m_{tot} = P_{tot} \frac{dm_p}{dA} \sin(\gamma) + m_{c,A} \quad (7-1)$$

In Equation (7-1), the total sticking probability (P_{tot}) takes into account the stickiness of the particle (P_p) and the surface (P_s) (Equation (7-2)). In particular, the stickiness of the surface derives from the vapour condensation which promotes fouling, especially on clean tubes. Moreover, the particle stickiness was function of the temperature and the chemical composition of ash particles.

$$P_{tot} = P_s(1 - P_p) + P_p(1 - P_s) + P_s P_p \quad (7-2)$$

In order to do this, previous models from the literature were considered, appropriately modified and combined as explained in this section. The condensation flux was calculated, as in Equations (2-19)-(2-23) assuming that the main vapour was Na_2SO_4 , where the constant 'S', with the inverse dimensions of deposition flux, was experimentally estimated on the basis of the maximum deposit accumulated on the probe during the experimental campaign ($\sim 24000 \text{ [kg/(m}^2 \text{ s)]}^{-1}$) (Tomeczek and Wacławiak, 2009). Different concentrations of Na_2SO_4 were investigated (1, 10 and 100 ppm) to determine the possible influence of the condensation on the total deposition flux (section 7.8).

The particle stickiness was calculated with the viscosity model in Equations (2-38) (Richards *et al.*, 1993), where the ash particle viscosity (μ_p) was compared with the reference viscosity (Equation (7-3)).

$$P_{stick}(T, X) = \frac{\mu_{ref}}{\mu_p} \text{ if } \mu_p > \mu_{ref} \quad (7-3)$$

$$1 \text{ if } \mu_p \leq \mu_{ref}$$

With $\mu_{ref} = 10^4$ Pa·s; which is a common value of viscosity at lower temperatures (Kleinhans *et al.*, 2018). This value was taken from the literature, but should be experimentally measured and verified.

In this case, the ash particle viscosity was obtained from the model of Urbain in Equation (7-4) (Browning *et al.*, 2003).

$$\mu_p = aT e^{1000b/T} \quad (7-4)$$

Where:

μ_p is the particle viscosity [Pa·s]; T is the temperature [K].

The constants necessary to calculate the particle viscosity (μ_p) were obtained using the ash chemical composition in Equations (7-5) to (7-11).

$$\ln(a) = -0.2812b - 11.8279T \quad (7-5)$$

Where a is function of b and the temperature T (calculated in Fluent[®]). Moreover, b is function of the mole fraction of silica, N , and β , is the ratio of the mole fraction of the main oxides in the ash. The expression used for β was developed by Urbain (Senior and Srinivasachar, 1995) and modified by Kalmanovitch who took into account additional species such as oxides of iron, magnesium, sodium, potassium and titanium (Browning *et al.*, 2003).

$$b = b_0 + b_1N + b_2N^2 + b_3N^3 \quad (7-6)$$

$$b_0 = 13.8 + 39.9355\beta - 44.049\beta^2 \quad (7-7)$$

$$b_1 = 30.481 - 117.1505\beta + 129.9978\beta^2 \quad (7-8)$$

$$b_2 = -40.9429 + 234.0486\beta - 300.04\beta^2 \quad (7-9)$$

$$b_3 = 60.7619 - 153.9276\beta + 211.1616\beta^2 \quad (7-10)$$

$$\beta = \frac{CaO + MgO + Na_2O + K_2O + FeO + TiO_2}{Al_2O_3 + CaO + MgO + Na_2O + K_2O + FeO + TiO_2} \quad (7-11)$$

The mole fractions of the oxides of the selected elements used for the calculations are in Table 7-3. These values are an average of the mole fractions obtained from the ash analysis of the samples collected from the ports where the probes were collected (Chapter 6). However, it is important to highlight that the oxide species required in this model were not the highest oxides (as in Chapter 6), therefore further calculations were necessary.

Table 7-3: Mole fraction percentage of the oxides of each element in the fly ash obtained from combustion of Daw Mill-12 wt.% Miscanthus and used for the calculation of the particle viscosity.

Component	%x _i
SiO ₂	50.61
Al ₂ O ₃	18.46
CaO	8.71
FeO	7.11
K ₂ O	2.33
MgO	3.71
Na ₂ O	1.90
TiO ₂	1.12
SO ₃	6.05

7.6 Deposit temperature

The methodology to predict the deposit temperature was explained in Chapter 3 and applied to the real probes used in Cranfield's combustion rig. Figure 7-15 represents a schematic of an air cooled ceramic probe used for deposition studies during the experimental campaign.

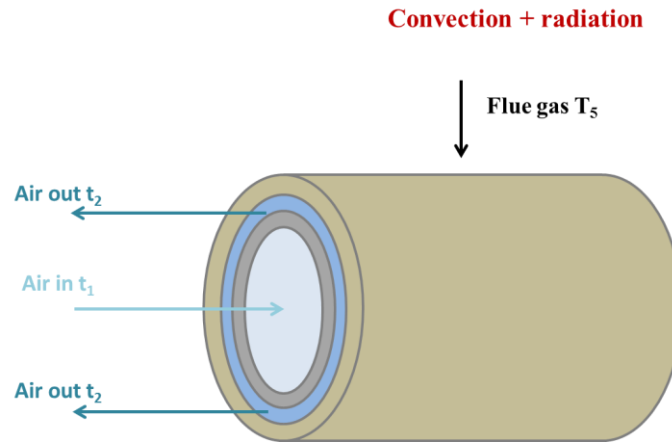


Figure 7-15: Schematic of an air cooled ceramic probe used to study deposition in the pilot scale combustor rig at Cranfield ($d_t = 39$ mm).

At the beginning of each test, the ceramic probe was clean but, during the combustion, solid ash particles and vapours deposited on the surface of the probe as shown in Figure 7-16.

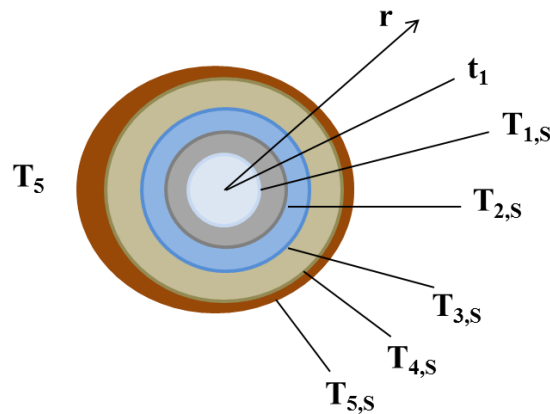


Figure 7-16: Cross section of the deposit accumulation on the ceramic probe and identification of the main temperatures for heat transfer calculations.

The deposit build-up represents a resistance towards heat transfer between the hot flue gas and the cooling air which can be summarised as follows (Figure 7-17) (Appendix G).

- 1) External hot flue gas convection and radiation (between T_5 and $T_{5,s}$)
- 2) Conduction into the deposit layer (between $T_{5,s}$ and $T_{4,s}$)
- 3) Conduction through the ceramic probe (between $T_{4,s}$ and $T_{3,s}$)

- 4) Convection air out (between $T_{3,s}$ and $T_{2,s}$)
- 5) Conduction into the stainless steel tube (between $T_{2,s}$ and $T_{1,s}$)
- 6) Convection air in (between $T_{1,s}$ and t_1).

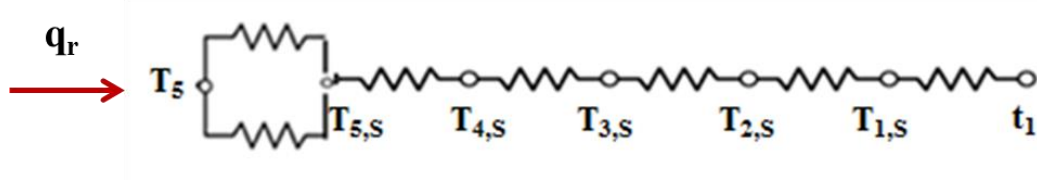


Figure 7-17: Thermal resistance schematic between the flue gas and the air cooling system.

The tube surface in the CFD geometry represented the ceramic probe surface (mullite) which was assumed to be at a constant temperature ($T_{4,s}$), therefore the calculation of the deposit temperature was carried out with the simplification in Figure 7-18 where the coolant and the metal tube were neglected.

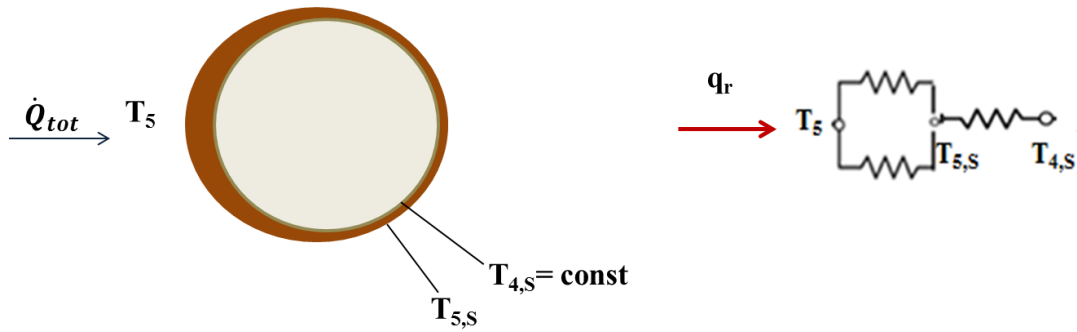


Figure 7-18: Simplification of a ceramic probe with a deposit layer (left) and thermal resistance for heat transfer calculations (right).

The main deposit properties used in this work are summarised below.

Deposit properties:

Deposit density $\rho_{dep} = 600 \text{ kg/m}^3$ (material density multiplied by the deposit porosity) (García Pérez, 2016)

Deposit porosity $\phi_{dep} = 0.7$ (Furmański, 1995);

Thermal Conductivity $k_{dep} = 3 \text{ W/(m K)}$ (Kleinhans *et al.*, 2018)

Emissivity $\sigma_{dep} = 0.91$ (The Engineering Toolbox, 2018)

The deposit properties could not be determined experimentally; therefore reasonable data were taken from the literature. This represents one of the model limitations and may have affected the accuracy of the model predictions.

7.7 Model predictions

7.7.1 Case study A

Firstly, the model explained in section 7.5 with Na_2SO_4 1 ppm was implemented in the modified DEFINE_DPM_EROSION UDF to identify the deposition locations and to calculate the deposition flux on the ceramic probes. In this case, the deposition was studied neglecting the effect of the deposit shape and of the increasing deposit temperature (considered in section 7.7.2).

The results were reported below for the different configurations and probe temperatures. During the simulations, the surface monitor option in Fluent[®] was used to observe the trend of the particle accumulation over time. The amount of deposit accumulated on the surface area [kg/m^2] was quite linear (Figure 7-19), while the deposition flux [$\text{kg/m}^2 \text{ s}$] tended to reach a plateau or at least to become flat after a while. This behaviour was more evident, and was obtained after a shorter time, when single ash particles were injected (Figure 7-20) compared to simulations where an ash particle size distribution was implemented (Figure 7-21).

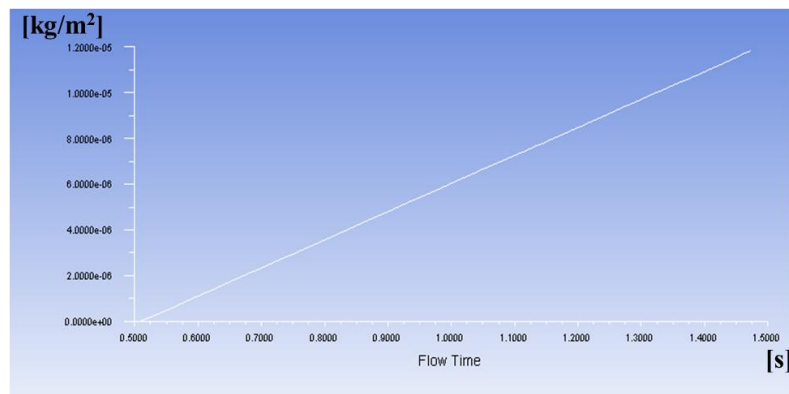


Figure 7-19: Typical trend of the kg/m^2 deposited on a ceramic probe ($d_t = 39 \text{ mm}$) at a constant temperature over time ($U_0 = 2 \text{ m/s}$).

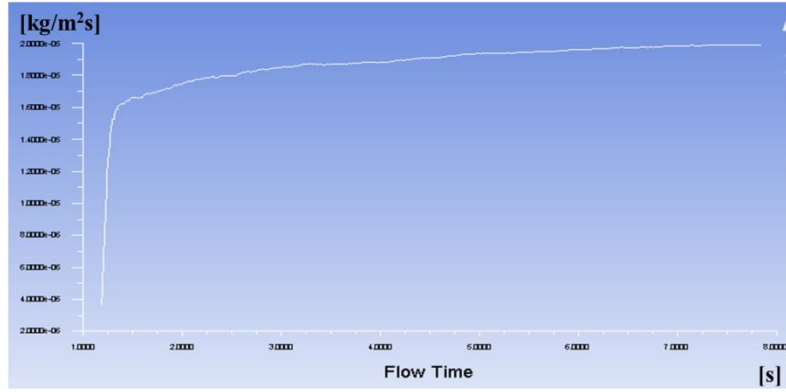


Figure 7-20: Typical trend of the deposition flux [kg/m² s] on a ceramic probe ($d_t = 39$ mm) over time for 100 μm particles ($U_0 = 2$ m/s).

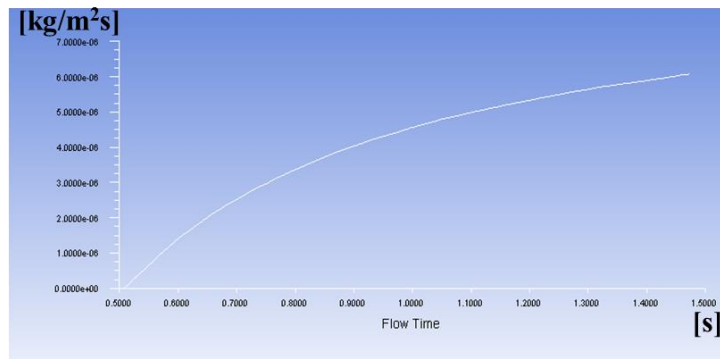


Figure 7-21: Typical trend of the deposition flux [kg/m² s] on a ceramic probe ($d_t = 39$ mm) over time for a particle size distribution ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

Therefore, once the deposition flux was stable, it was extrapolated and used to calculate the deposit thicknesses and the deposit temperatures after 2.5 hours and 5 hours (Equation (2-75)) assuming a constant external heat flux function of the flue gas convective and radiative contributions (Equations (2-64)).

These simulations were run for the first configuration with probe temperatures at 773 K and the second configuration with probe temperatures at 773 K, 873 K and 973 K. The latter value was not experimentally tested but it was included to have an additional comparison.

7.7.1.1 Configuration 1 at 773 K surface temperature

The aforementioned procedure was used to predict the deposition flux and shape using the first configuration of probes at a surface temperature of 773 K.

The deposition fluxes obtained from the modelling are reported in Figure 7-22 whose values are comparable with the experimental results in section 6.3.1. Moreover, the simulations were able to correctly predict the deposition location around the probes, higher on the upstream surfaces than side and downstream (Figure 7-23). However, the model seems to slightly overestimate the deposition on the upstreams and underestimate that on the rear sides of the probes; this can be attributed to some of the assumptions and simplifications made to approach such a complex phenomenon (e.g. 2D geometry, sticking model, etc.).

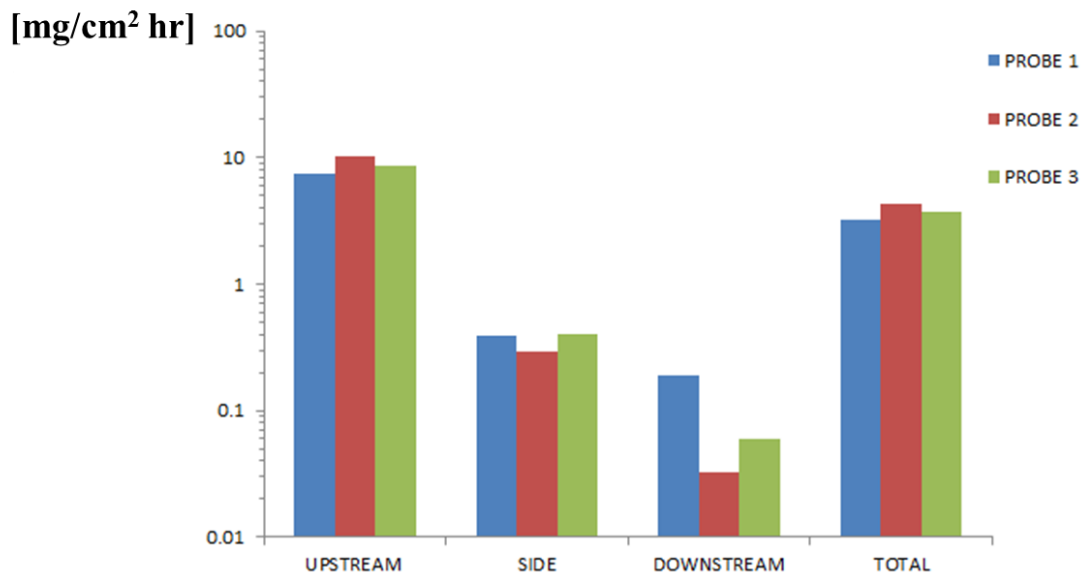


Figure 7-22: Predicted deposition fluxes on different sides of probes (773 K, $d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

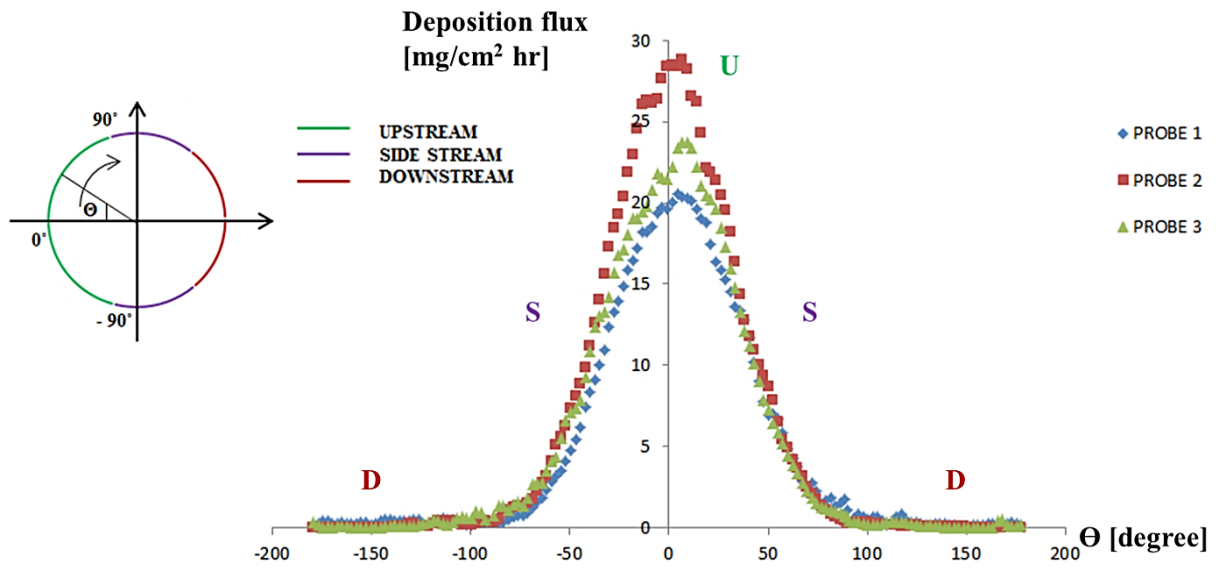


Figure 7-23: Predicted deposition fluxes around probes (773 K, $d_t=39$ mm) using the 1st probes' configuration ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$).

The presence of the bend $\sim 0.5\text{ m}$ downstream of the probes in Figure 7-1 was investigated and the results of simulations with and without the bend were compared with the experimental values and reported in Figure 7-24.

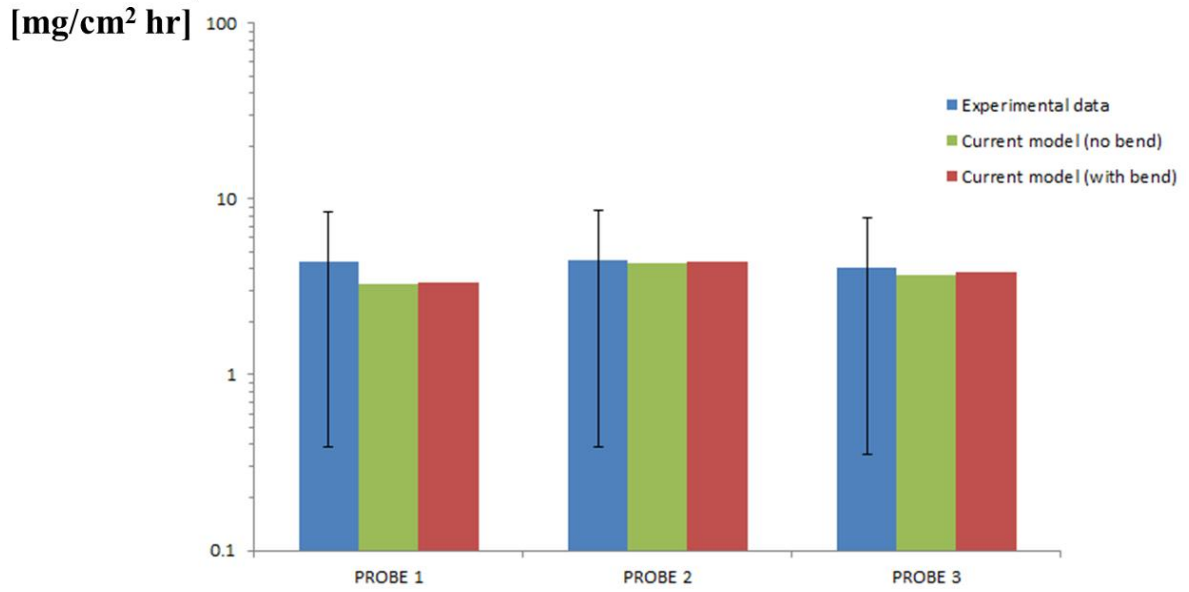


Figure 7-24: Comparison between experimental and modelling total deposition fluxes on probes (773 K, $d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

The shape of the deposit was predicted after 2.5 hours and 5 hours using Equations (3-6). The deposit looked thicker after 5 hours and only a very thin layer was found on the downstream (Figure 7-25), which was observed also in the experimental results (sections 6.3.1 and 6.3.2). Moreover, the deposits were thicker on the top of probes 2 and 3 than probe 1, probably because of the particle rebounds from probe 1 onto probes 2 and 3. The maximum thickness values calculated after 5 hours on probes 1, 2 and 3 were 3.52 mm, 4.09 mm and 3.83 mm respectively.

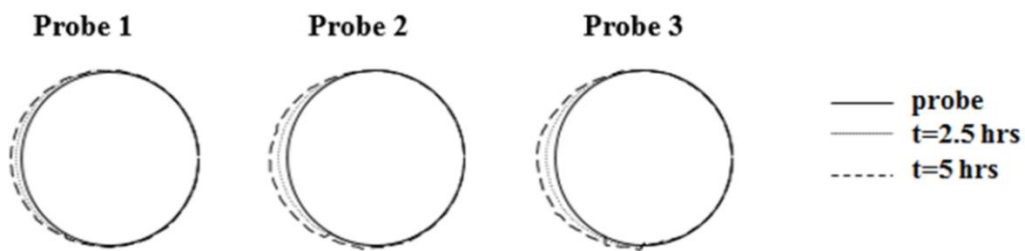


Figure 7-25: Predicted deposit shape after 2.5 and 5 hours of simulation with 1st configuration of probes (773 K, $d_t = 39$ mm, $d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

In Chapter 6, (e.g. Figure 6-19) it was noticed that the deposit shape varied along the probe length and had thicknesses in a range between ~ 0.05 cm and ~ 1.1 cm. This aspect cannot be appreciated in a 2D approach, and Figure 7-25 is only an example of how deposits build up on the probes. However, the predicted values were within the experimental error allowance.

Predictions of deposit surface temperatures after 2.5 and 5 hours of exposure were reported in Figure 7-26 as function of the angle described around probe 1. In agreement with previous results from the literature (Wacławiak, 2016), deposit accumulation represents a thermal resistance R which leads to an increasing deposit temperature; the highest temperature was identified on the surface of the upstream deposit, followed by the side and downstream.

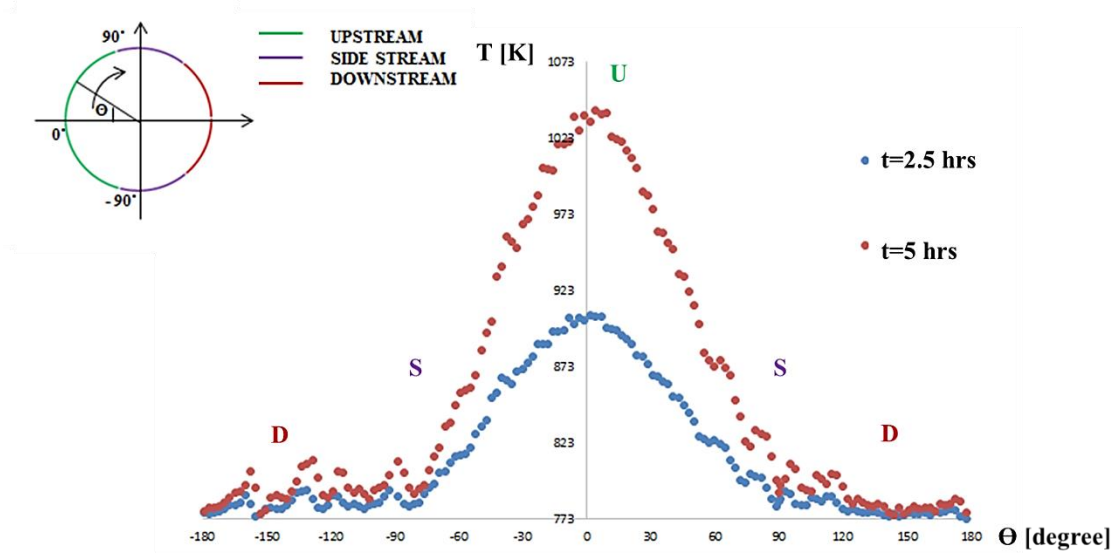


Figure 7-26: Predicted deposit temperature on probe 1 (1st configuration) at 773 K after 2.5 and 5 hours ($d_{min}=0.43$ μm , $d_{mean}=68$ μm , $d_{max}=535$ μm , polydispersion parameter $n=1.07$, $U_0=2$ m/s).

Moreover, Figure 7-27 describes the deposit temperatures on the three probes after 5 hours. It can be noticed that after 5 hours of exposure the deposit temperatures were closer to the gas temperature, which reduces the heat transfer and affects the thermal efficiency in industrial boilers. In addition, the deposit temperature profiles reflected the deposition flux trend, in fact probes 2 and 3, characterised by the highest deposition

fluxes and, as a consequence, deposit thicknesses, had the highest deposit surface temperatures.

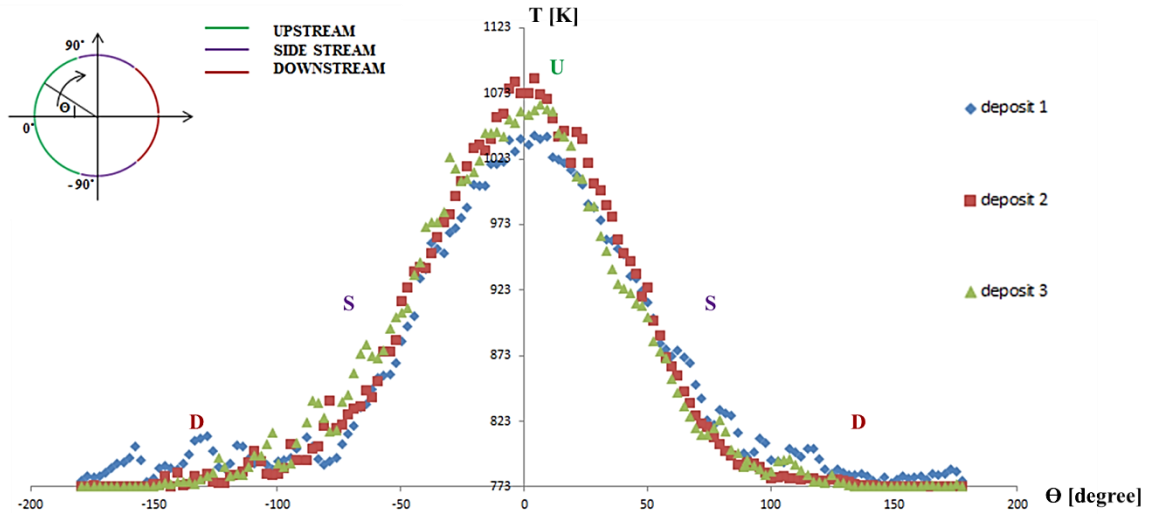


Figure 7-27: Predicted deposit temperature profile after 5 hours (1st configuration) on probes at 773 K ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$).

7.7.1.2 Configuration 2 at 773K surface temperature

The same procedure explained above was applied to predict deposition in the equivalent operating conditions of Experiment n°3 (2nd configuration of probes at 773 K).

The model was able to identify the main areas where deposition took place and also to predict the deposition fluxes, with more accuracy on the upstream than the side and downstream. In fact, some of the approximations made (e.g. 2D geometry) may have compromised the prediction of ash particle behaviour and the vortex shedding formation which is responsible for deposit formation on the downstream of tubes (Figure 7-28 and Figure 7-29).

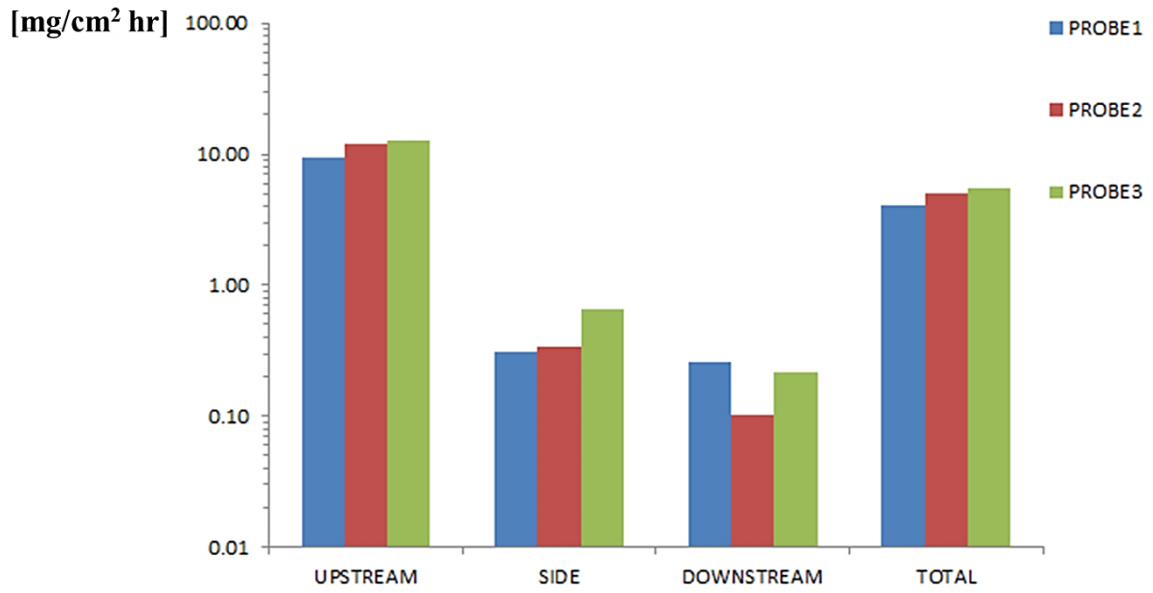


Figure 7-28: Predicted deposition fluxes on different sides of probes (~ 773 K, $d_t = 39$ mm) using the 2nd probes' configuration ($U_0 = 2$ m/s, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$).

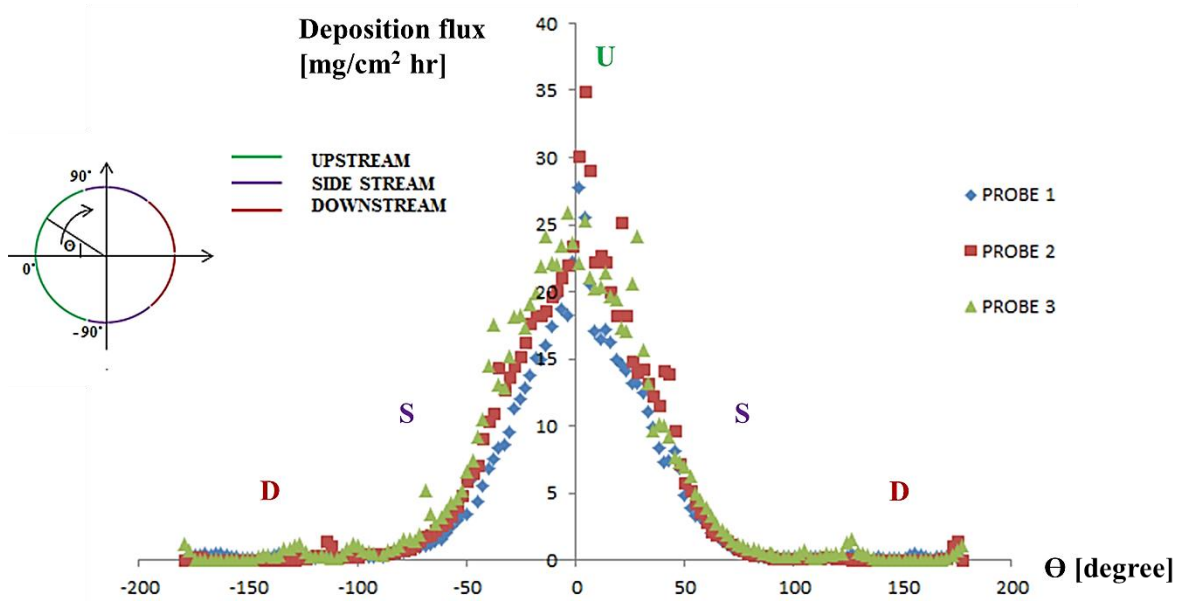


Figure 7-29: Predicted deposition fluxes around probes (~ 773 K, $d_t = 39$ mm) using the 2nd probes' configuration ($U_0 = 2$ m/s, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$).

In Figure 7-30, a comparison between the experimental results of deposition, using the second configurations of probes at 773 K during combustion of Daw Mill-12 wt.% Miscanthus, and modelling confirms that the presence of the bend does not have a significant influence on the particle behaviour.

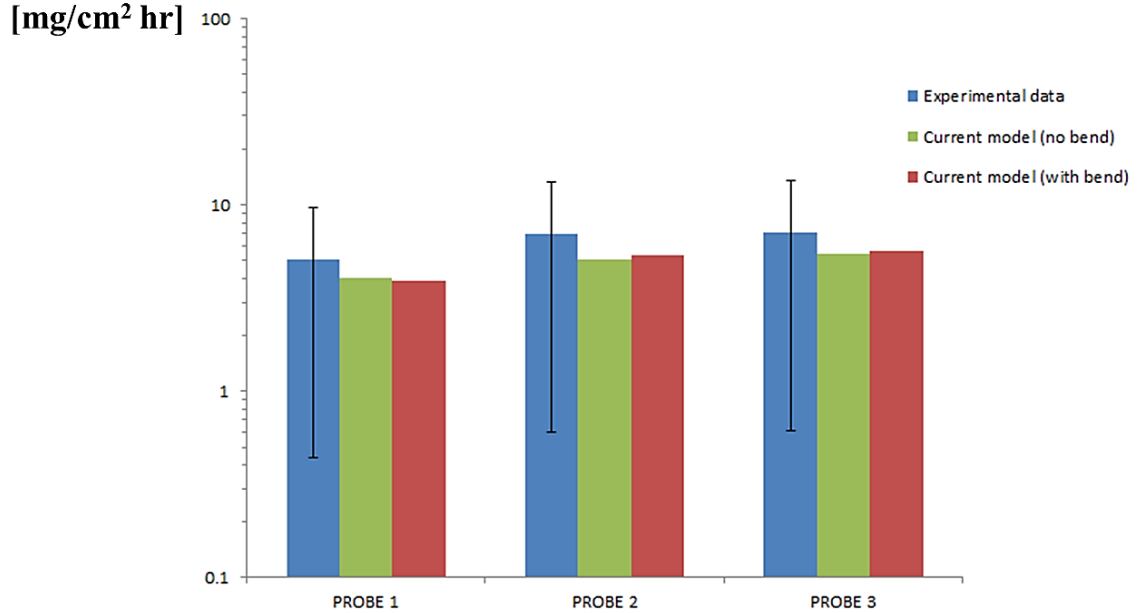


Figure 7-30: Comparison between experimental and modelling total deposition fluxes on probes (773 K, $d_t = 39$ mm) using the 2nd probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

The deposit shapes were predicted (Figure 7-31) and the maximum thickness was 3.47 mm, 4.37 mm and 3.23 mm on probes 1, 2 and 3 respectively.

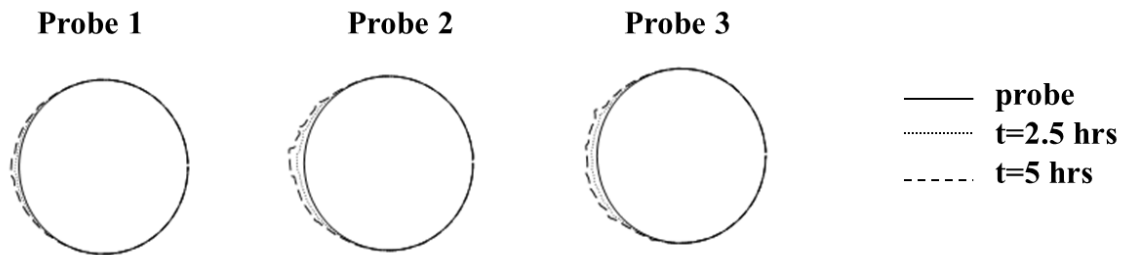


Figure 7-31: Predicted deposit shape after 2.5 and 5 hours of simulation with 2nd configuration of probes (773 K, $d_t = 39$ mm, $d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

As in 7.7.1.1, the deposit temperatures were calculated and they confirmed an increase with the deposit thickness (Figure 7-32) and, after 5 hours of exposure the temperatures were higher on probes 2 and 3 than probe 1, in agreement with the deposit thickness values (Figure 7-33).

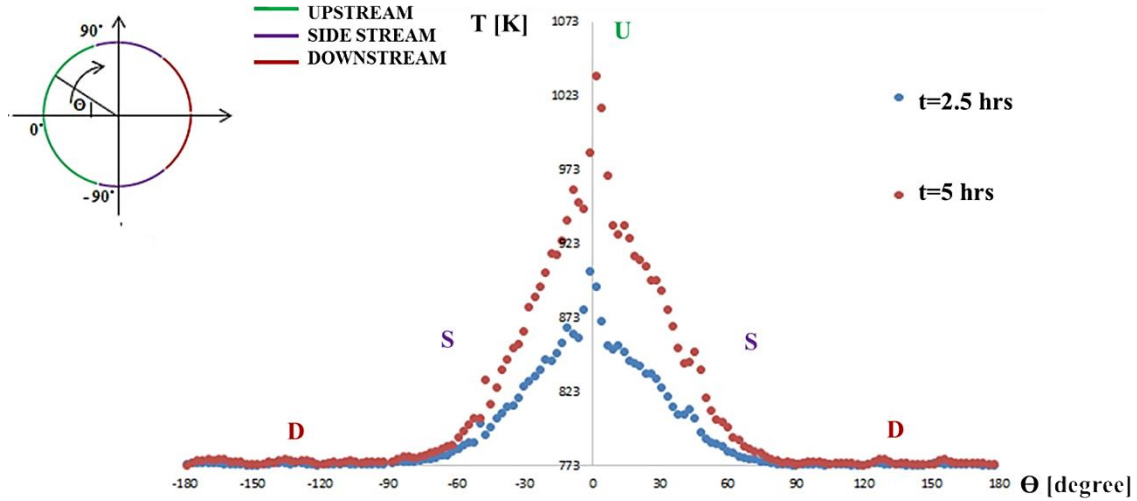


Figure 7-32: Predicted deposit temperature on probe 1 (2nd configuration) at 773 K after 2.5 and 5 hours ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$).

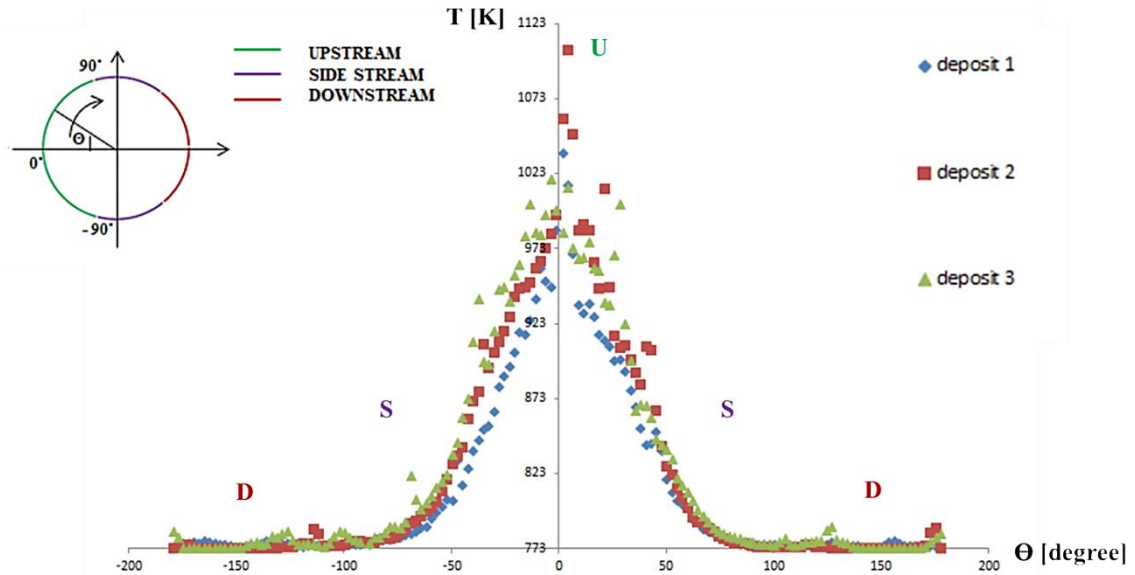


Figure 7-33: Predicted deposit temperature profile after 5 hours (2nd configuration) on probes at 773 K ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$).

7.7.1.3 Configuration 2 at 873 K surface temperature

During the experiments, the second configuration of probes was also used to test higher probe temperatures and study its effect on the deposit formation. The model provided a good prediction of the deposition flux around the probe, in particular on the upstream surfaces (Figure 7-34 and Figure 7-35).

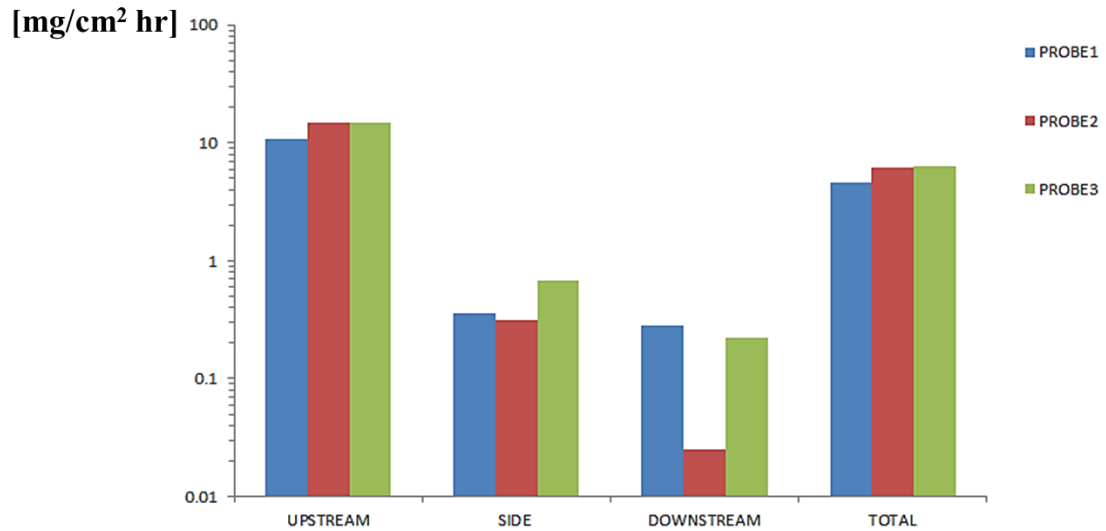


Figure 7-34: Predicted deposition flux on different sides of probes (873 K, $d_t = 39 \text{ mm}$) using the 2nd probes' configuration ($U_0 = 2 \text{ m/s}$, $d_{\min} = 0.43 \text{ }\mu\text{m}$, $d_{\text{mean}} = 68 \text{ }\mu\text{m}$, $d_{\max} = 535 \text{ }\mu\text{m}$, polydispersion parameter $n = 1.07$).

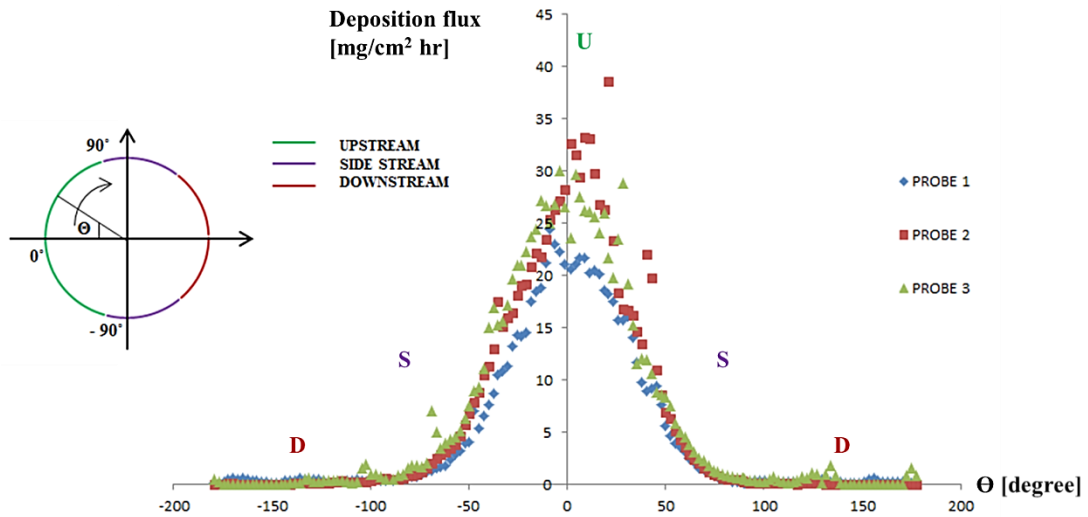


Figure 7-35: Predicted deposition flux around probes (873 K, $d_t = 39$ mm) using the 2nd probes' configuration ($U_0 = 2$ m/s, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$).

As for the previous simulations, the deposit shape is represented in Figure 7-36 and it reflected what observed at the end of the experiments, thicker deposit on the top than side and rear side with a maximum thickness of 3.05 mm, 4.82 mm and 3.74 mm for probes 1-3 respectively.

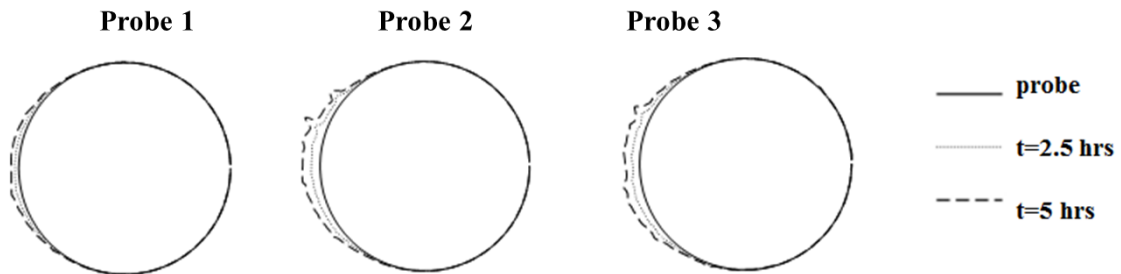


Figure 7-36: Predicted deposit shape after 2.5 and 5 hours of simulation with 2nd configuration of probes (873 K, $d_t = 39$ mm, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$).

Finally, deposit temperature predictions reflected the zones where the deposits were thicker and created a thermal insulation which implied higher surface temperatures (Figure 7-37 and Figure 7-38).

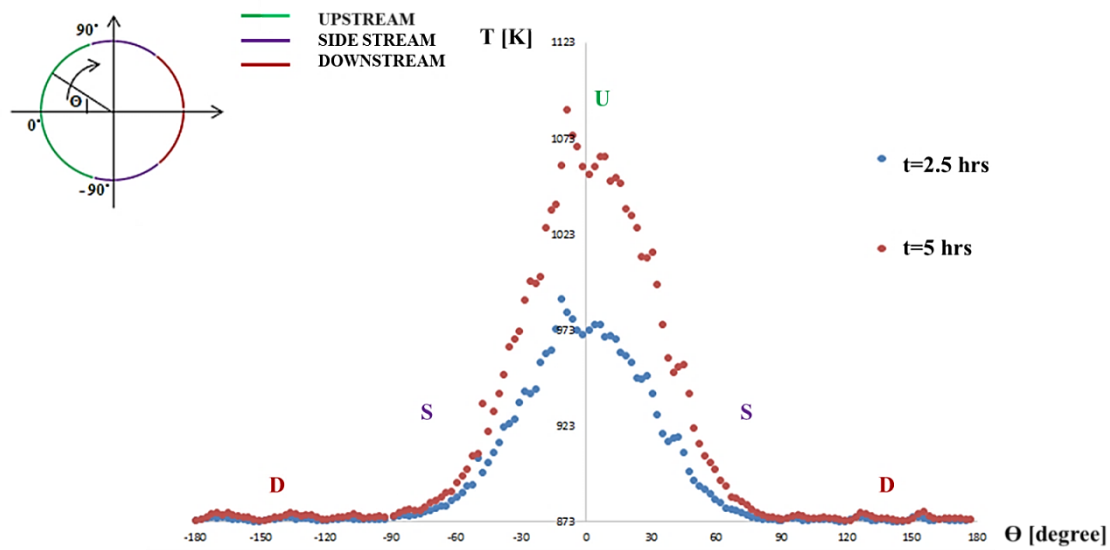


Figure 7-37: Predicted deposit temperature on probe 1 (2nd configuration) at 873 K after 2.5 and 5 hours ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$).

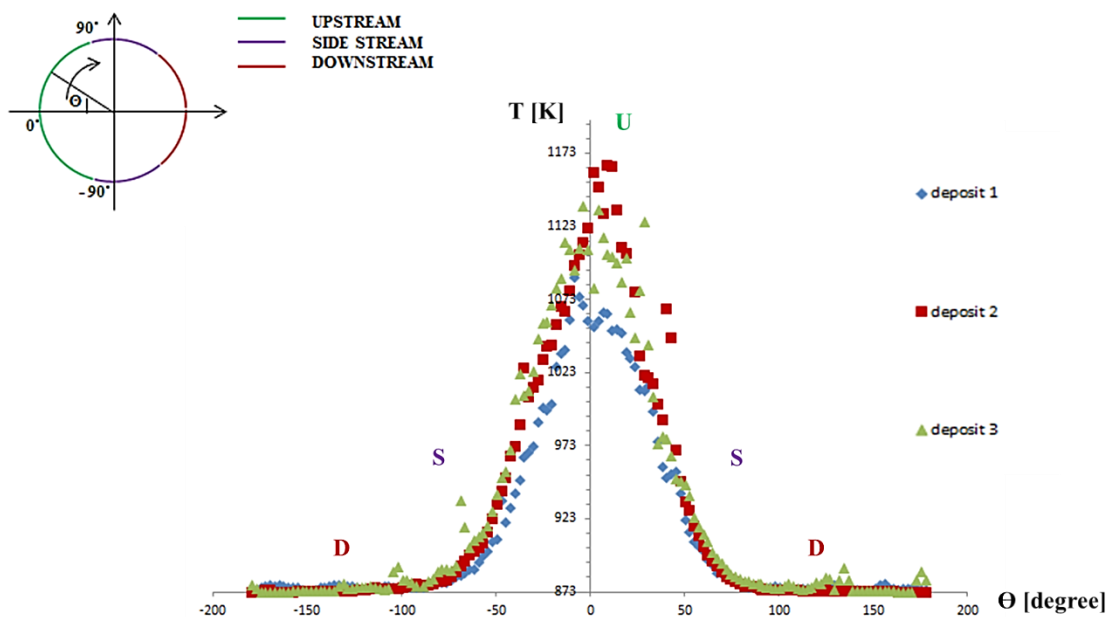


Figure 7-38: Predicted deposit temperature profile after 5 hours (2nd configuration) on probes at 873 K ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$).

7.7.1.4 Configuration 2 at 973 K surface temperature

An experiment with configuration 2 and probe temperature at 973 K was not carried out, however a simulation of this was included to allow a comparison with the previous two cases at different temperatures (sections 7.7.1.2 and 7.7.1.3).

The deposition flux on the three probes had the same trend as in the previous two cases with higher amounts of deposit on probes 2 and 3 than probe 1 (Figure 7-39 and Figure 7-40).

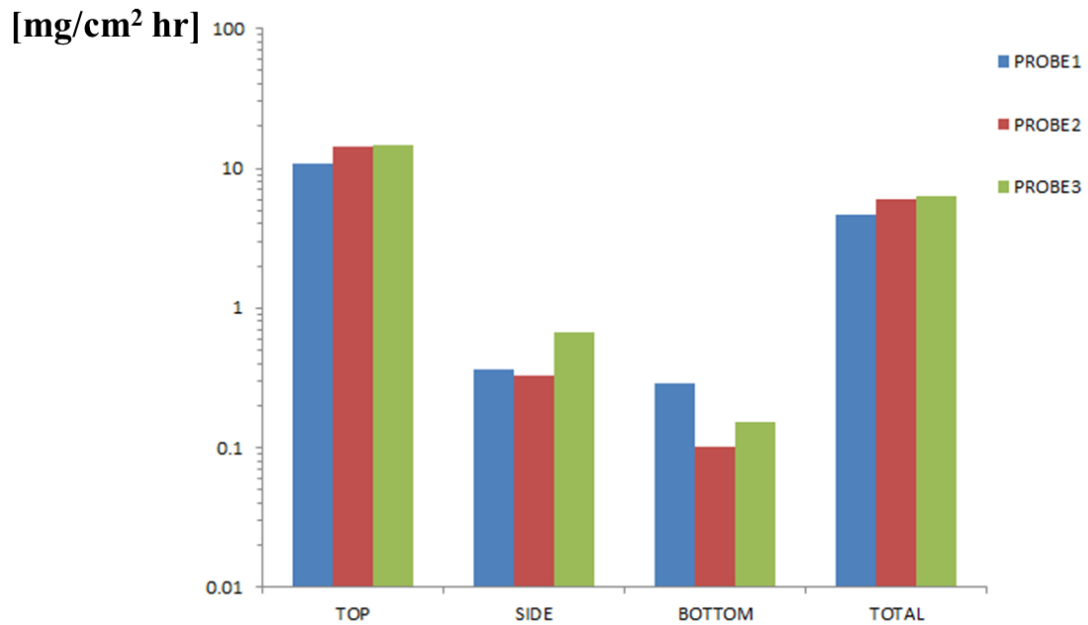


Figure 7-39: Predicted deposition flux on different sides of probes (~ 973 K, $d_t = 39$ mm) using the 2nd probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

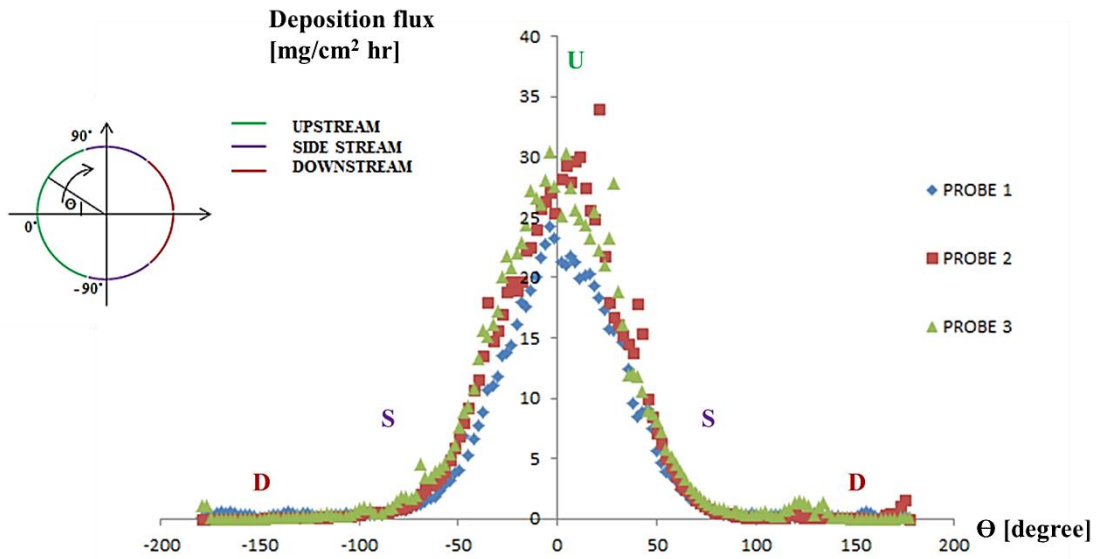


Figure 7-40: Predicted deposition flux around probes (~ 973 K, $d_i = 39$ mm) using the 2nd probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

As already observed before, this behaviour was reflected into the deposit shape for the three probes in Figure 7-41. Deposits were thicker on the upstream of probes 2 and 3 than probe 1, probably because particles rebounded from the top of probe 1 to probes 2 and 3 where they were more likely to deposit. The maximum deposit thickness was 3.04 mm, 4.25 mm and 3.79 mm for probes 1-3 respectively.

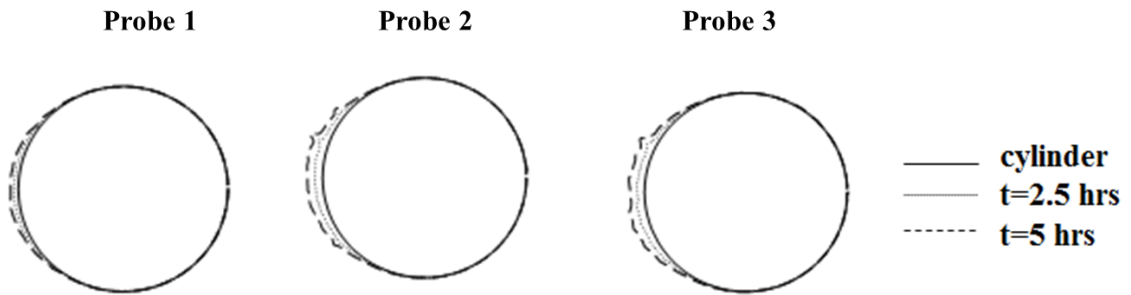


Figure 7-41: Predicted deposit shape after 2.5 and 5 hours of simulation with 2nd configuration of probes (973 K, $d_i = 39$ mm, $d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$).

Finally, the temperature profiles in Figure 7-42 and Figure 7-43 confirmed what has already been observed in the previous two cases.

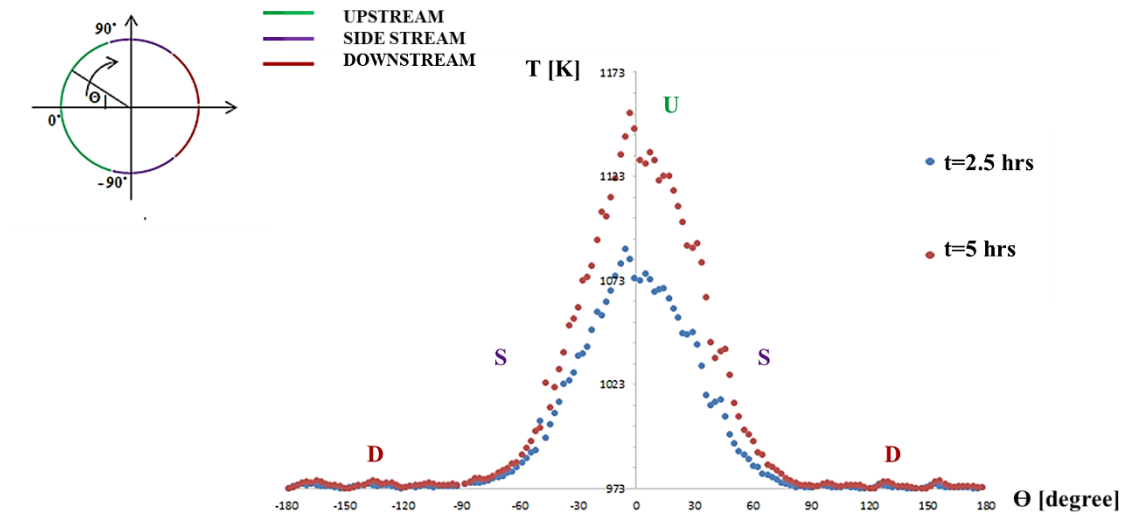


Figure 7-42: Predicted deposit temperature on probe 1 (2nd configuration) at 973 K after 2.5 and 5 hours using an ash particle size distribution ($d_{min}= 0.43 \mu\text{m}$, $d_{mean}= 68 \mu\text{m}$, $d_{max}= 535 \mu\text{m}$, polydispersion parameter $n= 1.07$, $U_0= 2 \text{ m/s}$).

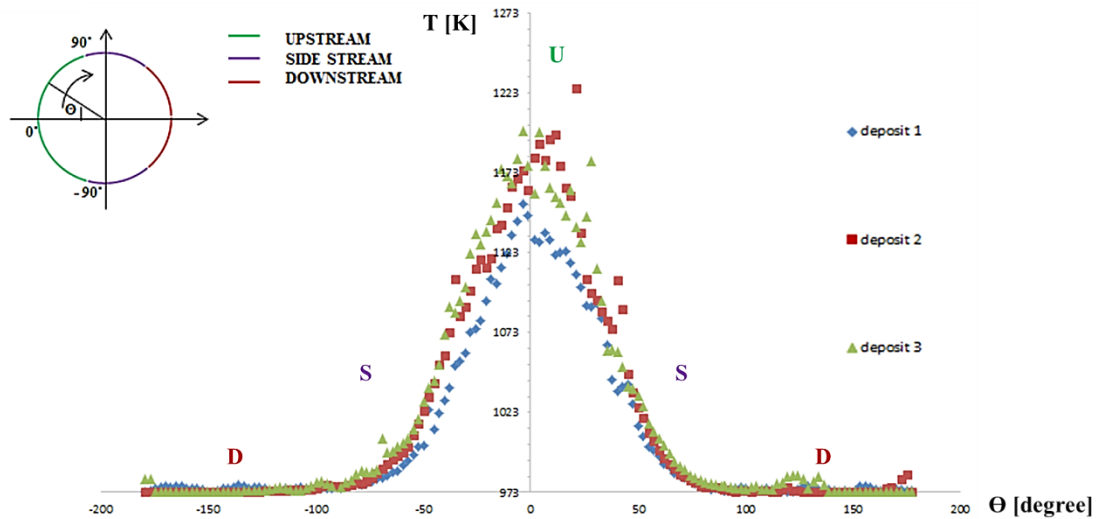


Figure 7-43: Predicted deposit temperature profile after 5 hours (2nd configuration) on probes at 973 K ($d_{min}= 0.43 \mu\text{m}$, $d_{mean}= 68 \mu\text{m}$, $d_{max}= 535 \mu\text{m}$, polydispersion parameter $n= 1.07$, $U_0= 2 \text{ m/s}$)

7.7.1.5 Summary

Generally, it is possible to state that, despite all the simplifications, the model was able to identify the main zones of deposition and to give a good prediction of the deposition flux around the ceramic probes for the different configurations and probe temperatures.

Probes 2 and 3 showed slightly higher deposition flux, especially on the upstream because of the rebound of particles from probe 1 to probes 2 and 3. Moreover, probe 3, closer to the chamber wall, was more affected by particle rebounds compared to probe 2.

The effect of the probe temperature did not generate considerable differences on the deposition flux; however the deposition increased slightly at higher probe temperatures. Generally, the vapour condensation and the thermophoresis are affected negatively by the increase of surface temperature; however these mechanisms give only a partial contribution to the total deposition flux. On the other hand, the ash particle sticking model used in this work included functions of the temperature and ash chemical composition. This latter did not change during the simulations (Table 7-3), but particles have a lower viscosity at higher temperature which implied higher sticking efficiency (Equations (2-38) and Figure 7-44).

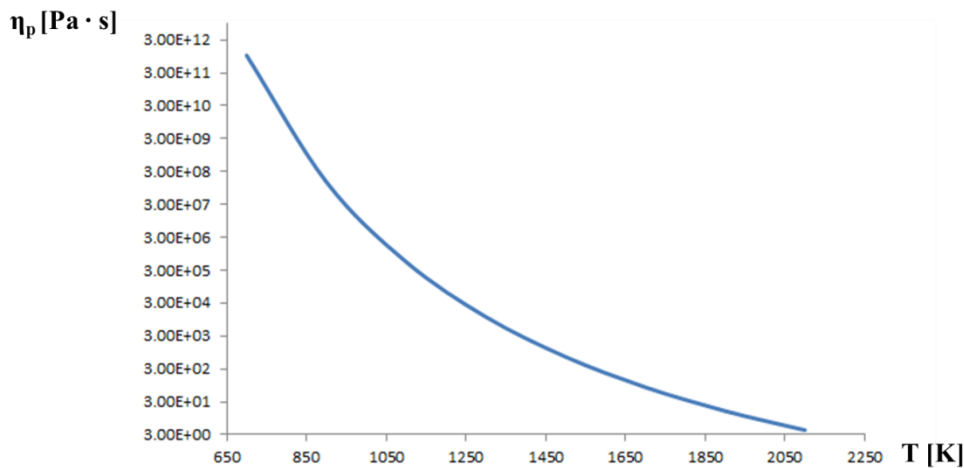


Figure 7-44: Particle viscosity as function of the temperature [K] and ash chemical composition (Equation (7-4)).

7.7.2 Case study B

In this section, the dynamic effects of deposit shape and temperature on the deposition accretion were taken into account. In fact, when the deposit temperature increases, some of the deposition mechanisms are affected (e.g. condensation, thermophoresis) and as a consequence the deposition process can be reduced. However, when the deposit builds

up, the flow dynamics around the probe changes as illustrated in Figure 7-45 which compares two different situations: at time zero, before injecting particles (left), and after a certain exposure time (right). This shows that the flow behaviour is quite different, in fact the deposit build-up generated a more aerodynamic shape, the flow attaches easily to the surface (Coanda effect (García Pérez, 2016)) and this reduced the deposition flux, in particular at the stagnation point where the contact area is smaller. As a consequence, when the deposit thickness increases, the dual effects of temperature and shape affect the deposit accretion.

For this reason, in the literature the effect of different tube shapes (i.e. circular, elliptic) have been investigated as solutions to reduce the fouling tendency (Bouris *et al.*, 2005; Haugen and Kragset, 2010). However, there are several problems linked to the use of alternative shapes and, among all, their high manufacturing costs make their promotion difficult.

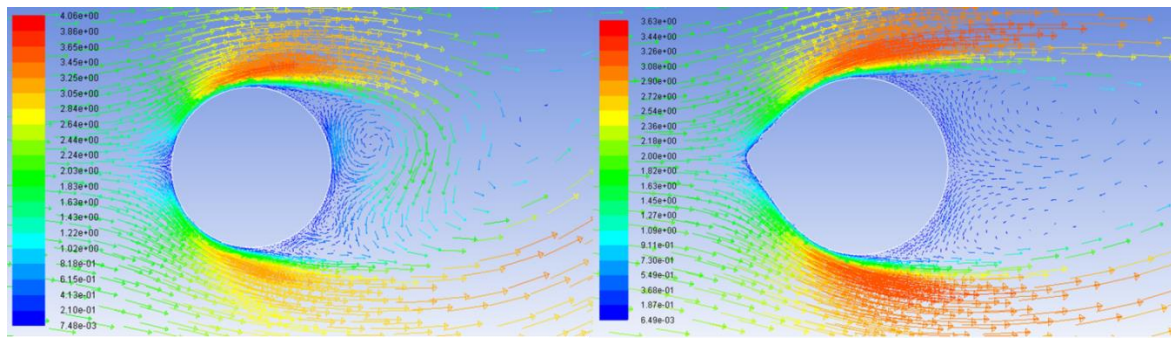


Figure 7-45: Gas velocity vectors around probe 1 (1st configuration) before deposit formation (left) and after deposit accretion (right) [m/s].

In the following simulations, these two factors were taken into account with the modified UDFs `DEFINE_GRID_MOTION` and `DEFINE_PROFILE` for the deposit shape and temperature predictions respectively. The UDFs (one `DEFINE_DPM_EROSION`, three `DEFINE_GRID_MOTION` and three `DEFINE_PROFILE`) for three probes had a total of ~ 700 lines. However, these UDFs made the simulations even more expensive and it was not reasonable to simulate five hours of exposure time with time step sizes of 10^{-3} s.

Therefore a solution to simulate the fouling for longer time was derived by observing that ash particle behaviour became stable after a few time steps and the deposition flux quasi- steady state once the particles and the flow were developed around the probes. This characteristic was used to update the mesh and the deposit temperature every certain number of time steps (e.g. 10-50 time steps). For example, the deposition flux was extrapolated and used to calculate the deposit thickness that would have accumulated after a few minutes. This value was then used to move the grid and increase the deposit temperature. After that, the deposition flux was set to zero and the same process was repeated again until the total exposure time was reached or until the simulation diverged.

This methodology was used for the model validation and the increment of the deposit thickness represented one of the biggest challenges. In fact, if the deposition flux calculated was used to predict the deposit accretion after a too long time, the mesh cells would overlap and degenerate into negative volumes or create areas with high temperatures which caused temperature divergence.

Some of the results applying the aforementioned methodology were reported below for the model validation.

7.7.2.1 Configuration 1 at 773 K surface temperature

The 3 modified UDFs were used to predict the deposition fluxes, the deposit shapes and temperatures. Figure 7-46 shows an example of temperature contour of the flue gas around probe 1, the shape of the deposit and its surface temperature after ~ 4.5 hours. Similar results were found for probes 2 and 3; the deposit temperature was higher on the upstream (thicker deposit) than sides and downstream which did not show almost any variations. The maximum deposit thickness was ~ 1.7 mm, 2.56 mm and 2.05 mm for probes 1-3.

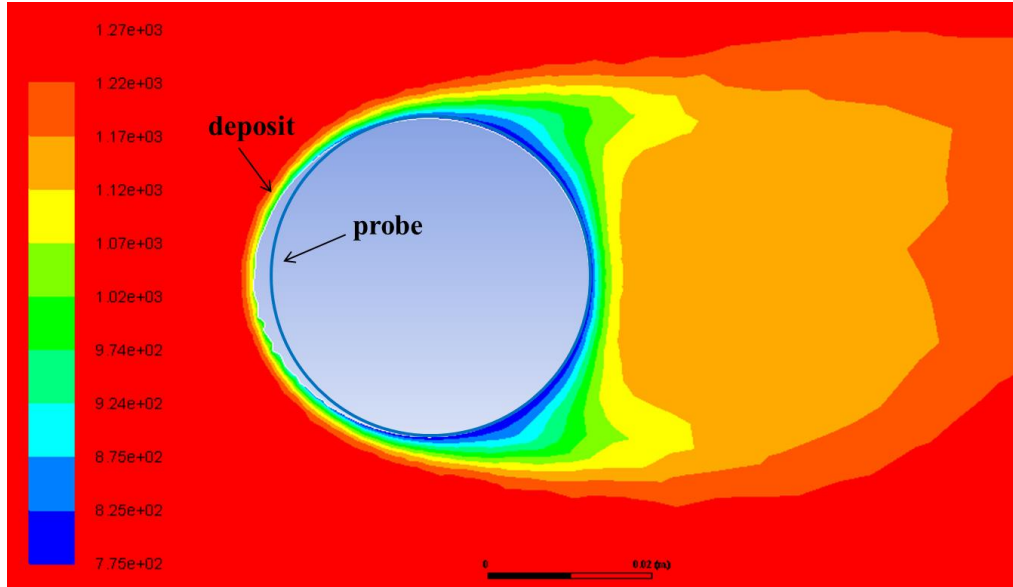


Figure 7-46: Temperature contour [K] around probe 1 (1st configuration, $d_t = 39$ mm) after ~ 4.5 hours of exposure time ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

The temperature values on the deposit surfaces were exported and plotted for the three probes in Figure 7-47. These results were similar to Figure 7-27 and had the same trend; in fact the temperature was higher on probes 2 and 3 than probe 1.

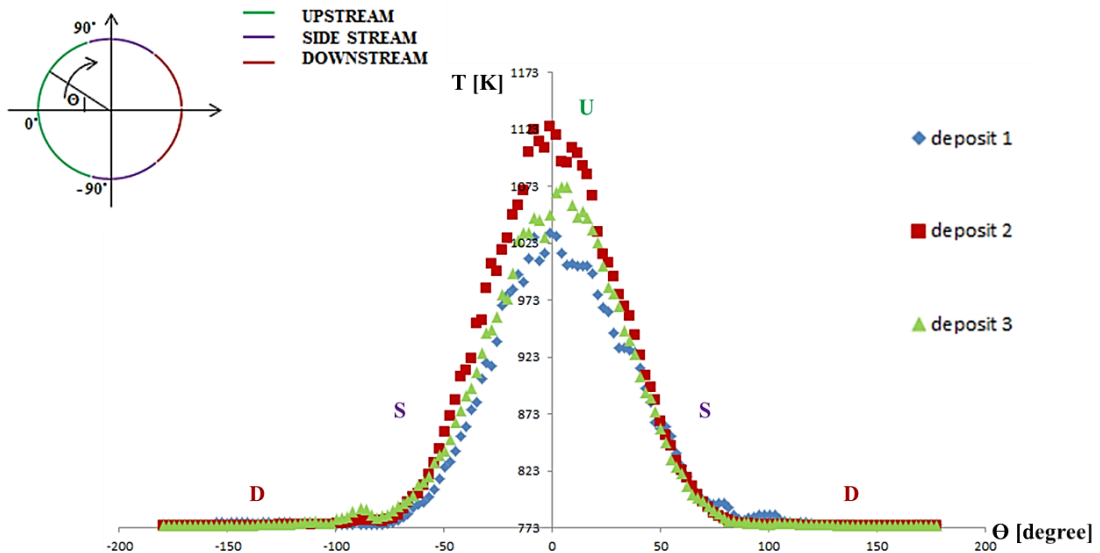


Figure 7-47: Predicted deposit temperature profile after ~ 4.5 hours on probes (1st configuration, $d_t = 39$ mm) at 773 K ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

In addition, an example of deposition flux around probe 1 has been plotted as function of the angle, after 3 hours and 4.5 hours (Figure 7-48). The results are comparable and this supports the methodology used to simplify simulations of deposit formation over a long exposure time introduced at the beginning of section 7.7.2. In fact, deposition fluxes were higher on the upstream than sides and downstream surfaces. However in Figure 7-48, it can be observed that deposition flux was higher on the sides of probe 1 at lower time which implies lower surface temperature and, therefore, more condensation.

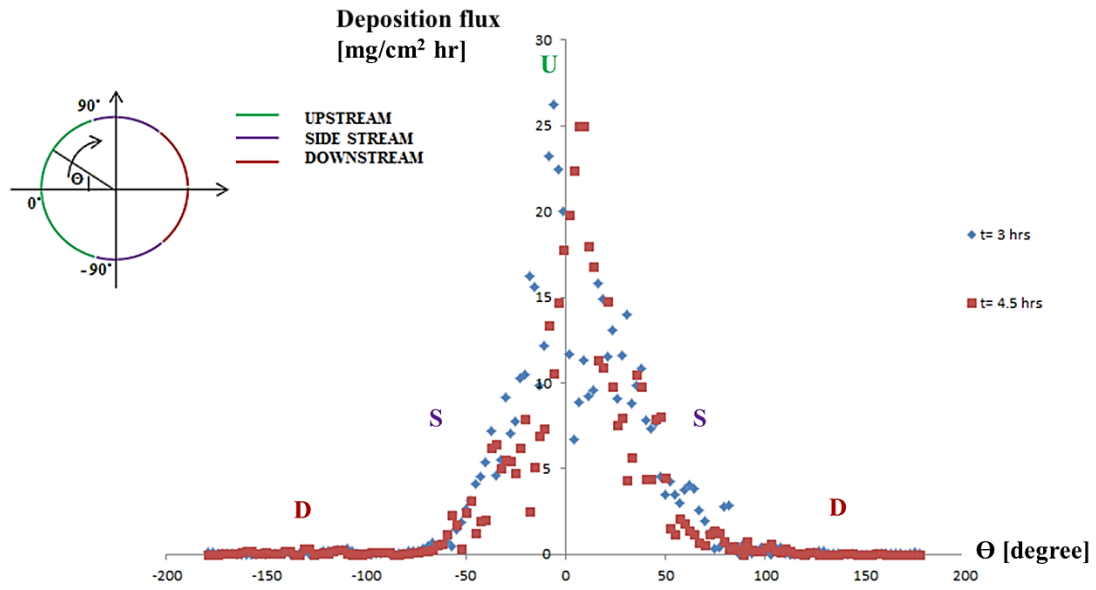


Figure 7-48: Predicted deposition flux after 3 hours and 4.5 hours on probe 1 (1st configuration, $d_t = 39$ mm) at 773 K ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

7.7.2.2 Configuration 2 at 773 K surface temperature

Figure 7-49 shows the contour of temperature for the gas and deposit accumulated on probe 1 in configuration 2 assuming a probe constant temperature of 773 K.

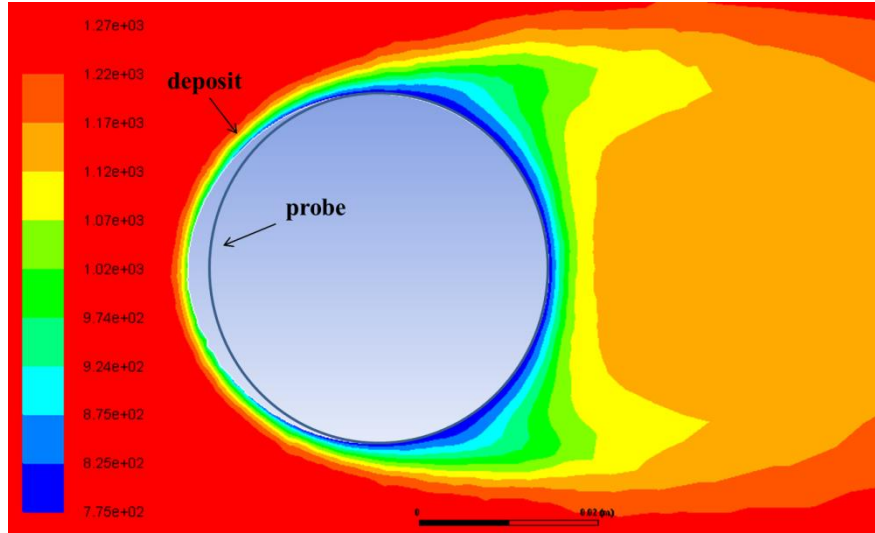


Figure 7-49: Temperature contour [K] around probe 1 (2nd configuration, $d_t=39$ mm) after ~ 4 hours of exposure time ($d_{min}=0.43$ μm , $d_{mean}=68$ μm , $d_{max}=535$ μm , polydispersion parameter $n=1.07$, $U_0=2$ m/s).

As expected, deposition was localised mainly on the upstream of the probes which implied a higher deposit surface temperature (Figure 7-50). The deposit temperature on the top was higher for probes 2 and 3 followed by probe 1. The maximum thickness values calculated after 5 hours on probes 1, 2 and 3 were 2.62 mm, 3.7 mm and 3.62 mm respectively.

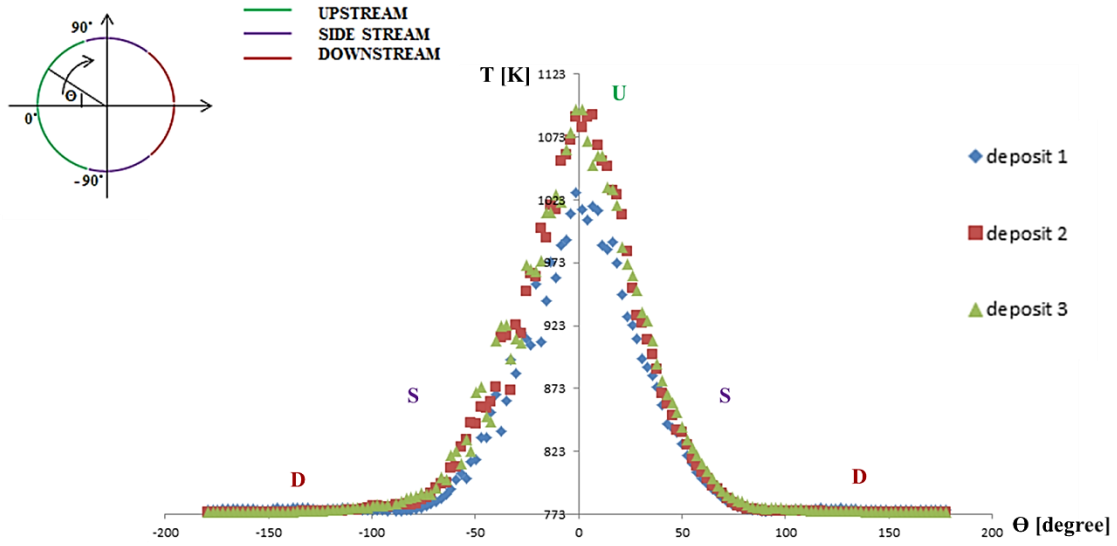


Figure 7-50: Predicted deposit temperature profile after ~ 4 hours on probes (2nd configuration, $d_t= 39$ mm) at 773 K ($d_{min}= 0.43$ μm , $d_{mean}= 68$ μm , $d_{max}= 535$ μm , polydispersion parameter $n= 1.07$, $U_0= 2$ m/s).

In this Chapter, the dynamic nature of deposition flux has been studied and, for this reason, deposition flux calculations included the combined effect of fluid dynamics (deposit shape) and temperature conditions around the probes.

Deposition fluxes were compared at different exposure times and the trend has demonstrated to be the same for all the probes, therefore an example of deposition flux has been plotted after 2.5 hours and 4 hours around probe 1 using the second configuration at 773 K (probe surface temperature). In Figure 7-51 the deposition fluxes were comparable at different exposure times; this confirms that the simplification used in this study, to carry out longer simulations, is acceptable. However, for lower times the deposit flux values on the sides and downstream surfaces were higher than after 4 hours. In fact, the deposit surface temperature increases over time because of the deposit accretion; this reduces the vapour condensation flux (considered particularly important for the deposit growth on the sides and rear sides). Whereas, on the upstream surfaces, inertial impaction is the main deposition mechanisms and, at higher temperatures (longer exposure time), particles are stickier; therefore they are characterised by higher deposition flux (as observed in 7.7.1.5).

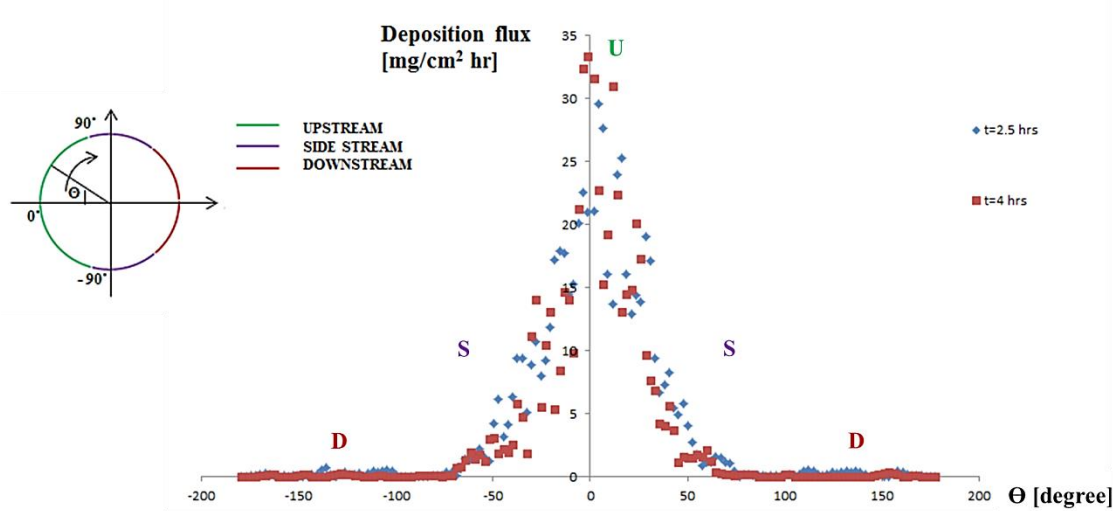


Figure 7-51: Predicted deposition flux after 2.5 hours and 4 hours on probe 1 (2nd configuration, $d_t = 39$ mm) at 773 K ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

7.7.2.3 Configuration 2 at 873 K surface temperature

Finally, similar simulations were run to study the deposit accretion on the probes in configuration 2 with probe temperatures at 873 K. In this case the simulation was stopped slightly before five hours because of a temperature divergence (Figure 7-52).

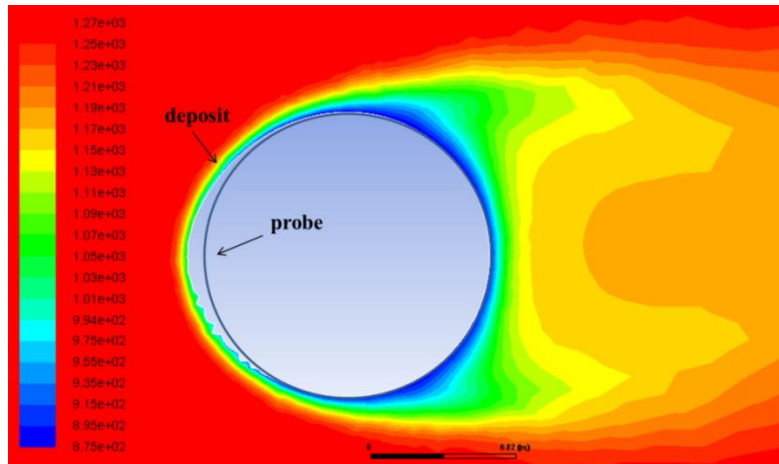


Figure 7-52: Temperature contour [K] around probe 1 (2nd configuration, $d_t = 39$ mm) after ~ 5 hours of exposure time ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

Also in this case the model was able to identify the main deposit location and the effect of the deposit build-up on the surface temperature for the three probes (Figure 7-53). The maximum thickness values calculated after 5 hours on probes 1, 2 and 3 were 2.62 mm, 3.7 mm and 3.62 respectively.

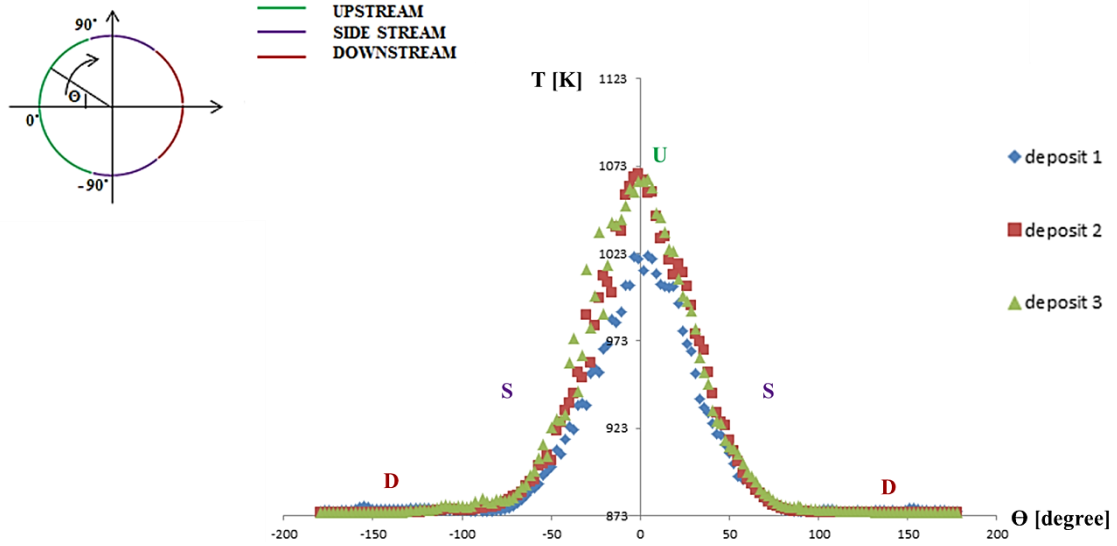


Figure 7-53: Predicted deposit temperature profile after ~ 5 hours on probes (2nd configuration, $d_t= 39$ mm) at 873 K ($d_{min}= 0.43$ μm , $d_{mean}= 68$ μm , $d_{max}= 535$ μm , polydispersion parameter $n= 1.07$, $U_0= 2$ m/s).

As in section 7.7.2.2, the total deposition flux was plotted as function of the angle around probe 3, after 3 and 5 hours (Figure 7-54). The results confirmed that, at higher surface temperatures (thicker deposits), deposit decreases more on the downstream surfaces than upstream surfaces as already commented in Figure 7-51.

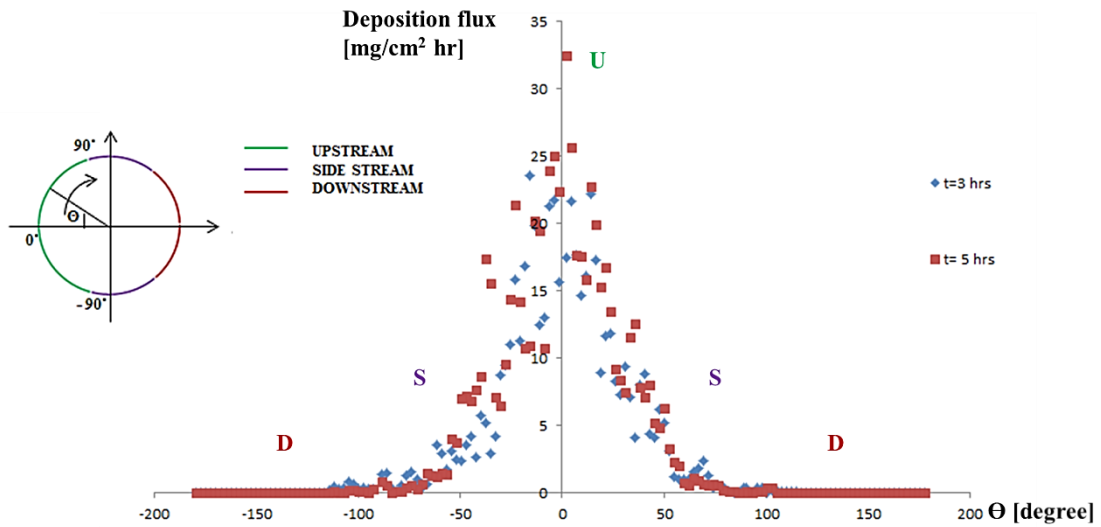


Figure 7-54: Predicted deposition flux after 3 hours and 5 hours on probe 3 (2nd configuration, $d_t = 39$ mm) at 873 K ($d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

7.7.2.4 Summary

The results in this section gave a good approximation of the deposit build-up, of the shape and the surface temperature which tend to become similar to the gas surrounding temperature. However, it is important to highlight that including the dynamic effect of deposit temperature and shape on the deposit formation, it was not always possible to cover the entire experimental exposure time (five hours). In fact, divergence of temperature and momentum, generally caused by the presence of areas at high temperatures or spiky shapes, did not allow the simulation completion.

The results generated by using this latter approach (case 2) were comparable to the first one (case 1), with deposit thicknesses thinner ($\sim 35\%$) than the ones in 7.7.1. This could be attributed to the effect of the increased surface temperature on the vapour condensation and on the thermophoresis. Moreover, the enhanced particle stickiness, at higher temperatures, could be balanced by the dynamic mesh effect which makes the deposit surface smoother and reduces the particle deposition. Finally, the numerical errors could be another reason for the discrepancy.

In Chapter 3, the double coupled wall was presented as additional method to predict the deposit temperature and study the temperature gradient inside the deposit layer. This

method was not used for the model validation and further studies are necessary to improve this approach (e.g. meshing, deposit properties, etc.).

7.8 Role of condensation

The presence of the alkali vapours in the hot flue gas has been investigated to understand their influence in the deposition process. During the experiments, it was not possible to measure the alkali vapour concentrations, therefore the species Na_2SO_4 was chosen and deposition was studied at different values (1, 10 and 100 ppm) using the first probes' configuration at different surface temperatures (i.e. 773, 873 and 973 K).

The amount of alkali compound vapours that condense on the surface of heat exchangers depends on their concentration in the flue gases and on the surface temperature. However, condensation is more likely to happen on the surfaces of probes at a temperature lower than the alkali compounds' dew point.

The total deposition fluxes were calculated on the three probes using Eq. (7-1) as function of the alkali vapour concentrations at probe surface temperature of 773 K and the results (Figure 7-55) show that deposition increases in the presence of higher vapour concentrations in the flue gas.

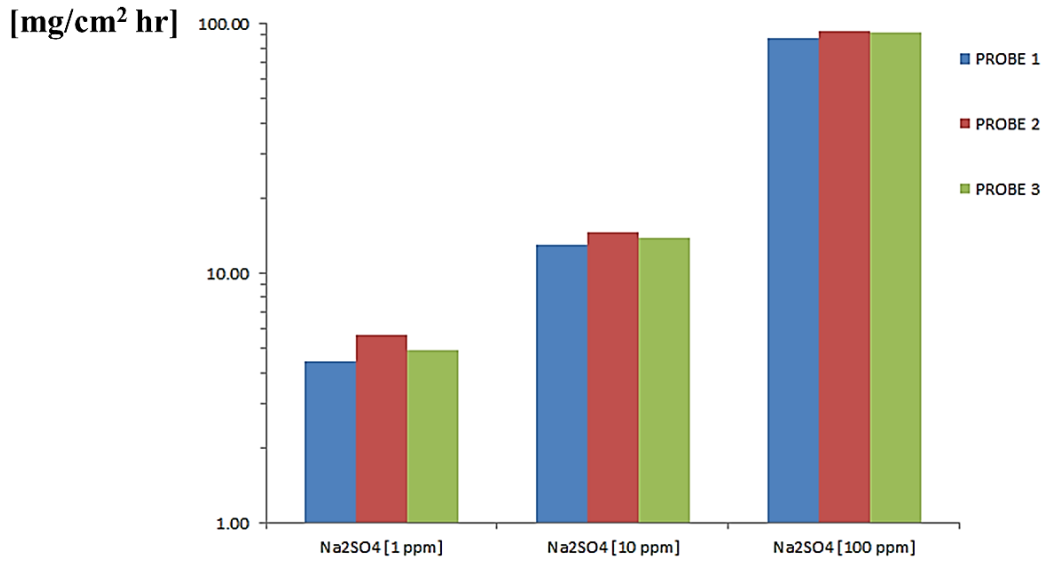


Figure 7-55: Total deposition fluxes at different concentrations of Na₂SO₄ on ceramic probes (1st configuration, $d_t = 39$ mm, at 773 K, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

In section 7.5, it was stated that vapours contribute to the surface stickiness and to the condensation flux itself. The contributions of the total deposition flux (m_{tot}) and the flux of particles deposited in the presence of a sticky surface (m_s) were calculated for the three probes at different concentrations of alkali vapour (Na₂SO₄) and three different probe temperatures and the results are given in Table 7-4. The numbers show that the total deposition fluxes obtained from the experiments were better predicted by models that used a concentration of Na₂SO₄ ~ 1 ppm (value used for all the simulations).

The deposition flux of particles deposited in the presence of a sticky wall (m_s) was calculated simplifying Eq. (7-1) (i.e. $(P_s \frac{dm_p}{dA} \sin(\gamma))$). The results show that the total deposition fluxes (m_{tot}) and the flux of particles deposited in the presence of a sticky surface (m_s) increase with the alkali vapour concentration (from 1 to 100 ppm) (Table 7-4). Moreover, the vapour condensation flux ($m_{c,A}$) was added to the particle deposition flux and its value contributed to the total deposition flux (m_{tot}).

At constant Na₂SO₄ concentrations (1 and 10 ppm) and increasing probe surface temperatures, m_s decreases (reduced driving force) and m_{tot} increases (increased particle stickiness). However, an inversion can be observed at Na₂SO₄ 100 ppm as the total

deposition flux increases from 773 K to 873 K but it decreases from 873 K to 973 K for all the probes. This may happen because, higher alkali concentrations (100 ppm) are more affected by an increase of temperature and have a bigger impact on the total deposition flux.

Table 7-4: Alkali sulphate vapour contributions to the total deposition flux (1st configuration, $d_t = 39$ mm, at 773 K, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

	T_{PROBE} [K]	PROBE 1 [mg/cm ² hr]		PROBE 2 [mg/cm ² hr]		PROBE 3 [mg/cm ² hr]	
Na_2SO_4		m_{tot}	m_s	m_{tot}	m_s	m_{tot}	m_s
1 ppm	773	4.76	$1.09 \cdot 10^{-3}$	6.03	$1.19 \cdot 10^{-3}$	5.28	$1.15 \cdot 10^{-3}$
	873	4.97	$9.52 \cdot 10^{-4}$	6.35	$1.06 \cdot 10^{-3}$	5.52	$9.76 \cdot 10^{-4}$
	973	5.27	$8.89 \cdot 10^{-4}$	6.65	$1.07 \cdot 10^{-3}$	5.80	$9.38 \cdot 10^{-4}$
10 ppm	773	13.9	$1.06 \cdot 10^{-2}$	15.7	$1.15 \cdot 10^{-2}$	15.1	$1.25 \cdot 10^{-2}$
	873	14.1	$1.05 \cdot 10^{-2}$	16.0	$1.12 \cdot 10^{-2}$	15.1	$1.06 \cdot 10^{-2}$
	973	14.2	$9.49 \cdot 10^{-3}$	16.3	$1.09 \cdot 10^{-2}$	15.3	$9.61 \cdot 10^{-3}$
100 ppm	773	107	$1.07 \cdot 10^{-1}$	113	$1.15 \cdot 10^{-1}$	112	$1.12 \cdot 10^{-1}$
	873	109	$1.01 \cdot 10^{-1}$	117	$1.10 \cdot 10^{-1}$	116	$1.08 \cdot 10^{-1}$
	973	105	$9.71 \cdot 10^{-2}$	112	$1.10 \cdot 10^{-1}$	111	$9.85 \cdot 10^{-2}$

From previous modelling results (Chapter 4), it was noticed that the presence of alkali sulphate vapours makes the deposit more uniform around the probes (Figure 4-8). However, with the operating conditions used in this study (Na_2SO_4 [1 ppm] and probe surface temperatures 773/873 K), alkali vapour condensation partially contributes to the total deposition flux ($m_s \sim 0.02\%$ and $m_{c,A} \sim 16\%$), whose main mechanism is related to be the inertial impaction of solid ash particles.

7.9 Summary

In this Chapter, the procedures shown in Chapter 3 and tested for simple cases in Chapter 4 were applied to the probe configurations used during the experiments with more realistic boundary conditions. The sticking model to predict deposition was derived from previous correlations found in the literature which were modified and combined. In fact, this thesis aimed at developing a model to predict deposit formation on heat exchanger tubes by combining several deposition mechanisms (only the chemical reactions and Brownian motion were neglected) and the stickiness of the ash

particles and vapour condensation (which is among the main initiators of fouling, in particular on a clean tube surface).

Despite the approximations (i.e. 2D geometry, material properties, sticking criteria etc.), the model developed in this work produced acceptable predictions of deposit formation on ceramic air cooled probes during combustion of Daw Mill-12 wt.% Miscanthus. Firstly, the deposition flux was calculated assuming a constant deposit shape and temperature. Successively, the dynamic effect of the deposit growth and, as a consequence, its increasing temperature was included. This step added some challenges such as solutions that sometimes diverged, high computational costs, additional coding etc. However, the results were promising and represented a good starting point for future model improvements.

8 GENERAL DISCUSSION

8.1 Introduction

This chapter brings together discussions on the work done during the course of this research, focussed on developing models for deposit formation on heat exchangers. Some of the choices and approximations made to develop the CFD models and to run the experiments are discussed in the following sections and a sensitivity analysis has been included.

8.2 Methodology-targeted modelling and experiments

In this work, deposition on heat exchangers has been investigated combining CFD modelling with an experimental approach. CFD, with recent computer technology, has overtaken previous models (e.g. empirical indices and mechanistic models) and is now recognised to be one of the best tools to study deposition (Tomeczek and Waclawiak, 2009; García Pérez, 2016; Yang *et al.*, 2018). In fact, it can be used to characterise the gas flow and ash particle trajectories, predict the deposit accumulation and the heat and mass transfer. The software Fluent[®] has been used since it is commercially available; it was integrated with modified UDFs, functions in C language that were compiled in Fluent[®] to describe properties, boundary conditions, etc.

The experimental and modelling approaches have been demonstrated to be often complementary and their combination has helped understanding aspects of the phenomenon when one of the approaches was not satisfactory. In fact, the experiments gave tangible results but the CFD simulations were useful to clarify some details that could not be observed during the experiments (e.g. fly ash trajectories, deposit accretion, temperature profile, etc.). Moreover, the experiments provided data to be used as boundary conditions and material properties which were fundamental to recreate the physical conditions of the CFD domain and improve the quality of the predictions. However, in absence of real material properties (e.g. deposit properties), data from the literature were used and this may have had an impact on the surface temperature and, as a consequence, on the deposition flux predictions.

8.3 Limitations of this study

In this work, some of the results previously obtained from the experiments have been applied to build a CFD model (e.g. geometry, ash particle size distribution and composition, gas and particle velocity, probe temperature, etc.) and for its validation in particular conditions. The main challenges faced during the development of the framework model and its application to particular conditions have already been highlighted in Chapters 3, 4 and 7.

Under the particular conditions investigated, the model has been demonstrated to identify the right locations of deposition on the ceramic probes and to get deposition fluxes comparable with the experimental results also when the bend ~ 0.5 m downstream of the last probe was neglected ($< 4\%$ of deposition flux).

In addition, the geometry was simplified to a 2D domain to reduce the high computational costs that a 3D geometry would have determined. In fact, already with a 2D geometry, simulations took up to a week (or more) to be completed, in particular when the Rosin Rammler ash particle size distribution was included and the modified UDFs `DEFINE_PROFILE` and `DEFINE_GRID_MOTION` were used.

This simplification has been already widely used in the literature (e.g. by Manuel Garcia Perez, Jerzy Tomeczek, Krzysztof Waclawiak, Xin Yang, Roman Weber, etc.) and it has been demonstrated to correctly identify the main areas where deposition takes place and to give a good prediction of the experimental results.

3D geometries have been used in the literature and in industry to study the extent of deposition, generally in different areas of boilers rather than specific zones (Schulze *et al.*, 2003; Kær *et al.*, 2006; Magda, 2012), and to identify the most critical areas where deposition takes place by changing some operating conditions and using different fuels. This was out of the scope of this work which was focussed on studying fouling in specific areas of the combustion rig and on the identification of the main deposit formation mechanisms.

However, experimental results have emphasized the 3D nature of deposit formation; in fact it was observed that the deposit thickness varies along the ceramic probe (as can be

observed from the pictures of deposits in Chapter 6) and a 2D geometry can only show a single average value of the thickness. Moreover, the vortex shedding has a 3D nature already for Reynolds number > 200 and a 2D domain represents a simplification which could influence in particular the behaviour of small particles on the rear side of the tubes and, as a consequence, predictions of their deposition. In fact, the model developed in this work generally underestimated the deposition flux on the sides and downstream (up to $\sim 90\%$ of deposition flux) and overestimated the deposition flux on the upstream surfaces (up to $\sim 30\%$ of deposition flux).

The development of this model required a deeper knowledge not only about fouling in combustion of pulverised fuels but also in CFD and coding. In fact, the need for coding and debugging the UDFs for the prediction of the shape and deposit temperature proved to be particularly time consuming.

Material properties have demonstrated to be significant for deposit predictions. However, in the absence of experimental measurements, they were found from previous works in the literature, where the gap in terms of fuel characterisation (especially for biomass) is still quite big.

Another limitation was represented by the ash particle size distribution which was obtained collecting ash from the ports along the vertical section of the combustor. Ideally fly ash samples should have been extracted from the combustor using an isokinetic sampling to characterise the ash particle distribution present in the flue gas and impacting the ceramic probes (Srinivasachar *et al.*, 1990; Beckmann *et al.*, 2016). This solution was not available and the fly ash collected from the ports where the ceramic probes were located was taken to represent the fly ash that caused deposition. These samples were analysed with a laser diffraction particle sizer by Doosan Babcock and the experimental measurements were used to fit the Rosin Rammler model and to determine the parameters needed in Fluent[®] (d_{min} , d_{max} , d_{mean} and n) (Bailey *et al.*, 1983). These latter were implemented in the software and, despite the approximation, they gave a good prediction of the deposition fluxes.

In the following paragraphs, some of the main parameters studied during the PhD have been discussed.

8.4 Ash particle trajectories

Ash particles were studied with the DPM model as single injections (one diameter) and Rosin Rammler ash particle size distribution. Trajectories of particles with diameter $d_p > 10 \mu\text{m}$ were characterised by bounces on the surface of the probe and rebounds whose energy increased with their diameters. Particles smaller than $10 \mu\text{m}$ followed the flue gas streamlines around the probe and hit the rear side because of their low inertia.

Different geometries have been used in the course of the study, from single tube to multiple probes in Cranfield's combustor rig. However, in the presence of other probes or if the geometry was narrower, bigger particle trajectories were modified. In fact, after bouncing on the upstream surfaces they rebounded onto the neighbouring probes or were deviated by the presence of the chamber walls towards other probes. Moreover, simulations showed that bigger particles can hit the downstream surfaces of the upstream probes after rebounding from the upstream surfaces of the downstream probes. This was also confirmed by SEM images of deposits around different sides of the probes (section 6.3.2); particle measurements with Image J showed that bigger particles deposited on the upstream of probes or on the sides of upstream probes and medium and smaller particles were found in the deposits on the sides and on the back of the probes.

The analysis of single particle size injections allowed a good understanding of the particle behaviour. However, in real boilers ash particles are present as distributions with different particle diameters. The Rosin Rammler particle size distribution model was chosen as it has frequently been used to characterise fly ash size distributions, is available in Fluent[®] and widely used in the literature (Wacławiak and Kalisz, 2011; Beckmann *et al.*, 2016; García Pérez, 2016).

One of the view ports along the combustor in Cranfield was used to observe the fly ash "rain" in the flue gas and the deposit accretion on probe 1, which was almost at the same height as the view port (Figure 8-1 a, b, c). The pictures taken from the view port show the incandescent ash particles and some of their hits on the deposit surface. In Figure 8-1, b it is also possible to observe a particle which seems to be rebounding and Figure 8-1, c shows the instant when a particle was settling. These images do not distinguish the particles, therefore the CFD model supported the experimental evidence

and showed the trajectories of the ash particle size distribution obtained by fitting the Rosin Rammler model with the experimental results (Figure 8-1, d). Simulations were all transient but, only for an illustrative purpose, Figure 8-1, d shows the trajectories for different ash particle diameters with a steady approach which allows a clear picture of single particle paths. In fact, it can be seen that bigger particles (green) bounce on the surface of the probe and rebound, while smaller particles (blue) follow the gas path around the probe (and they do not hit the rear side if the gas is steady).

The use of a Rosin-Rammler particle size distribution increased substantially the computational costs and, in the post-processing, it was more difficult to distinguish single particle trajectories but it was still possible to observe the different trends between bigger and smaller particles (section 7.4).

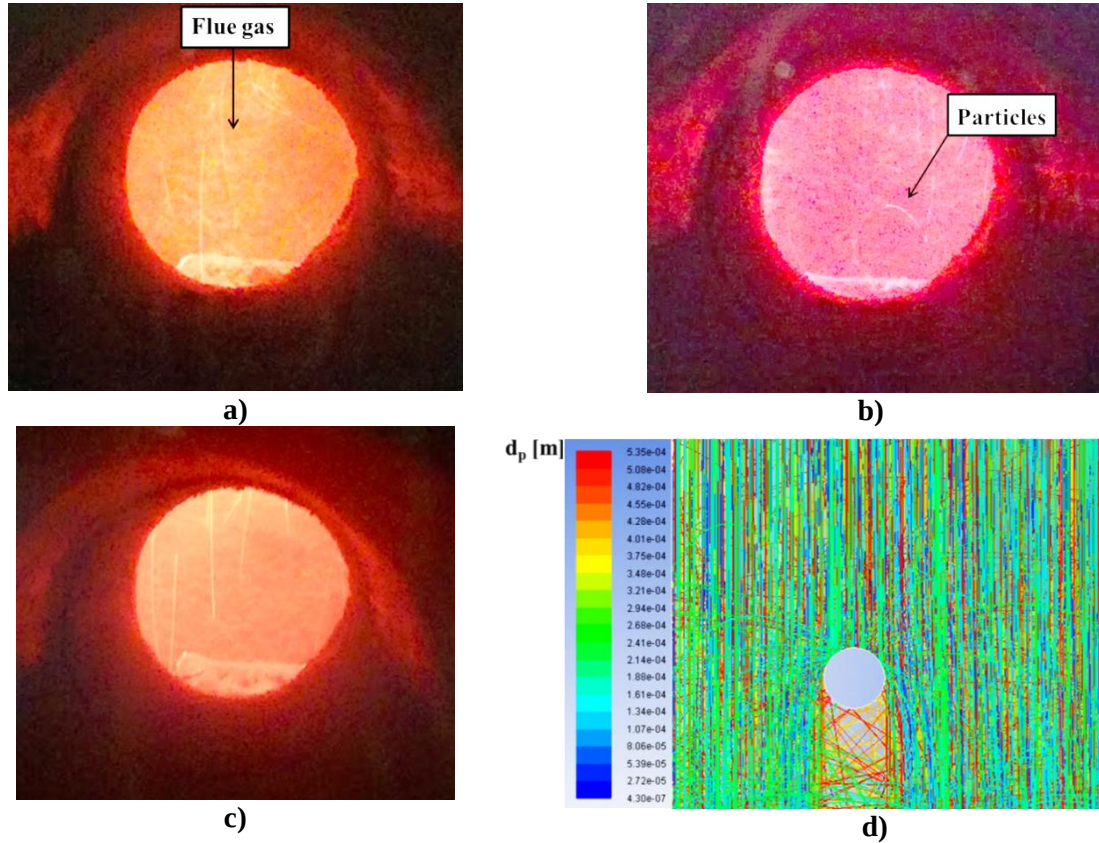


Figure 8-1: a, b, c) Fly ash particle trajectories and impaction observed from one of the view ports during combustion of Daw Mill-12 wt.% Miscanthus; d) steady ash particle trajectories from CFD simulations (773 K, $d_t = 39$ mm, $d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2\text{m/s}$).

8.5 Alkali vapour concentration

The presence of alkali compound vapours in the flue gas was investigated as their condensation is generally responsible for the formation of an initial sticky layer on clean surfaces; this can enhance the particle deposition and make it more uniform around the probes. Moreover, the condensation flux was added to the particle deposition flux for the determination of the total deposition flux.

The measurement of the alkali vapour concentration in the flue gas during the experiments was not carried out and it was difficult to predict the amount of vapours released during combustion. This depends on the fuel and the ratio of coal and biomass. Higher biomass content may release more vapours and determine the formation of deposits with different chemical compositions and deposition fluxes. However, during all the experiments, the same blend of coal and biomass was used and, as a consequence, the results in terms of deposition fluxes and chemical composition were not remarkably different.

Therefore, the effect of the vapour condensation was simulated and deposition was studied at different concentrations of Na_2SO_4 (1, 10 and 100 ppm), which was chosen as examples of potential vapour levels. The results of the simulations showed that with increasing amounts of Na_2SO_4 vapour, the total deposition flux increased all around the probe but with the highest value still on the upstream surface (Figure 8-2).

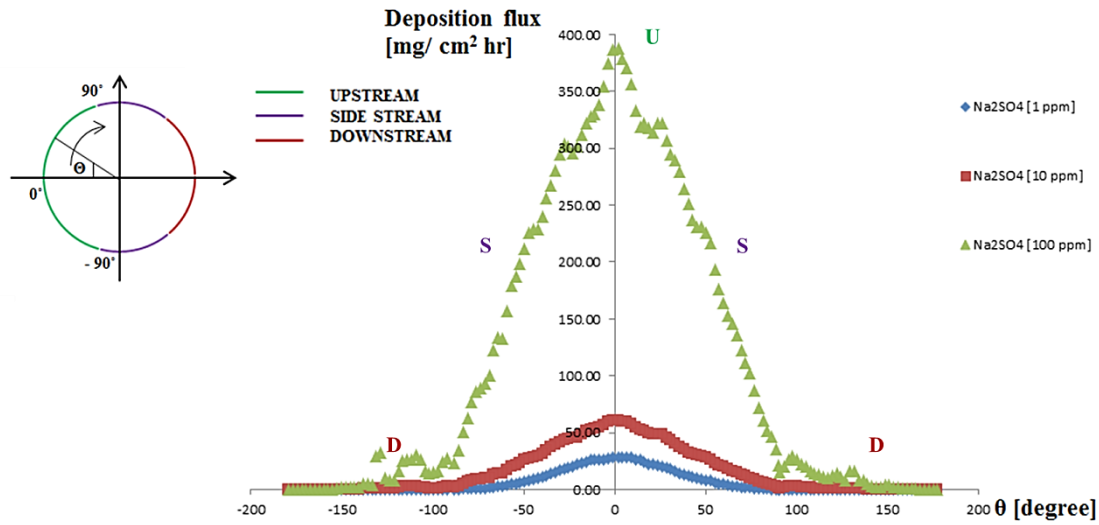


Figure 8-2: Predicted total deposition flux around probe 2 (773 K, $d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43 \mu\text{m}$, $d_{mean} = 68 \mu\text{m}$, $d_{max} = 535 \mu\text{m}$, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at different concentrations of Na_2SO_4 .

The total deposition fluxes calculated at 1, 10 and 100 ppm of Na_2SO_4 (Figure 8-3) showed that the experimental results were better predicted by models that used a concentration of $\text{Na}_2\text{SO}_4 \sim 1$ ppm (value used for all the simulations). However, it needs to be highlighted that in the reality several alkali vapours are present in the gas and this study has simplified the phenomenon to understand the role of condensation on the total deposition flux.

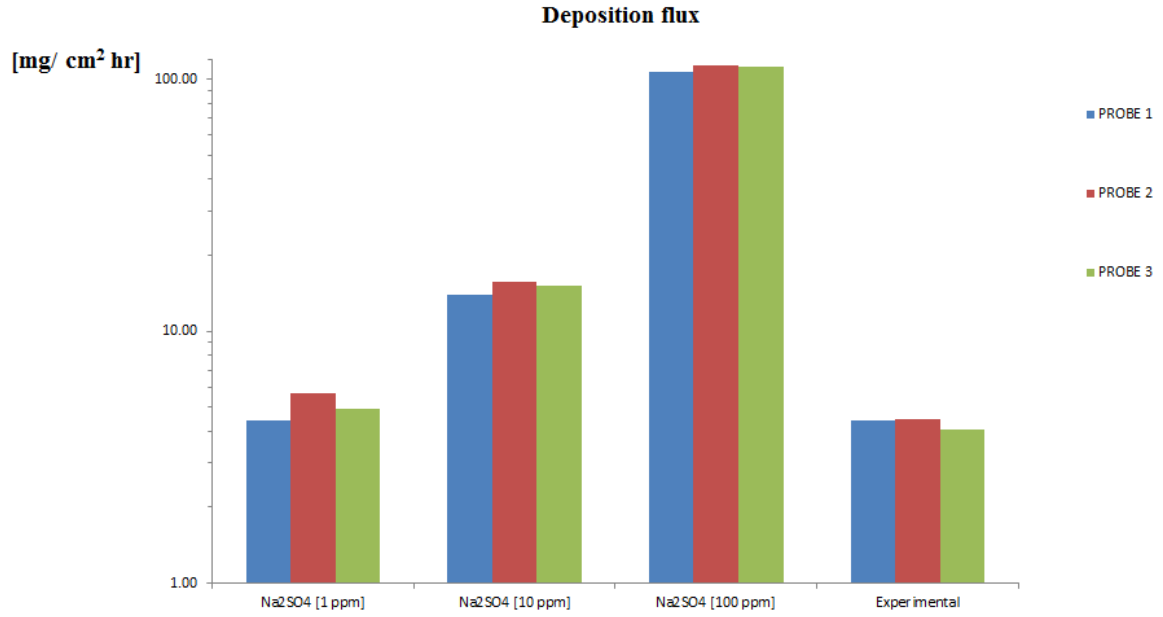


Figure 8-3: Total deposition fluxes around probes (773 K, $d_t = 39$ mm) using the 1st probes' configuration from experiments and model predictions ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at different concentrations of Na_2SO_4 .

The results about the alkali vapour concentration obtained for the model validation (Chapter 7) were different from some preliminary qualitative predictions in (Chapter 4, Figure 4-30-Figure 4-33). In that case, deposition was studied on four probes ($d_t = 39$ mm) at 773 K for a given Rosin Rammler ash particle size distribution ($d_{min} = 1$ μm , $d_{mean} = 40$ μm , $d_{max} = 200$ μm , $n = 0.8$), at increasing Na_2SO_4 concentrations (1, 10 and 100 ppm), $T_g = 1273$ K, and $U_0 = 4$ m/s. The model took into account the stickiness of the surface (m_s) and the particles (calculated with the model suggested by Beckmann *et al.*, (2016) for Middelburg coal). The condensation flux ($m_{c,A}$) was not included and the normalised deposition flux did not vary significantly with the alkali concentration. The discrepancy between the trends obtained in Figure 4-30-Figure 4-33 and Figure 8-2 highlights that the condensation flux ($m_{c,A}$) contributes to the total deposition (included in the model validation) and demonstrates the importance of selecting the right sticking models and boundary conditions for the model predictions.

8.6 Effect of the surface temperature

Deposition was studied at different probe surface temperatures; simulations were run at 773 K, 873 K and 973 K while experiments were run only at 773 K and 873 K using the second configuration of probes varying the cooling air flow rate. However, from the experimental results it was difficult to understand the effect of the ceramic surface temperature on the deposition flux because of ash loss (e.g. probe 2 at 873 K) and measurement errors. Moreover, while in the simulations the ceramic probe was at a constant temperature, in the reality there is always a radial distribution of the temperature which was found to be more fluctuating (e.g. $500^{\circ}\text{C} \pm 19\%$). Therefore, CFD simulations were run to clarify the role of the surface temperature in the deposition process and a comparison between experimental and modelling results is in Figure 8-4 for the second probes' configuration.

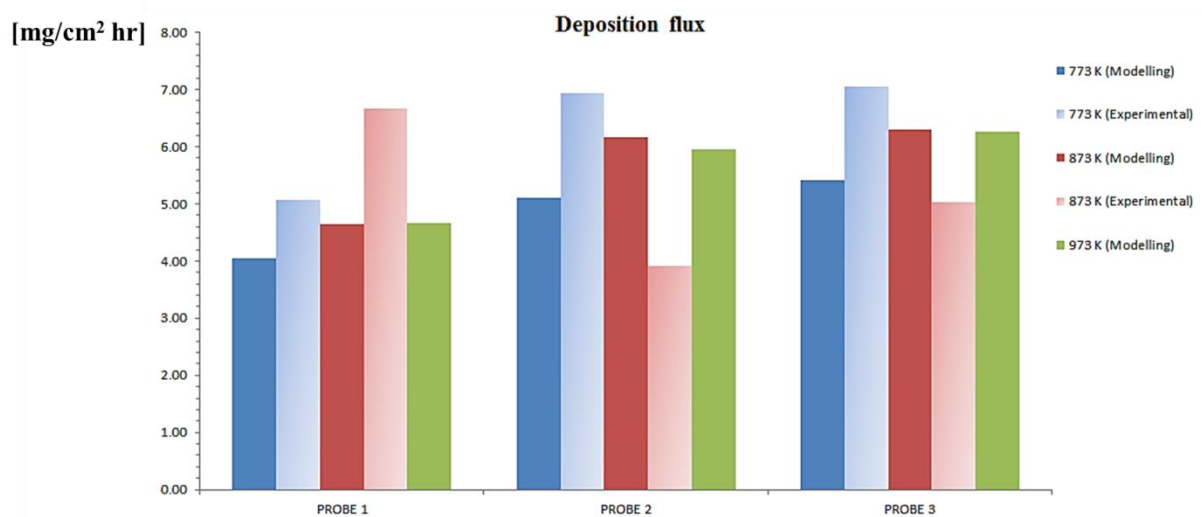


Figure 8-4: Measured and predicted total deposition fluxes around probes ($d_t = 39$ mm) using the 2nd probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at Na_2SO_4 [1 ppm] and different probe surface temperatures.

These simulations were run also for the first probes' configuration (Figure 8-5). The modelling results showed that deposition fluxes tended to increase with the surface temperature. In fact, even if the surface stickiness depends on the vapour condensation, negatively affected by an increase of the surface temperature, the total deposition flux

increment may be due to the ash particles whose stickiness is enhanced at higher temperatures (lower viscosity).

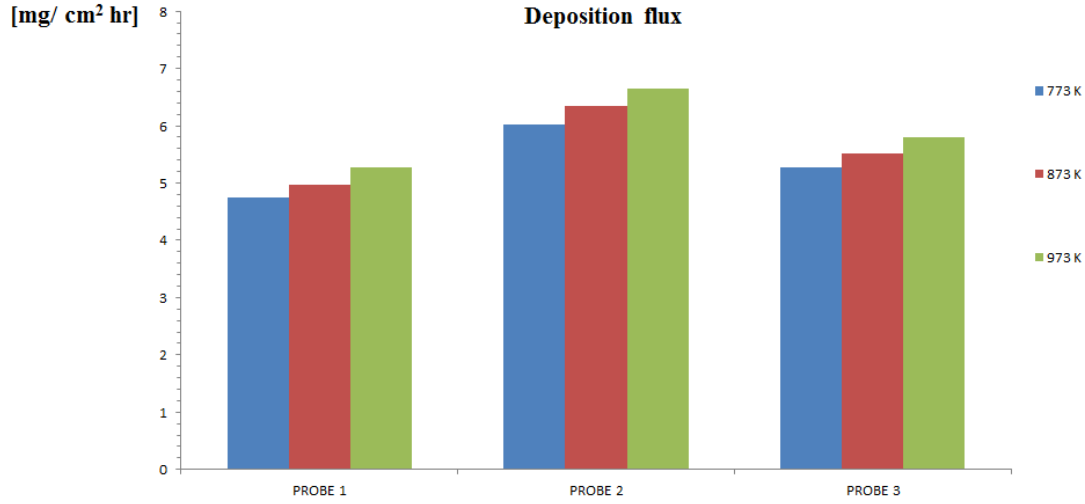


Figure 8-5: Predicted total deposition fluxes around probes ($d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at Na_2SO_4 [1 ppm] and different probe surface temperatures.

Additional simulations were run to predict the amount of ash particles that deposit in the presence of an alkali vapour layer (m_s) at different surface temperatures (773, 873 and 983 K) and vapour concentrations (1, 10 and 100 ppm). The results showed that the flux of particles deposited for previous vapour condensation ($\sim 10^{-3}$ - 10^{-1} mg/cm² hr), was affected by an increase of the surface temperature, in particular on the sides and downstream surfaces (section 7.8). An example is in Figure 8-6 for Na_2SO_4 1 ppm (Appendix F).

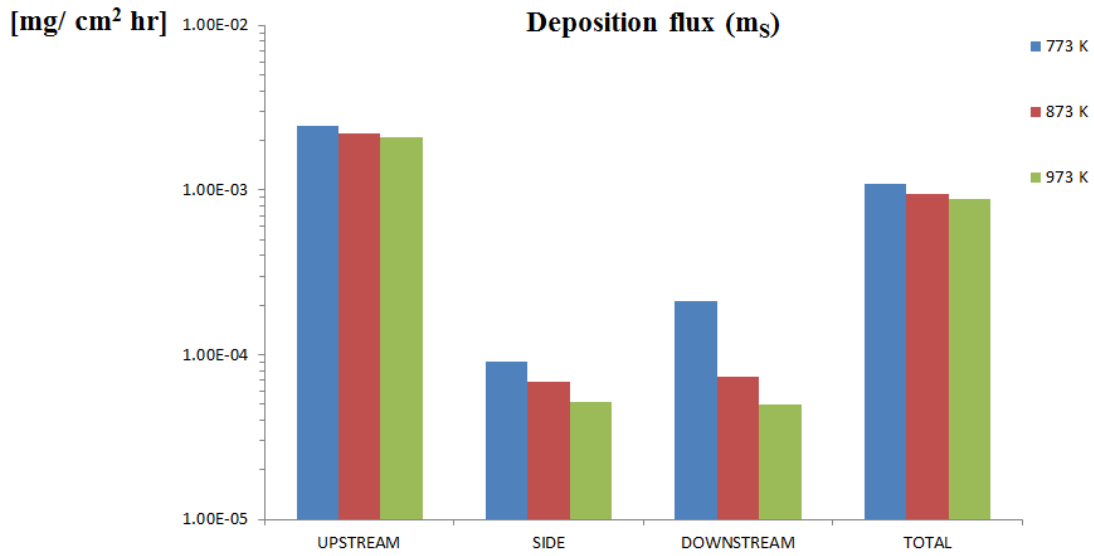


Figure 8-6: Predicted deposition fluxes due to the stickiness of the surface around probe 1 ($d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at Na₂SO₄ [1 ppm] and different probe surface temperatures.

Finally, condensation increases the total amount of deposit but the main mechanism responsible for deposition is represented by the impaction of solid ash particles whose deposition depends on their stickiness at the moment of the impact.

8.7 Grid motion

Predictions of deposit shape were carried out by modifying DEFINE_DPM_EROSION UDF to calculate the deposit thickness and update the cylinder nodes in DEFINE_GRID MOTION UDF. However, the dynamic mesh with “remeshing” option required the use of a triangular mesh rather than a structured one.

The use of an unstructured mesh can compromise the quality of the results and the convergence; therefore solutions had to be found to improve the predictions of deposit formation (e.g. mesh refinement around probes, using interiors to make the mesh finer around probes, etc.) (section 7.2). In this study, three different meshes were realised varying the number of nodes around the cylinder and it was verified that the variation of the grid would not affect the deposition results (Appendix B). However, it was not possible to verify the adequacy of all the meshes realised in the work (different

geometries, one and multiple probes) to study deposition. In fact, this operation is very time consuming and computationally expensive.

One of the biggest challenges while studying the grid motion was the generation of negative volumes which had also been reported in previous researches (e.g. Waławiak and Kalisz, 2012; García Pérez, 2016). In fact, it was found that if the deposit was accumulated for too long before activating the grid motion option, the mesh movements were too big (with a spiky shape) and caused an overlap of the neighbouring faces, also called negative volume error, which did not allow the completion of the simulation.

DEFINE_GRID MOTION UDF can be applied at each time step; however this method would not be feasible to predict deposition after a long exposure time. In fact, this problem arose during the model validation activity and it was overcome by updating the mesh every a certain number of time steps (e.g. 20 to 50). An example of gradual deposit accretion and its shape is given in Figure 8-7.

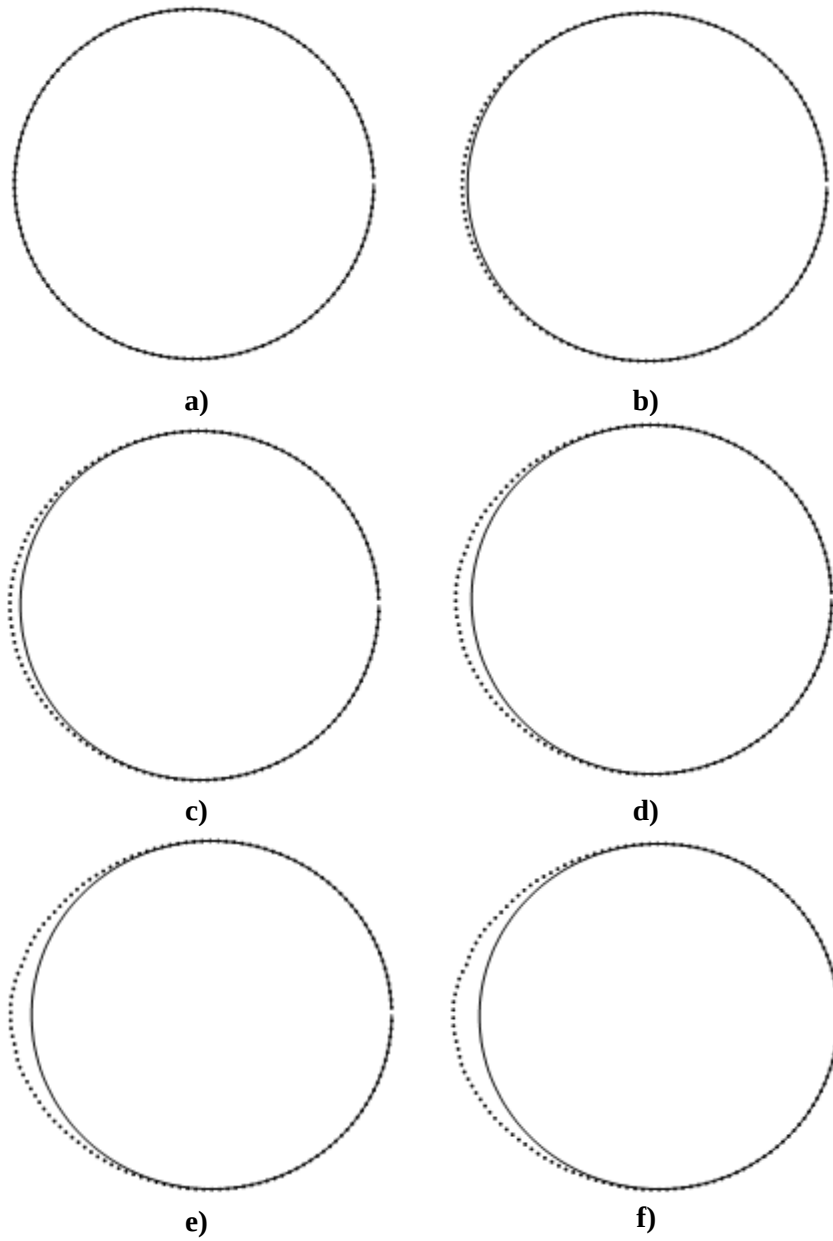


Figure 8-7: Deposit shape on probe 2 ($d_t = 39$ mm, 773 K) using the 1st probes' configuration: a) $t = 0$ hr, b) $t = 1$ hr, c) $t = 2$ hrs, d) $t = 3$ hrs, e) $t = 4$ hrs, f) $t = 5$ hrs ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s, Na_2SO_4 [1 ppm]).

8.8 Effect of combined mechanisms

In this work, deposition was studied including several deposition mechanisms for solid ash particles and alkali vapours whose stickiness was taken into account combining

previous models from the literature which were refined applying specific experimental conditions (e.g. ash chemical composition, temperature, etc.).

The comparison between experimental and modelling results was promising; in fact the model was able to capture the main deposition areas with a good approximation of the deposition fluxes around the probes (e.g. Figure 8-8).

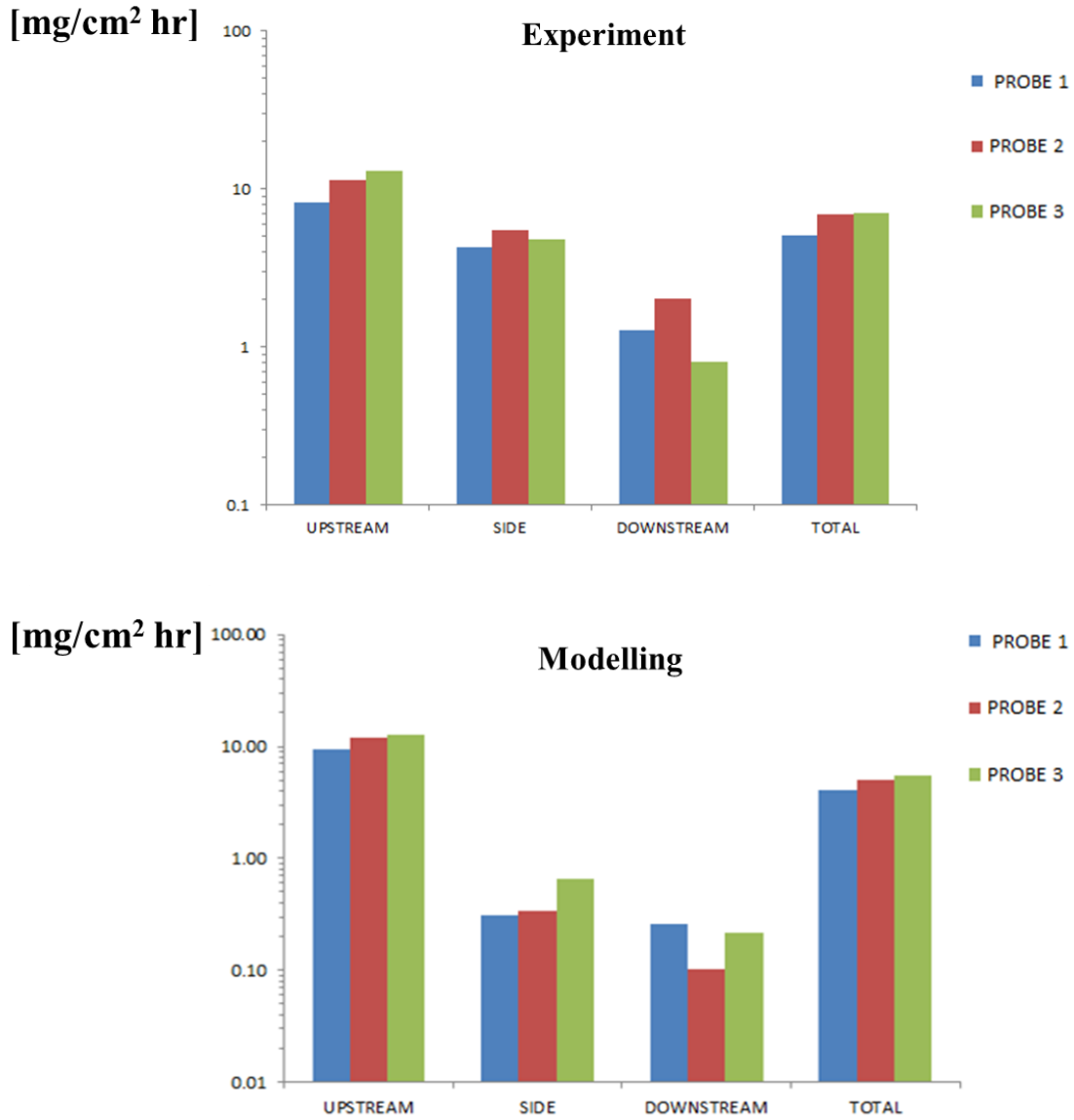


Figure 8-8: Comparison between experimental and modelling predictions (case study A) of deposition flux on different sides of probes (~ 773 K, $d_t = 39$ mm) using the 2nd probes' configuration ($U_0 = 2$ m/s, $d_{min} = 0.43$ μ m, $d_{mean} = 68$ μ m, $d_{max} = 535$ μ m, polydispersion parameter $n = 1.07$).

Moreover, the dynamic nature of deposit formation has been taken into account updating the temperature and deposit shape in the course of the simulation to include their effects on the deposition flux. In fact, the deposit build-up changes the fluid dynamics around the probe and the deposit surface temperature.

The layer of deposit formed on the probe represents the new surface that is exposed to the flue gas and to the ash particle hits; however this surface has chemical and thermal properties that are different from the initial clean surface (Figure 8-9). This highlights the dynamic nature of the deposit formation which requires a wider knowledge in terms of material properties (e.g. deposit, fly ash, etc.) for different fuels and at different temperatures.

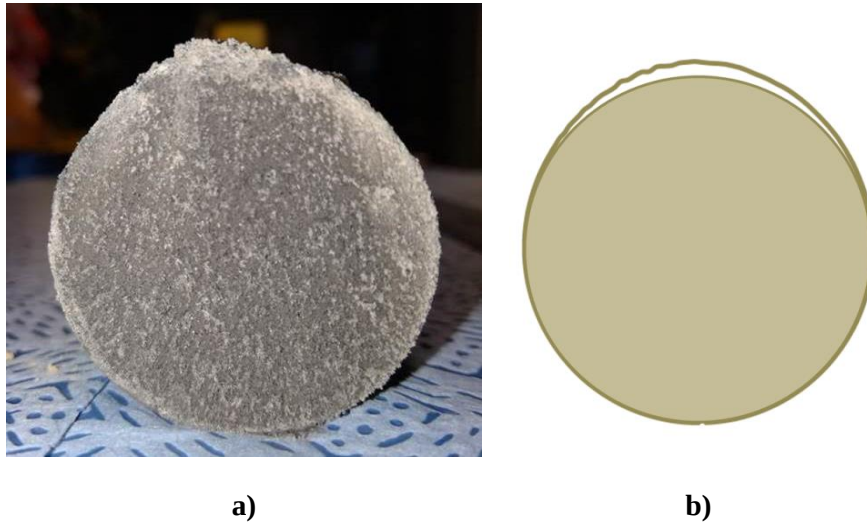


Figure 8-9: a) Deposit shape on one of the probes after combustion of Daw Mill-12 wt.% Miscanthus (2.5 hours of exposure); b) predicted deposit shape after 2.5 hours (773 K, $d_t= 39$ mm, $d_{min}= 0.43$ μ m, $d_{mean}= 68$ μ m, $d_{max}= 535$ μ m, polydispersion parameter $n= 1.07$, $U_0= 2$ m/s).

In this study, the effect of the deposit surface temperature and deposit shape on the total deposition flux was included combining modified UDFs DEFINE_GRID_MOTION and DEFINE_PROFILE. Results showed that the deposit was always thicker on the upstream than sides and downstream surfaces and, as a consequence, the deposit surface temperature was higher where the deposit was thicker and its values tended to become more similar to the surrounding gas temperature (section 7.7).

Fluent[®] can also predict the deposit surface temperature and the temperature gradient inside the deposit using the double couple wall. This method is highly demanding in terms of mesh quality and material properties. However, only a few simulations were carried out using this technique on a single probe and it was not used to validate the model. In fact, further studies are necessary to improve this approach (e.g. meshing, deposit properties, etc.) (section 4.3.6).

8.9 Comparison with previous models

This work aimed to develop improved models to predict deposit formation on clean air cooled probes by combining different deposition mechanisms (inertial impaction, Eddy impaction, thermophoresis and vapour condensation). The role of condensation is quite relevant to start the deposit build up (Zhou, Jensen and Frandsen, 2007). For this reason it has been taken into account and it was combined with the ash particle stickiness calculated with the particle viscosity based on the real ash chemical composition. However, one of the criticisms of the viscosity based approach is the absence of the particle kinetic energy (Yang *et al.*, 2018).

In previous works (section 2.8.2), deposition has been studied according to several sticking criteria based on the physical properties of particles and surfaces. Waclawiak and Kalisz, 2011, 2012 studied a model for “powdery” deposits which is more suitable when a dry particle hits a clean surface in low temperature regions. In this case, the deposition is due to a force balance that involves the particle and tube material properties, van der Waals force and the gravity force. Moreover, “bonded” deposits, made from sticky or molten/semimolten ash particles, have been predicted with sticking probability correlations based on the ash particle softening temperature or viscosity (Tomeczek, Palugniok and Ochman, 2004; Tomeczek and Waclawiak, 2009; Kleinhans *et al.*, 2018). Yang *et al.*, 2018 in their model took into account the sticking/rebounding particle behaviour after the impaction on tubes with an energy conservation analysis which includes the ash chemistry, particle and surface properties and furnace operating conditions. However, only a limited number of studies have investigated the vapour condensation contribution and one of the common issues was the prediction of material properties (in particular for biomass) and constants used in the model equations.

Therefore, more experiments are necessary to provide data of deposition flux and deposit properties, in particular when alternative fuels, such as biomass, are used.

A comparison between the models developed in this study and previous models from the literature has been carried out using the first probes' configuration at 773 K (Figure 8-10). However, in the absence of some determining material properties and constants, they were taken from the literature. This limitation was already flagged in Chapter 4, where preliminary CFD model results were presented.

The model developed by Yang *et al.*, 2018 was applied with the properties of soda-lime glass particles (section 2.8.2.3) since data for deposit derived from Daw Mill and Miscanthus combustion were not available.

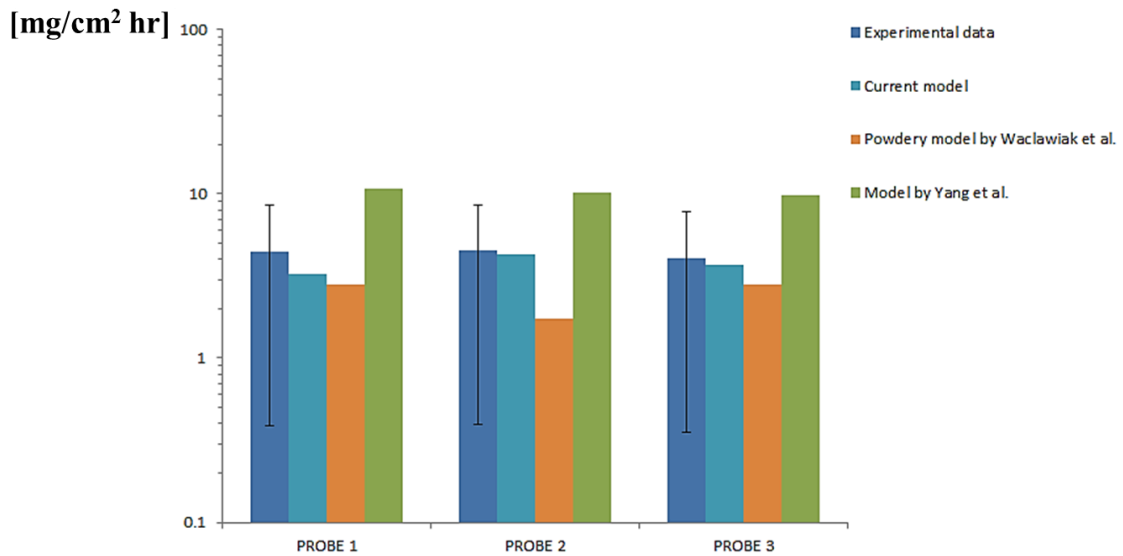


Figure 8-10: Comparison of the total deposition fluxes between the experiments and several sticking models on ceramic probes (773 K, $d_t = 39$ mm) using the 1st probes' configuration ($U_0 = 2$ m/s, $d_{min} = 0.43$ μ m; $d_{mean} = 68$ μ m; $d_{max} = 535$ μ m; polydispersion parameter $n = 1.07$).

The results in Figure 8-10 show an overestimate of the total deposition flux on the ceramic probes when the viscous-elastic model is used ($\sim 58\%$, 56% and 59% for probes 1, 2 and 3 respectively). However, such model (Yang *et al.*, 2018) is more suitable for slagging predictions rather than fouling formation on clean probe surfaces.

In addition, the powdery deposition model developed by Waclawiak and Kalisz, 2011, 2012 was used with the same constants suggested in the paper and it was shown to underestimate the deposit predictions ($\sim 36\%$, 61% and 30% for probes 1, 2 and 3 respectively).

This model was used to test the influence of the gas velocity on the deposition flux and it demonstrated that deposition decreases at higher velocity for bigger particles while smaller particles are less affected by the variation of the gas velocity (section 4.3.5).

Finally, predictions from the models developed in the current work give under predictions of $\sim 25\%$, 4% and 8% for probes 1, 2 and 3 respectively. Therefore, future studies should include an investigation of the deposit physical properties for different fuels and optimize the constants used in the model equations to improve the quality and reliability of alternative model predictions.

8.10 Technological impact

Deposit formation represents a serious issue in industrial power plants since thick deposits can restrict heat transfer and so reduce the boiler efficiency and can induce fireside corrosion that leads to tube failures, adding substantially to maintenance and repair costs. The model developed in this study has been used to predict the formation of deposits on cooled ceramic probes in a pilot scale combustor rig. However the combination of modelling and targeted experiments has been shown to be fundamental in providing realistic boundary conditions and data for the model set-up to achieve promising results.

These models could be further applied to predict the deposition on heat exchanger tubes in different combustion environments (e.g. different fuel blends, geometries, surface temperatures, boiler upgrade), as well as to identify preferred plant and heat exchanger operating conditions. Moreover, a CFD approach represents a cheaper solution than running experimental tests, especially on a bigger scale.

In addition, the CFD tools (Fluent[®] and UDFs), as well as the methodological approach used in this study, can be applied to predict different types of deposition in other scientific fields such as: predictions of ice accretion over airfoils (Fornasier, 2016),

aerosol deposition in airways during breathing (Guha, 2008; Scheinherr, 2015), deposition in gas and steam turbines (Guha, 2008; Barker, 2010), electro-aerodynamic nanoparticle printing on metal grid transparent electrodes (Nasrabadi and Hwang, 2018).

8.11 Summary

Deposition on heat exchangers has been studied combining experimental and CFD modelling approaches. The outcomes can be summarised as follows:

- 2D geometries and different probe configurations have been investigated to study ash particle trajectories and deposition flux.
- Structured and unstructured meshes were developed but the use of a triangular mesh was necessary to predict the shape of deposit with grid motion setting (section 3.3). Moreover, three different meshes were generated to identify the optimum between mesh quality and computational costs (section 4.3.2).
- Ash particle trajectories were studied for single particle injections and ash particle size distribution in the presence of single or multiple tubes (Chapter 4).
- Vapour condensation increased the total deposition flux and made the deposit more uniform around the probe as it creates a sticky layer which enhances particle deposition (sections 4.2.4 and 7.8). At higher surface temperatures, the amount of particles that deposited on a sticky surface on the sides and downstream was reduced. However, in this study, ash inertial impaction resulted to be the main deposition mechanism and the total deposition flux increased at higher surface temperature.
- Deposit temperature predictions showed that increasing the deposit thickness, its temperature tended to be similar to the surrounding gas temperature (section 7.7).
- Compared to previous studies, this model included different deposition mechanisms for solid ash particles and alkali vapours using a transient approach. The results were promising as the model gave good predictions of the deposit locations and fluxes detected in the combustor rig at Cranfield. However, it could be used for deposit predictions in different combustion environments. The

main limitations of this work have been highlighted and alternative applications of the methodology have been illustrated.

9 CONCLUSIONS AND FUTURE WORK

9.1 Conclusions

This PhD was focussed on the study of deposit formation on superheater/reheater tubes during co-firing of coal and biomass to improve current knowledge, understanding and modelling in this field. Experimental work was carried out to generate experimental data of deposit accretion in terms of deposition flux. Investigations of gas composition, fly ash particle size distribution, fly ash and deposit chemical composition were included. CFD modelling was carried out to develop models for predictions of deposition flux, deposit shape and heat transfer.

This chapter summarises the main findings of this research in terms of the modelling and experimental activities, as well as highlighting the development of new knowledge and understanding.

9.1.1 Improved models

A CFD approach was used to simulate the movement of flue gas and ash particles as well as the formation of deposits on heat exchanger surfaces. As part of the learning process, simulations were carried out with an increasing level of difficulty; from deposition on one probe with single deposition mechanisms and boundary conditions taken from the literature, to more complex models to predict deposits on various air cooled ceramic probes in the combustion rig at Cranfield University.

- CFD simulations were run using Fluent[®] (16.2 and 17.1), enhanced with specifically modified UDFs, to predict the formation of deposits on heat exchangers and their surface temperature.
- Particle trajectories were studied injecting single ash particle sizes as well as particle size distributions, which are more representative of real boilers. In both cases, it was observed that bigger particles have more momentum and tend to follow their own trajectories. In fact, they can bounce on the surface of the tube and rebound with an energy that increases with their diameter. The stochastic tracking model was enabled to include the influence of the gas turbulence on the

particles and therefore predict smaller particle trajectories as they tend to follow the gas streamlines and hit the rear side of the probes.

- Particle trajectories can be altered by the chamber walls or in the presence of other tubes. Different probe configurations were studied and it was observed that bigger particles can rebound from the upstream surfaces of downstream tubes and hit the downstream surfaces of upstream tubes.
- The deposition flux was calculated modifying the DEFINE_DMP_EROSION UDF and the value obtained was used to predict the deposit shape with a modified DEFINE_GRID_MOTION UDF and the deposit temperature using a modified DEFINE_PROFILE UDF. In particular, the use of “remeshing” option required a triangular mesh rather than a structured one. Deposition was studied with a transient approach which included the effect of an increasing surface temperature and dynamic deposit shape on the deposition flux.
- Preliminary qualitative results showed that deposit was more likely to happen on the upstream surfaces than sides and downstream and this trend was reflected in the temperature profile which had higher temperatures where the thermal resistance exerted by the deposits was higher (thicker deposit).

(Relates to objectives 1 and 4, with more details given in Chapters 3 and 4).

9.1.2 Deposition experiments

Experiments were carried out in the pilot scale combustion rig 100 kW_{th} at Cranfield University using a blend of Daw Mill coal-12 wt.% Miscanthus and the main findings are highlighted below:

- FTIR was used during all the tests to analyse the flue gas major and minor components (CO₂, H₂O, O₂, CO, NO, NO₂, N₂O, SO₂, HCl).
- Gas and surface temperatures were measured at different locations in the rig with particular focus on the air-cooled ceramic probes whose temperatures were controlled (e.g. to ~ 500 and 600 °C) by varying their compressed air cooling flow rates to reproduce real heat exchanger surface temperatures.

- Fly ash and deposits were analysed with SEM/EDX to capture images and calculate their chemical compositions in terms of highest oxides of elements (SiO_2 , Al_2O_3 , CaO , Fe_2O_3 , K_2O , MgO , Na_2O , TiO_2 , SO_3 , P_2O_5 , SO_3 , P_2O_5 , Mn_3O_4). Moreover, XRD analyses provided the crystalline composition of the deposits. The analyses did not show any difference in terms of deposit composition on the different zones around the probe, sign that the deposition process did not affect the chemical composition.
- Fly ash samples were analysed to get ash particle size distributions and the average values of the Rosin Rammler distributions identified were used in the CFD model validation (Chapter 7).
- Deposition was studied as function of the probe location (e.g. the relative position of the probes and their vicinity to the chamber wall), the surface temperature of the probes and the exposure time. Deposits were always thicker on the top of the probes compared to the sides and downstream surfaces. Moreover, deposits looked quite powdery and only on the downstream stickier, probably because of the vapour condensation. However, it was difficult to identify remarkable differences in terms of deposit chemical compositions and deposition fluxes in relation to the probe temperature, the probe configuration or the exposure time. This could be attributed to the operating conditions, the deposit loss during the probes' extraction or to the measurement errors. The use of CFD modelling helped understand better these aspects.

(Relates to objectives 2 and 4, as discussed in detail in Chapters 5 and 6).

9.1.3 Model validation

- Some of the experimental results and operating conditions were used to set-up the model and fix the boundary conditions (e.g. geometry, probe configurations, flue gas temperature, gas velocity, ash chemical composition, fly ash particle size distribution, etc.). Some other results were used to validate the model (e.g. deposition flux, deposit shape and thickness).

- The model predicted fly ash trajectories according to different diameters and in the presence of other probes in the computational domain. It included three UDFs which were modified to predict the deposition flux, the deposit shape and temperature respectively. It took into account several deposition mechanisms for alkali vapours and solid ash particles of different diameters (e.g. vapour condensation, inertial impaction, thermophoresis, Eddy impaction). The stickiness of the particle (calculated with a viscosity model) and of the probe surface (for vapour condensation) were included.
- The model could give quantitative predictions of what had been observed from the experiments. As expected, deposition was more likely to occur on the upstream zone of the probe, where inertial impaction is the main deposition mechanism, and only a thin layer of deposit was found on the sides and downstream zones. In some cases the model slightly overestimated the deposition fluxes on the upstream surfaces and underestimated the ones on the sides and downstream surfaces. These differences could be due to the approximations made to approach this complex phenomenon (e.g. boundary conditions, material properties, 2D geometry, sticking criteria, etc.).
- The role of condensation was investigated and it demonstrated to be more significant on a clean surface probe and to enhance the particle deposition flux at increasing alkali vapour concentration.

(Relates to objectives 3 and 4, more details are given in Chapter 7. Objective 3 could be met only once the first two objectives had been completed).

9.1.4 Overall findings and technological impact

Deposit formation is a serious issue in industrial power plants. This work has used a combination of experimental methods and CFD modelling to produce improved predictions of deposit formations on heat exchanger tubes in pulverised fuel fired combustion plants. The resulting models represent a significant development of those previously reported in the literature. They combine a variety of deposition mechanisms for a real ash particle size distribution using a transient approach. This showed the

development of deposition around the probes for different configurations. Moreover it allowed the study of some of the deposition mechanisms at different exposure times and therefore thermal conditions.

The experiments have been used to generate data for model validation and to define boundary conditions including deposition flux, gas composition and temperature, fly ash and deposit chemical composition and fly ash particle size distribution.

This combined approach has the flexibility to be applied to other fuel mixes, boiler geometry, etc. In addition, such methods could be used to investigate other similar phenomena such as ice accretion over airfoils, deposition in gas and steam turbines, etc.

9.2 Recommendations for future research

The work accomplished during this PhD has contributed to improve the current understanding of deposit formation on heat exchangers in co-fired boilers including different deposition mechanisms and using transient simulations. This approach is not commonly used because of the high computational costs that it requires. The sticking model used to predict deposition was derived from previous correlations found in the literature which were modified with experimental data (if available) and combined to include the ash particle and tube surface stickiness. However, the analysis of the results has identified some limitations which could represent interesting starting points for future research. Some of these are summarised as follows:

- The use of fuel blends with increasing biomass content should be investigated considering also the current interest toward renewable sources of energy. This would clarify the impact that different types of fuel may have on the deposition flux, fly ash distribution, deposit chemical composition, role of condensation, etc. Moreover, this study would generate material properties and boundary conditions to test the model predictions in different combustion environments.
- Include the dependence of material properties on the temperature.
- Include the effect of the particle shape and surface roughness.
- Model predictions at different time step sizes.

- Upgrade of the model to a 3D geometry to verify its influence on the predictions of deposit formation on the downstream and sides of the probes.
- Implement in Fluent[®] a Rosin Rammler ash particle size distribution obtained by an isokinetic sampling during experiments of combustion.
- Further study to predict deposit formation and heat transfer using the double coupled walls.
- Carry out a more detailed grid independence study for all the deposition models applied.
- Improve the sticking model accounting for real material properties, ash particle velocity and additional deposition mechanisms (e.g. chemical reactions, nucleation, etc.).
- Further investigation of the role of thermophoresis on the total deposition flux.
- Study the presence of additional vapours in the flue gas and their effect on the total deposition flux.

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APPENDICES

Appendix A

This section includes basic knowledge which was necessary for the development of the CFD methodology (Chapter 3).

A.1 Governing Equations for CFD

CFD is based on the governing equations of fluid dynamics, which are the conservation laws of physics reported below (Tu *et al.*, 2007c):

A.1.1 Mass Conservation

According to this law “matter may neither be created nor destroyed”. The mass conservation in the Cartesian coordinate system can be expressed as Equation (A-1) (Tu *et al.*, 2007c):

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} + \frac{\partial(\rho w)}{\partial z} = 0 \quad (\text{A-1})$$

Where the fluid velocity at any point in the flow field is described by the local velocity components u , v and w , which are, in general, functions of location (x , y , z) and time (t).

A.1.2 The Momentum Equation

Newton's second law of motion states that the sum of forces that is acting on the fluid element equals the product between its mass and acceleration. Even if there are three scalar relations along the x , y and z directions, in Equation (A-2) it is reported only the x component of Newton's second law (Tu *et al.*, 2007c).

$$\sum F_x = m a_x \quad (\text{A-2})$$

where F_x and a_x are the force and acceleration along the x direction.

On the left side of Equation (A-2), there are two sources of this force: body forces and surface forces. The body forces are: gravity, centrifugal, Coriolis, and electromagnetic

forces and they can influence the fluid momentum (they can be added as source terms into the momentum equations). The surface forces for the velocity component u , that deform the fluid element are due to the normal stress (σ_x) and tangential stresses (τ_{yx} and τ_{zx}) acting on the fluid element surfaces. The normal stresses (σ_{xx} , σ_{yy} , σ_{zz}) are due to the combination of pressure p and normal viscous stress components (τ_{xx} , τ_{yy} , τ_{zz}) acting perpendicular to the control volume. The remaining terms contain the tangential viscous stress components. Considering the continuity equation, the momentum equations with the stress-strain relationships can be reduced to Equations (A-3)-(A-4) (Tu *et al.*, 2007c):

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = - \frac{1}{\rho} \frac{\partial p}{\partial x} + \nu \frac{\partial^2 u}{\partial x^2} + \nu \frac{\partial^2 u}{\partial y^2} \quad (\text{A-3})$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = - \frac{1}{\rho} \frac{\partial p}{\partial y} + \nu \frac{\partial^2 v}{\partial x^2} + \nu \frac{\partial^2 v}{\partial y^2} \quad (\text{A-4})$$

These equations derived from Newton's second law, where ν is the cinematic viscosity ($\nu = \mu/\rho$), describe the conservation of momentum in the fluid flow and are also known as Navier-Stokes equations.

In Equations (A-3)-(A-4) the terms on the left are the local acceleration (first term) and advection (second and third terms), whereas on the right there are the pressure gradient (first term) and diffusion terms (second and third).

A.1.3 The Energy Conservation

The equation for the conservation of energy derives from the first law of thermodynamics: the rate of change of energy equals the sum of rate of heat added and the rate of work done on the fluid. Generally, the energy of a fluid is the sum of the internal energy, kinetic energy and gravitational potential energy. The equation for the conservation of energy in two dimensions can be expressed as Equation (A-5) (Tu *et al.*, 2007c):

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{k}{\rho C_p} \frac{\partial^2 T}{\partial x^2} + \frac{k}{\rho C_p} \frac{\partial^2 T}{\partial y^2} \quad (\text{A-5})$$

Where the term in Equation (A-5) are: the local acceleration (first term on the left), advection (second and third terms on the left) and the two diffusion terms are on the right side.

A.2 Turbulence modelling

The Navier-Stokes equations describe the continuity and momentum equations for laminar flows. However, small disturbances, originated from the free stream of the fluid motion or the surface roughness, can generate chaotic and random motions also known as turbulent conditions (Tu *et al.*, 2007c). The Reynolds number is used to describe turbulence; it is a dimensionless number defined as the ratio of the inertia force to viscous force. When the inertial forces are big enough they generate turbulence. The transient velocity in the conservation equations is defined as an instantaneous velocity and is decomposed into a steady mean value ($\bar{u}$) and a fluctuating component ($u'(t)$) as in Equation (A-6) (Figure A-1).

$$u(t) = \bar{u} + u'(t) \quad (\text{A-6})$$

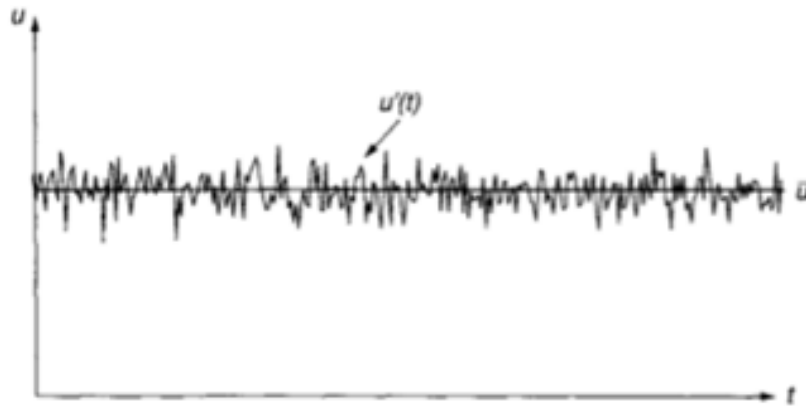


Figure A-1: Velocity fluctuating with time at some point in a turbulent flow (Tu *et al.*, 2007c).

In the presence of turbulent flow, the mean velocity is used in the continuity and conservative (momentum and energy) equations which are also known as the time

averaged governing equations Reynolds-Averaged Navier-Stokes (RANS) equations (7-7)-(7-10) (Tu *et al.*, 2007c).

$$\frac{\partial \bar{u}}{\partial x} + \frac{\partial \bar{v}}{\partial y} = 0 \quad (\text{A-7})$$

$$\frac{\partial \bar{u}}{\partial t} + \frac{\partial(\bar{u}\bar{u})}{\partial x} + \frac{\partial(\bar{v}\bar{u})}{\partial y} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial x} + \frac{\partial}{\partial x} \left(\nu \frac{\partial \bar{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\nu \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial x} \left(\nu \frac{\partial \bar{u}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\nu \frac{\partial \bar{v}}{\partial x} \right) - \left[\frac{\partial(\bar{u}'u')}{\partial x} + \frac{\partial(\bar{u}'v')}{\partial y} \right] \quad (\text{A-8})$$

$$\frac{\partial \bar{v}}{\partial t} + \frac{\partial(\bar{u}\bar{v})}{\partial x} + \frac{\partial(\bar{v}\bar{v})}{\partial y} = -\frac{1}{\rho} \frac{\partial \bar{p}}{\partial y} + \frac{\partial}{\partial x} \left(\nu \frac{\partial \bar{v}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\nu \frac{\partial \bar{v}}{\partial y} \right) + \frac{\partial}{\partial x} \left(\nu \frac{\partial \bar{u}}{\partial y} \right) + \frac{\partial}{\partial y} \left(\nu \frac{\partial \bar{v}}{\partial y} \right) - \left[\frac{\partial(\bar{u}'v')}{\partial x} + \frac{\partial(\bar{v}'v')}{\partial y} \right] \quad (\text{A-9})$$

$$\frac{\partial \bar{T}}{\partial t} + \frac{\partial(\bar{u}\bar{T})}{\partial x} + \frac{\partial(\bar{v}\bar{T})}{\partial y} = \frac{\partial}{\partial x} \left(\frac{k}{\rho C_p} \frac{\partial \bar{T}}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{k}{\rho C_p} \frac{\partial \bar{T}}{\partial y} \right) - \left[\frac{\partial(\bar{u}'T')}{\partial x} + \frac{\partial(\bar{v}'T')}{\partial y} \right] \quad (\text{A-10})$$

Where $\bar{u}$, $\bar{v}$, $\bar{p}$, $\bar{T}$ are the mean values and u' , v' , p' , T' are turbulent fluctuations. The term $\frac{k}{\rho C_p}$ is the thermal diffusivity (α) of the fluid. The equations above are similar to the ones formulated for laminar flows, except for the presence of additional terms of the form $\overline{a'b'}$.

As a result there are three unknowns (nine in three dimensions) which are the Reynolds stresses, in the time-averaged momentum equations. Also in the time averaged temperature equation there are some extra terms $\overline{u'T'}$ and $\overline{v'T'}$. The time averaged equations can be solved if the Reynolds stresses and extra temperature transport terms can be related to the mean flow and heat quantities (Tu *et al.*, 2007c).

In 1868, Boussinesq proposed a relation between the Reynolds stresses and the mean rates of deformation (Equations (A-11)-(A-13)).

$$-\rho \overline{u'u'} = 2\mu_T \frac{\partial \bar{u}}{\partial x} - \frac{2}{3} \rho k \quad (\text{A-11})$$

$$-\rho \overline{v'v'} = 2\mu_T \frac{\partial \bar{v}}{\partial y} - \frac{2}{3} \rho k \quad (\text{A-12})$$

$$-\rho \overline{u'v'} = \mu_T \left(\frac{\partial \bar{v}}{\partial x} + \frac{\partial \bar{u}}{\partial y} \right) \quad (\text{A-13})$$

These equations look very similar to the Newton's law of viscosity, except for the turbulent or eddy viscosity μ_T and turbulent kinetic energy k .

In Equations (A-11)-(A-13) the turbulent momentum transport is proportional to the mean gradient of velocity. Therefore, the turbulent transport of temperature is proportional to the gradient of the mean value of the transported quantity (Equations (A-14) and (A-15)) (Tu *et al.*, 2007c):

$$-\rho \overline{u'T'} = T_T \frac{\partial \bar{T}}{\partial x} \quad (\text{A-14})$$

$$-\rho \overline{v'T'} = T_T \frac{\partial \bar{T}}{\partial y} \quad (\text{A-15})$$

Where T_T is the turbulent diffusivity. Considering the same mechanisms behind the turbulent transport of momentum and heat (eddy mixing), a correlation was found which links the turbulent diffusivity (T_T) and the turbulent viscosity (μ_T) using the turbulent Prandtl number as in Equation (A-16) (Tu *et al.*, 2007c).

$$-Pr_T = \frac{\mu_T}{T_T} \quad (\text{A-16})$$

In many cases it is assumed that Pr_T is equal to one.

Turbulence is a very complex phenomenon which can be studied with several turbulence models. Commonly, the most used, at least in the first stage of research, is the $k - \varepsilon$ model, where k is the turbulent kinetic energy and ε is the dissipation rate of kinetic energy. A variation of this model is the $k - \omega$ turbulence model which uses ω , the turbulent frequency defined as $\omega = \varepsilon/k$, which can predict the near-wall flow better. The turbulent kinetic energy k and rate of dissipation ε can be defined in Cartesian tensor notation as in Equations (A-17) and (A-18) (Tu *et al.*, 2007c):

$$k = \frac{1}{2} u'_i u'_i \quad (\text{A-17})$$

$$\varepsilon = \nu_T \overline{\left(\frac{\partial u'_i}{\partial x_j} \right) \left(\frac{\partial u'_i}{\partial x_j} \right)} \quad i, j = 1, 2, 3 \quad (\text{A-18})$$

Using the local values of k and ε , a local turbulent viscosity μ_T is defined as in Equation (A-19) (Tu *et al.*, 2007c):

$$\mu_T = \frac{C_\mu \rho k^2}{\varepsilon} \quad (\text{A-19})$$

And the kinematic turbulent or eddy viscosity is defined as $\nu_T = \mu_T/\varepsilon$.

The non-conservative governing equations can be expressed as in Equations (A-20)-(A-23).

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \quad (\text{A-20})$$

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial x} + \frac{\partial}{\partial x} \left[(v + \nu_T) \frac{\partial u}{\partial x} \right] + \frac{\partial}{\partial y} \left[(v + \nu_T) \frac{\partial u}{\partial y} \right] + \frac{\partial}{\partial x} \left[(v + \nu_T) \frac{\partial u}{\partial x} \right] + \frac{\partial}{\partial y} \left[(v + \nu_T) \frac{\partial v}{\partial x} \right] \quad (\text{A-21})$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{1}{\rho} \frac{\partial p}{\partial y} + \frac{\partial}{\partial x} \left[(v + \nu_T) \frac{\partial v}{\partial x} \right] + \frac{\partial}{\partial y} \left[(v + \nu_T) \frac{\partial v}{\partial y} \right] + \frac{\partial}{\partial x} \left[(v + \nu_T) \frac{\partial u}{\partial y} \right] + \frac{\partial}{\partial y} \left[(v + \nu_T) \frac{\partial v}{\partial y} \right] \quad (\text{A-22})$$

$$\frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} + v \frac{\partial T}{\partial y} = \frac{\partial}{\partial x} \left[\left(\frac{\nu}{Pr} + \frac{\nu_T}{Pr_T} \right) \frac{\partial T}{\partial x} \right] + \frac{\partial}{\partial y} \left[\left(\frac{\nu}{Pr} + \frac{\nu_T}{Pr_T} \right) \frac{\partial T}{\partial y} \right] \quad (\text{A-23})$$

The additional differential transport equations required for the standard $k - \varepsilon$ model, for a constant fluid property and in non-conservation form are (Tu *et al.*, 2007c):

- For turbulent kinetic energy k

$$\frac{\partial k}{\partial t} + u \frac{\partial k}{\partial x} + v \frac{\partial k}{\partial y} = \frac{\partial}{\partial x} \left(\frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\nu_T}{\sigma_k} \frac{\partial k}{\partial y} \right) + P - D \quad (\text{A-24})$$

- For dissipation ε

$$\frac{\partial \varepsilon}{\partial t} + u \frac{\partial \varepsilon}{\partial x} + v \frac{\partial \varepsilon}{\partial y} = \frac{\partial}{\partial x} \left(\frac{\nu_T}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial x} \right) + \frac{\partial}{\partial y} \left(\frac{\nu_T}{\sigma_\varepsilon} \frac{\partial \varepsilon}{\partial y} \right) + \frac{\varepsilon}{k} (C_{\varepsilon 1} P - C_{\varepsilon 2} D) \quad (\text{A-25})$$

Where the production term P is formulated as in Equation (A-26).

$$2P = \nu_T \left[\left(\frac{\partial u}{\partial x} \right)^2 + \left(\frac{\partial v}{\partial y} \right)^2 \right] + \nu_T \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right)^2 \quad (\text{A-26})$$

And the destruction term D is given by ε .

The meaning of the equations reported above is that “the rate of change and the advection transport of k or ε equals the diffusion transport combined with the rate of production and destruction of k or ε ” (Tu *et al.*, 2007c). The equations contain five constants $C_\mu, \sigma_k, \sigma_\varepsilon, C_{\varepsilon 1}, C_{\varepsilon 2}$ whose values have been calculated by data fitting for a wide range of turbulent flows.

$$C_\mu=0.09, \sigma_k = 1.0, \sigma_\varepsilon = 1.3, C_{\varepsilon 1} = 1.44, C_{\varepsilon 2} = 1.92.$$

The production and destruction terms are proportional to the production and destruction terms of the k - ε equations; ε increases rapidly if k increases rapidly and it decreases fast to avoid nonphysical (negative) values of turbulent kinetic energy if k decreases. The factor $\frac{\varepsilon}{k}$ in the production and destruction terms makes these terms dimensionally correct in the ε equation.

There are three types of k - ε turbulence model available (ANSYS FLUENT, 2006c):

1) Standard

- Widely used in engineering turbulence model for industrial applications
- Robust and reasonably accurate
- Contains sub-models for compressibility, combustion, etc.

Limitations:

- The ε equation contains a term that cannot be calculated at the wall. Therefore, wall function must be used
- Generally performs poorly for flow with strong flow separation, reattachment, large streamline curvature and large pressure gradient
- It over predicts the gas turbulence kinetic energy k in the recirculation zone which leads to a higher turbulent viscosity

2) RNG (Renormalisation group)

- Constants in the k - ε equations are derived using renormalisation group theory
- Contains the following sub models:
 - Differential viscosity model to account for low Re effects
 - Analytically derived algebraic formula for turbulent Prandtl/Schmidt number
 - Swirl modification

- Performs better than standard k - ε for more complex shear flows and flows with high strain rates, swirl and separation.

Considering the renormalisation group theory, the new constant in the turbulence model are (Tu *et al.*, 2007e):

$$C_\mu=0.0845, \sigma_k = 0.718, \sigma_\varepsilon = 0.718, C_{\varepsilon 1} = 1.42, C_{\varepsilon 2} = 1.68.$$

3) Realizable

- The term realizable means that the model satisfies certain mathematical constraints on the normal stresses, consistent with the physics of turbulent flows
 - Positivity of normal stresses: $\overline{u'v'} > 0$
 - Schwarz' inequality for Reynolds shear stresses: $\overline{(u'v')^2} \leq \overline{u'v'}$
 - Neither the standard k - ε model nor the RNG k - ε model is realizable
 - Benefits:
 - Better prediction of the spreading rate of both planar and round jets
 - Provide superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients, separation and recirculation

This realizable model involves new eddy viscosity formula including C_μ in the turbulent viscosity relationship. Moreover, the transport ε equation (based on the dynamic equation of the mean square vorticity equation and C_μ is not a constant anymore). Some constants for this model are (Tu *et al.*, 2007e):

$$C_2=1.9, \sigma_k = 1, \sigma_\varepsilon = 1.2.$$

The k - ε standard equations are the same as k - ε RNG and Realizable except for the constants.

The prediction of flow separation from a smooth surface is one of the main problems in turbulence modelling and the amount of flow separation under adverse pressure gradient conditions cannot be predicted by standard two-equations turbulence models (e.g. aerodynamics). In general, turbulence models based on the ε equation predict the onset of separation too late and under-predict the amount of separation. Some models have been developed for a better prediction of the separation and, currently, the most

promising two-equation models in this area are the $k - \omega$ based models of Menter where ω is a frequency of the large eddies.

This model can describe quite well the boundary layer flows under strong adverse pressure gradients. As well as the $k-\varepsilon$ model, there is a transport equation to solve ω and its local distribution within the fluid flow. The model is very sensitive to the free-stream value of ω and it is important to take care of this value in boundary layer flows and free shear flows. The standard $k-\varepsilon$ is less sensitive to the free stream values and can be inadequate under adverse pressure gradients. To overcome these problems, Menter suggested a combination of the standard $k-\varepsilon$ model and the $k-\omega$. This model keeps the properties of $k-\omega$ close to the wall and uses the advantages of $k-\varepsilon$ far away from the wall.

The Shear Stress Transport (SST) variation of Menter's model allows to improve non equilibrium boundary layer regions such as those close to separation. This model is recommended for flow separation as the real flow is more likely to be much closer to separation (or more separated) than the calculations from the standard $k-\varepsilon$ model suggest. However, this model is less able to cope with flow recovery following flow reattachment.

These models are quite popular because (ANSYS FLUENT, 2006c):

- The model equations do not contain terms which are undefined at the wall, i.e. they can be integrated to the wall without using wall functions.
- They are accurate and robust for a wide range of boundary layers flows with pressure gradient.

There are two types of $k-\omega$ turbulence models (ANSYS FLUENT, 2006c):

- Standard $k-\omega$ (SKW) model
 - Very used in aerospace and turbo-machinery
 - Several sub models/options of $k-\omega$: compressibility effects, transitional flows and shear- flow corrections
- Shear Stress Transport $k-\omega$ (SST $k-\omega$) model

- This model uses a blending function for a gradual transition from the standard k - ω model near the wall to the high Reynolds number version of the k - ε model in the outer portion of the boundary layer
- Contains a modified turbulent viscosity formulation to account for the transport effects of the principal turbulent shear stress

A.3 Eulerian-Lagrangian model

The Eulerian-Lagrangian model splits the particulate modelling into two phases. The first phase (Eulerian) solves the flow solution (without particulate) with the Navier-Stokes equations. The second phase tracks particles dispersed in the flow (ANSYS FLUENT, 2009c). There can be three types of coupling for solid phase particles in turbulent flows (Sofialidis, 2013). The first coupling is One-Way: the turbulence in the flow affects the particle trajectories and dispersion. The second coupling is Two-Way and has the particles affecting the turbulence. The third coupling is Four-Way and includes the particles interacting with each other. Figure A-2 shows the various gas-solid flows where each coupling method is appropriate.

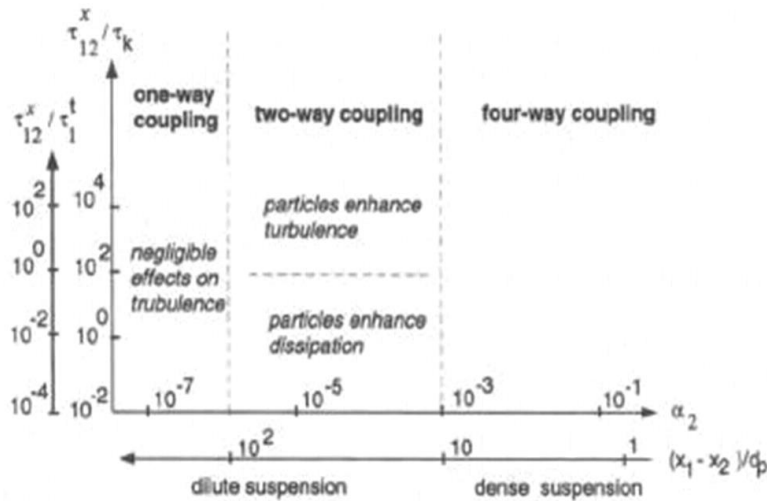


Figure A-2: Classification of flow regimes for gas-solid flows (Elghobashi, 1991).

Where α_2 is the volume fraction of the dispersed phase, τ_k , is the Kolmogorov time scale in seconds, τ_1^t is the Lagrangian Integral time scale in seconds and τ_{12}^x is the particle relaxation time (Barker, 2010).

Typically, ash particulate has a much higher density than the fluid and the number of particles is low enough for inter-particle collisions to be neglected (Fluent, 2001).

A.3.1 Trajectory calculations

Fluent[®] predicts the trajectory of a discrete phase particle (or droplet or bubble) by integrating the force balance on the particle, which is written in a Lagrangian reference frame. This force balance equates the particle inertia with the forces acting on the particle, and can be written (for the x direction in Cartesian coordinates) as (Fluent, 2001):

$$\frac{du_p}{dt} = F_D(u_g - u_p) + \frac{g_x(\rho_p - \rho_g)}{\rho_p} + F_x \quad (\text{A-27})$$

Where $F_D(u_g - u_p)$ is the drag force per unit particle mass and

$$F_D = \frac{18\mu_g}{\rho_p d_p^2} \frac{C_D Re}{24} \quad (\text{A-28})$$

Where u_g is the fluid phase velocity, u_p is the particle velocity, μ_g is the molecular viscosity of the fluid, ρ_g is the fluid density, ρ_p is the density of the particle and d_p is the particle diameter.

Re is the relative Reynolds number, defined as:

$$Re = \frac{\rho_g d_p |u_p - u_g|}{\mu_g} \quad (\text{A-29})$$

The drag coefficient is:

$$C_D = a_1 + \frac{a_2}{Re} + \frac{a_3}{Re^2} \quad (\text{A-30})$$

where a_1 , a_2 , and a_3 are constants that apply for smooth spherical particles over several ranges of Re given by Morsi and Alexander, or for non-spherical particles the relation is (Fluent, 2001):

$$C_D = \frac{24}{Re} (1 + b_1 Re^{b_2}) + \frac{b_3 Re}{b_4 + Re} \quad (\text{A-31})$$

Where:

$$b_1 = \exp(2.3288 - 6.4581\phi + 2.4486\phi^2) \quad (\text{A-32})$$

$$b_2 = 0.00964 + 0.5565\phi \quad (\text{A-33})$$

$$b_3 = \exp(4.905 - 13.8944\phi + 18.4222\phi^2 - 10.2599\phi^3) \quad (\text{A-34})$$

$$b_4 = \exp(1.4681 - 12.2584\phi + 20.7322\phi^2 + 15.8855\phi^3) \phi \quad (\text{A-35})$$

The shape factor ϕ , is defined as in Equation (A-36):

$$\phi = \frac{s}{S} \quad (\text{A-36})$$

Where s is the surface area of a sphere having the same volume as the particle, and S is the actual surface area of the particle.

For sub-micron particles, F_D is given in

$$F_D = \frac{18\mu_g}{C_C \rho_p d_p^2} \quad (\text{A-37})$$

The factor C_C is the Cunningham correction to Stokes' drag law, which can be computed from:

$$C_C = 1 + \frac{2\lambda}{d_p} (1.257 + 0.4e^{-(1.1d_p/2\lambda)}) \quad (\text{A-38})$$

Where λ is the molecular mean free path. Some more expressions of the drag laws are available for particle Mach number greater than 0.4 or a particle Reynolds number greater than 20.

In Fluent[®], the force of gravity on the particle g_x can be included, as the default value of gravitational acceleration is zero. The additional forces term, F_x , are: Thermophoretic Force, Brownian Force and Saffman's Lift Force.

A.3.2 Including the Gravity Term

In Fluent[®], the default gravitational acceleration is zero. To include the gravity force it is necessary to define the magnitude and the direction of the gravity vector in the Operating Conditions panel (Fluent, 2001).

A.3.3 Other forces

1) Virtual mass force

It is the force required to accelerate the fluid surrounding the particle. This force can be written as in Equation (A-39) (Fluent, 2001).

$$F_x = \frac{1}{2} \frac{\rho_g}{\rho_p} \frac{d}{dt} (u_g - u_p) \quad (\text{A-39})$$

and is important when $\rho_g > \rho_p$. An additional force arises due to the pressure gradient in the fluid (Equation (A-40)).

$$F_x = \left(\frac{\rho_g}{\rho_p} \right) u_p \frac{\partial u_g}{\partial x} \quad (\text{A-40})$$

2) Force in rotating reference frames

These forces arise in models of flows in rotating frames of reference.

3) Thermophoretic force

This force is due to the presence of a gradient of temperature which moves small particles suspended in a gas in the direction opposite to that of the gradient. In Fluent[®], this force can be included and its expression is given in Equation (A-41) (Fluent, 2001).

$$F_x = -D_{T,p} \frac{1}{m_p T} \frac{\partial T}{\partial x} \quad (\text{A-41})$$

Where $D_{T,p}$ is the thermophoretic coefficient. The coefficient can be constant, polynomial, user-defined function or the Talbot model can be selected (Talbot, 1980) (Equation (A-42)).

$$F_x = -\frac{6\pi d_p \mu_g^2 C_s (K + C_t Kn)}{\rho(1 + 3C_m Kn)(1 + 2K + 2C_t Kn) m_p T} \frac{1}{\partial x} \frac{\partial T}{\partial x} \quad (\text{A-42})$$

Where:

$Kn = 2\lambda/d_p$ (Knudsen number)

λ (mean free path of the fluid)

$K = k_g/k_p$

$k_g = (\frac{15}{4})\mu R$ (fluid thermal conductivity based on translational energy only) [W/ m K]

k_p (particle thermal conductivity [W/m K]), m_p (particle mass [kg]), T_g (local fluid temperature [Pa]), μ_g (fluid viscosity [Pa·s]).

$C_s = 1.17$

$C_t = 2.18$

$C_m = 1.14$

According to this expression the particle is a sphere and the fluid is an ideal gas.

4) Brownian force

An additional force term for sub-micron particle is the effect of Brownian motion. The components of the Brownian force are modelled taking into account the Kronecker delta function, the absolute temperature of the fluid T_g , the kinematic viscosity ν_g and the Stefan-Boltzmann constant σ (Fluent, 2001).

5) Saffman's lift force

The Saffman's lift force or lift due to shear, can also be included in the additional force term for small particles (Fluent, 2001).

A.4 Laws for heat and mass exchange

When the Discrete Phase model is enabled in Fluent[®] it is possible to select the type of heat and mass transfer laws according to the type of particle. For inert ash particle Law 1 and Law 6 are available (ANSYS FLUENT, 2009b).

These equations can be used to correlate the particle temperature $T_p(t)$ to the convective heat transfer and the absorption/emission of radiation at the particle surface (Equation (A-43)).

$$m_p c_p \frac{dT_p}{dt} = h A_p (T_\infty - T_p) + \varepsilon_p A_p \sigma (T_R^4 - T_p^4) \quad (\text{A-43})$$

Where:

m_p = particle mass [kg]

c_p = particle heat capacity (J/kg K)

A_p = particle surface area [m²]

T_∞ = gas temperature [K]

h = convective heat transfer coefficient [W/m² K]

ε_p = particle emissivity [-]

σ = Stefan-Boltzmann constant (5.67 10⁻⁸ W/m² K⁴)

T_R = radiation temperature

Radiation is included if the P-1 model is enabled and the radiation heat transfer to particles included.

A.5 Near wall flow

Near-wall regions are characterised by larger gradients in the solution variables, and momentum (Salim and Cheah, 2009). Generally, the region close to the wall is described by dimensionless variables. For example, y is the normal distance from the

wall and U is the time averaged velocity parallel to the wall. Therefore the dimensionless velocity U^+ and wall distance y^+ can be described as follows:

$$y^+ = yU_\tau/\nu \quad (\text{A-44})$$

$$U^+ = U/U_\tau \quad (\text{A-45})$$

Where:

μ dynamic viscosity [Pa s]

ν kinematic viscosity [m^2/s]

U_τ friction velocity= $(\tau_w/\rho)^{1/2}$ [m/s]

τ_w wall shear stress [$\text{kg}/\text{m s}^2$]

Figure A-3 shows that the *inner layer* (viscosity-affected region) can be divided in three zones (with their corresponding wall y^+) (Salim and Cheah, 2009):

- Viscous sublayer ($y^+ < 5$)
- Buffer layer or blending region ($5 < y^+ < 30$)
- Fully turbulent or log-law region ($y^+ > 30$ to 60)

The y^+ evaluation is often carried out in CFD modelling to identify the best mesh (coarser or finer) for a particular problem. This dimensionless number is the ratio between the turbulent and laminar influences in a cell. Viscous damping reduces the tangential velocity fluctuations close to the wall, while kinematic blocking reduces the normal fluctuations. In the outer part of the near-wall region, the turbulence is rapidly increased by the production of turbulent kinetic energy due to the large gradients in mean velocity. Generally, $y^+ \approx 30$ is appropriate for wall functions whereas $y^+ \approx 1$ can be used for near-wall modelling (Salim and Cheah, 2009).

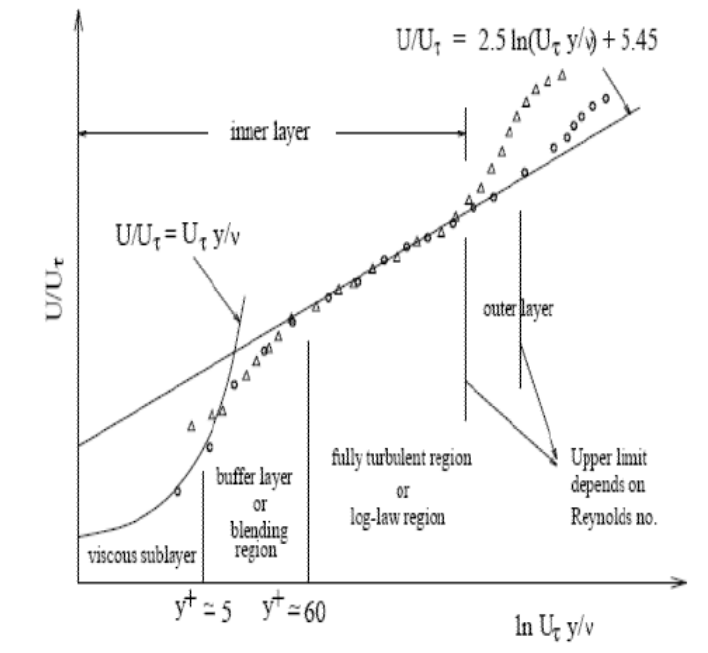


Figure A-3: Subdivisions of near-wall region (Salim and Cheah, 2009).

A.6 Flow around a cylinder and time step size calculation

Flow around a cylinder represents one of the main problems of fluid mechanics. At low Reynolds number the flow is symmetric but when the Reynolds number increases, flow begins to separate behind the cylinder and vortex shedding is created (typical of unsteady phenomenon) (Figure A-4).

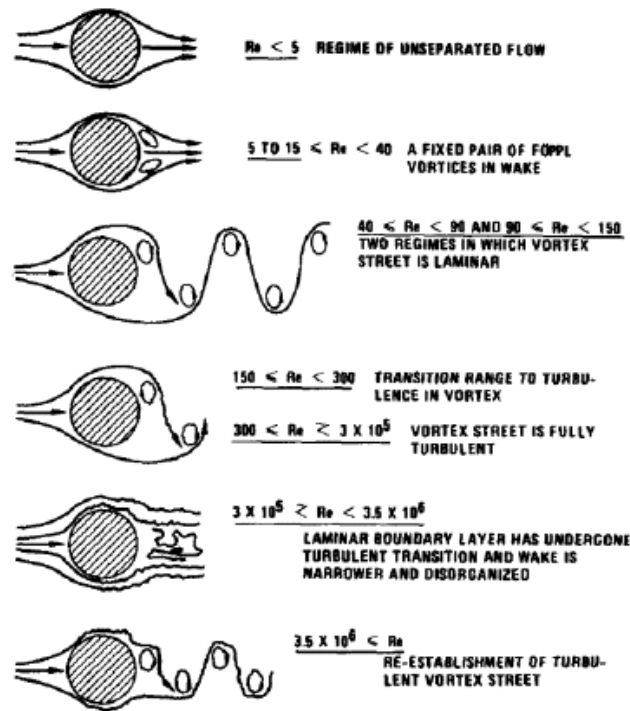


Figure A-4: Reynolds regimes for flow around a cylinder (Blevins, 1990).

For $40 < Re < 150$, there is a laminar vortex shedding in the wake of the cylinder. The laminar wake transient to turbulence in the region of $Re = 150$ to 300 . In the subcritical region $150 < Re < 3 \times 10^5$ the wake behind the circular cylinder becomes completely turbulent and a laminar boundary layer separation occurs.

The vortex shedding is calculated considering a dimensionless number, Strouhal number which is function of Reynolds as shown in Figure A-5 (Lienhard, 1966).

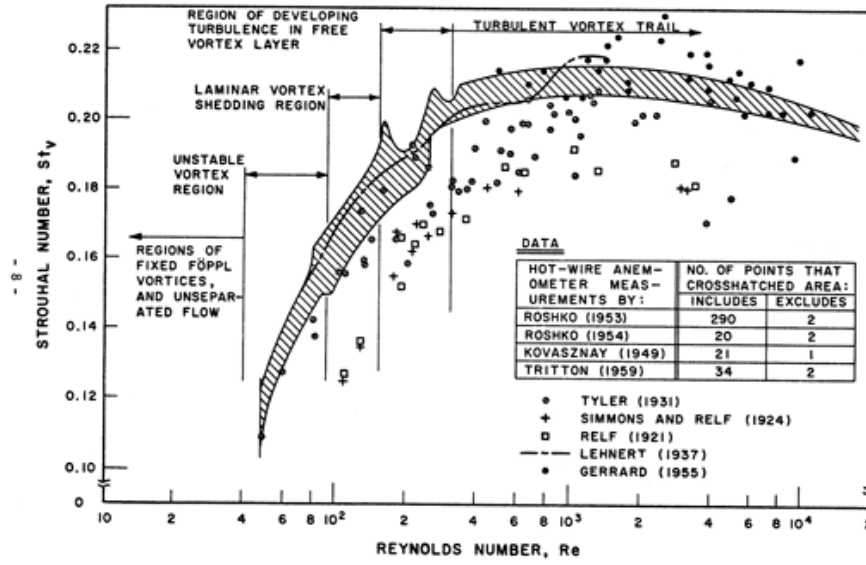


Figure A-5: Strouhal - Reynolds number data for circular cylinders, $40 < Re < 2 \cdot 10^4$ (Lienhard, 1966).

$$St = \frac{f d_t}{u} \quad (A-46)$$

Where:

f = frequency of vortex shedding [s^{-1}];

d_t = tube diameter [m];

u = free stream velocity [m/s].

From Figure A-5, knowing the Reynolds number, the Strouhal number is obtained and the frequency of vortex shedding can be calculated as follows (Fluent, 2017):

$$f = \frac{St u}{d_t} \quad (A-47)$$

The time period is:

$$T = \frac{1}{f} \quad (A-48)$$

In order to capture the shedding correctly, it is important to have at least 20-25 time steps in one shedding cycle (Fluent, 2017). Therefore, the time step size is defined as in Equation (A-49).

$$\Delta t = \frac{T}{n} \quad (\text{A-49})$$

Appendix B

B.1 Grid convergence

This section reports the results of simulations run using the geometry in Figure 4-12 with different number of nodes (Table B-1, Figure B-1). The mesh chosen has 150 nodes on the cylinder wall.

Table B-1: Total deposition flux values around probe 2 (773 K, $d_t=39$ mm) with different number of nodes ($d_{min}=0.43$ μm , $d_{mean}=68$ μm , $d_{max}=535$ μm , polydispersion parameter $n=1.07$, $U_0=2$ m/s) applying the model in section 7.5.

Cylinder nodes	100	150	200
Deposition flux [mg/(cm ² hr)]	7.80	3.83	3.79

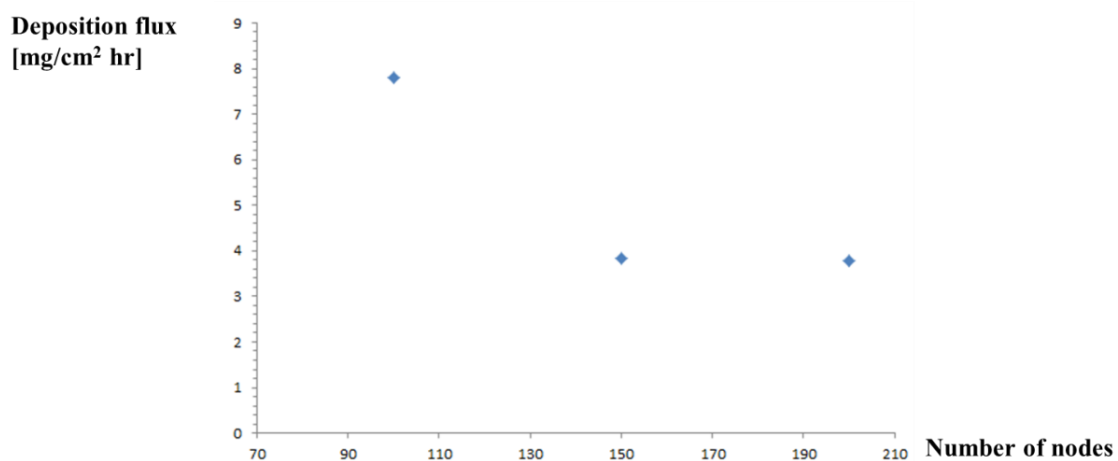


Figure B-1: Total deposition flux around probe 2 (773 K, $d_t=39$ mm) with different number of nodes ($d_{min}=0.43$ μm , $d_{mean}=68$ μm , $d_{max}=535$ μm , polydispersion parameter $n=1.07$, $U_0=2$ m/s) applying the model in section 7.5.

B.2 Configuration with bend

In this section, the presence of the bend downstream from the probes has been taken into account for configurations 1 and 2 at 773 K probe surface temperature (section 7.2). The geometries, meshes and ash particle tracking are reported for the two configurations

in Figure B-2 to Figure B-7, the mesh details in Table B-2 and Table B-3. Finally, the deposition flux values in Table B-4 to Table B-7.

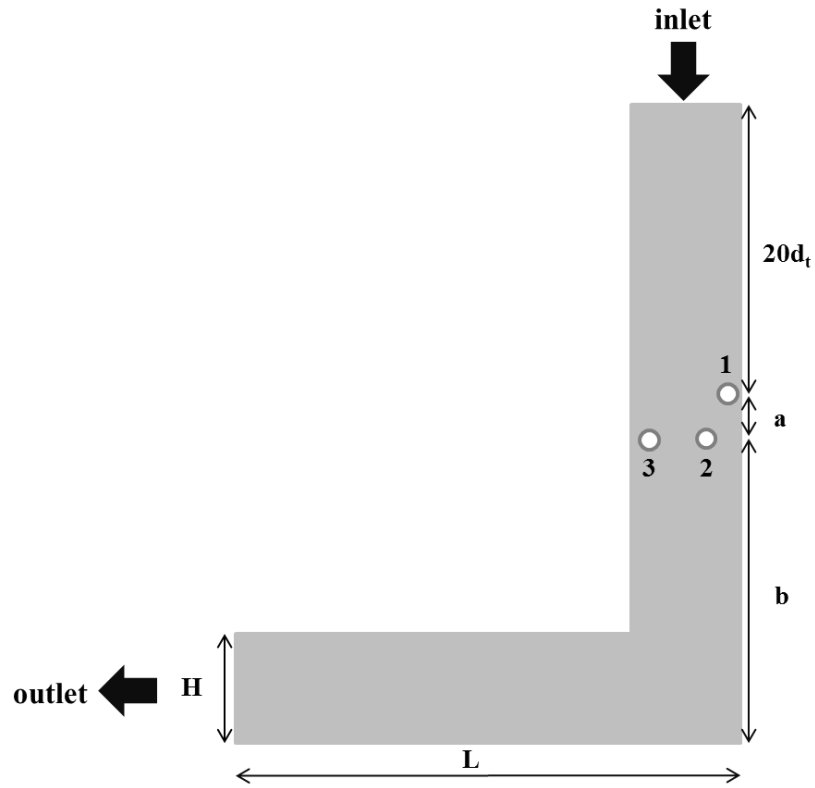


Figure B-2: 1st probes' configuration in the presence of the bend ($L= 1407.527$ mm, $H= 305.054$ mm, $a= 113.538$ mm, $b= 837.22$ mm, $d_t= 39$ mm).

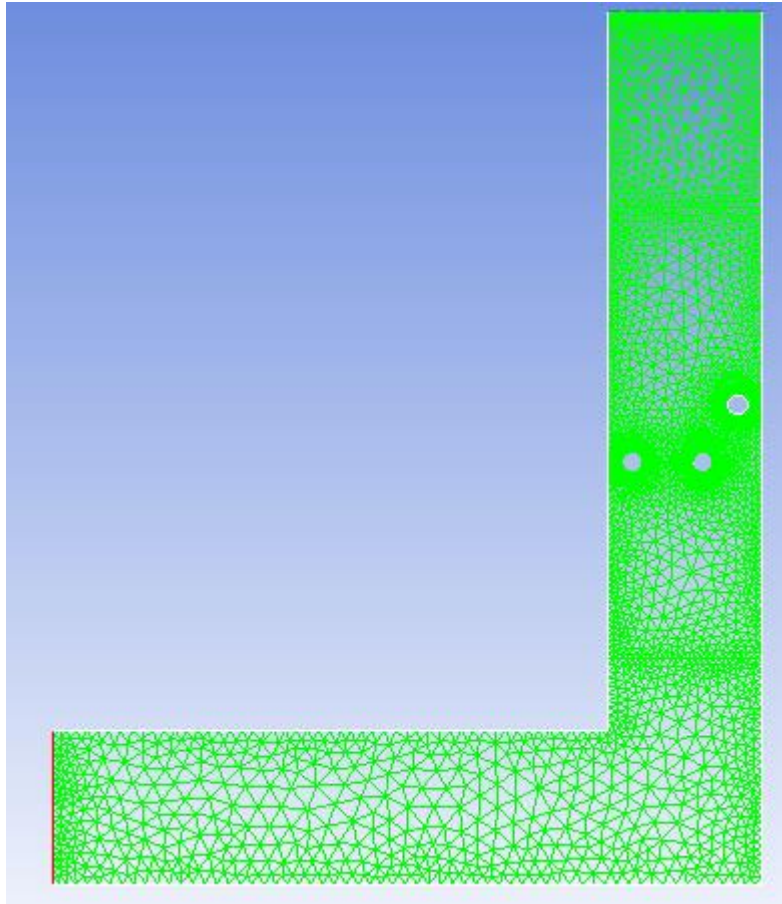


Figure B-3: Triangular mesh for the 1st probes' configuration in the presence of the bend.

Table B-2: Mesh features for the 1st probes' configuration in the presence of the bend.

Cylinder nodes	Nodes	Elements/Cells	Faces
150	6270	11613	17885

The estimated mesh quality is:

- Minimum Orthogonal Quality= $4.66 \cdot 10^{-1}$ (Orthogonal Quality ranges from 0 to 1, where values close to 0 correspond to low quality).
- Maximum Ortho Skew= $3.24 \cdot 10^{-1}$ (Ortho Skew ranges from 0 to 1, where values close to 1 correspond to low quality).
- Maximum Aspect Ratio= 4.87 (ideally equal to 1).

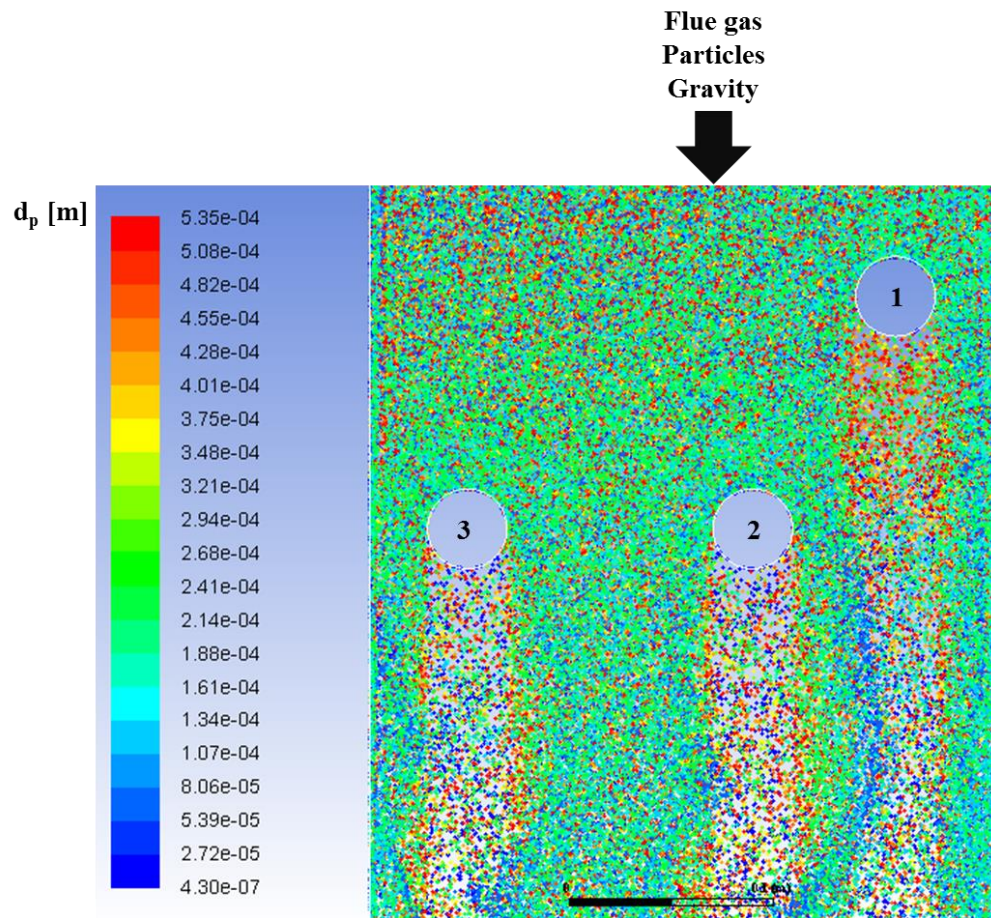


Figure B-4: Tracking of ash particles around the probes ($d_t = 39$ mm) using the 1st probes' configuration in the presence of the bend ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

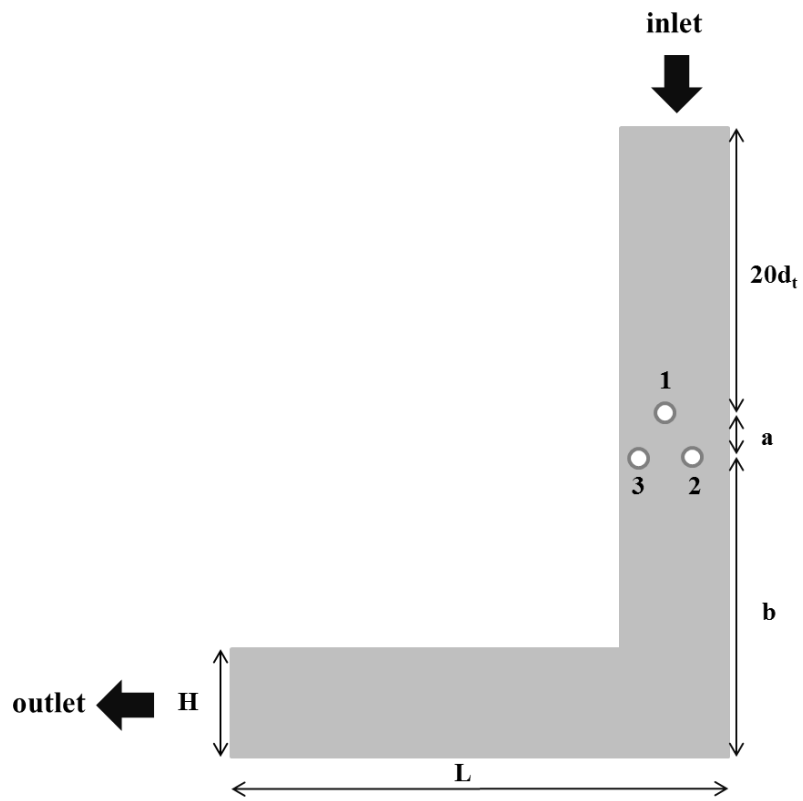


Figure B-5: 2nd probes' configuration in the presence of the bend ($L= 1407.527$ mm, $H= 305.054$ mm, $a= 113.538$ mm, $b= 837.22$ mm, $d_t= 39$ mm).

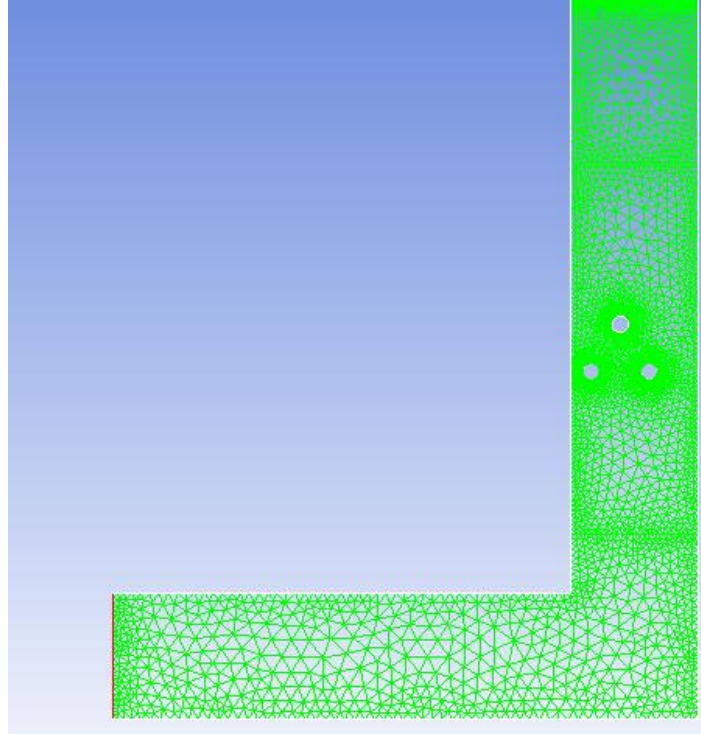


Figure B-6: Triangular mesh for the 2nd probes' configuration in the presence of the bend.

Table B-3: Mesh features for the 2nd probes' configuration in the presence of the bend.

Cylinder nodes	Nodes	Elements/Cells	Faces
150	6334	11746	18082

The estimated mesh quality is:

- Minimum Orthogonal Quality= $4.77 \cdot 10^{-1}$ (Orthogonal Quality ranges from 0 to 1, where values close to 0 correspond to low quality).
- Maximum Ortho Skew= $3.67 \cdot 10^{-1}$ (Ortho Skew ranges from 0 to 1, where values close to 1 correspond to low quality).
- Maximum Aspect Ratio= 4.97 (ideally equal to 1).

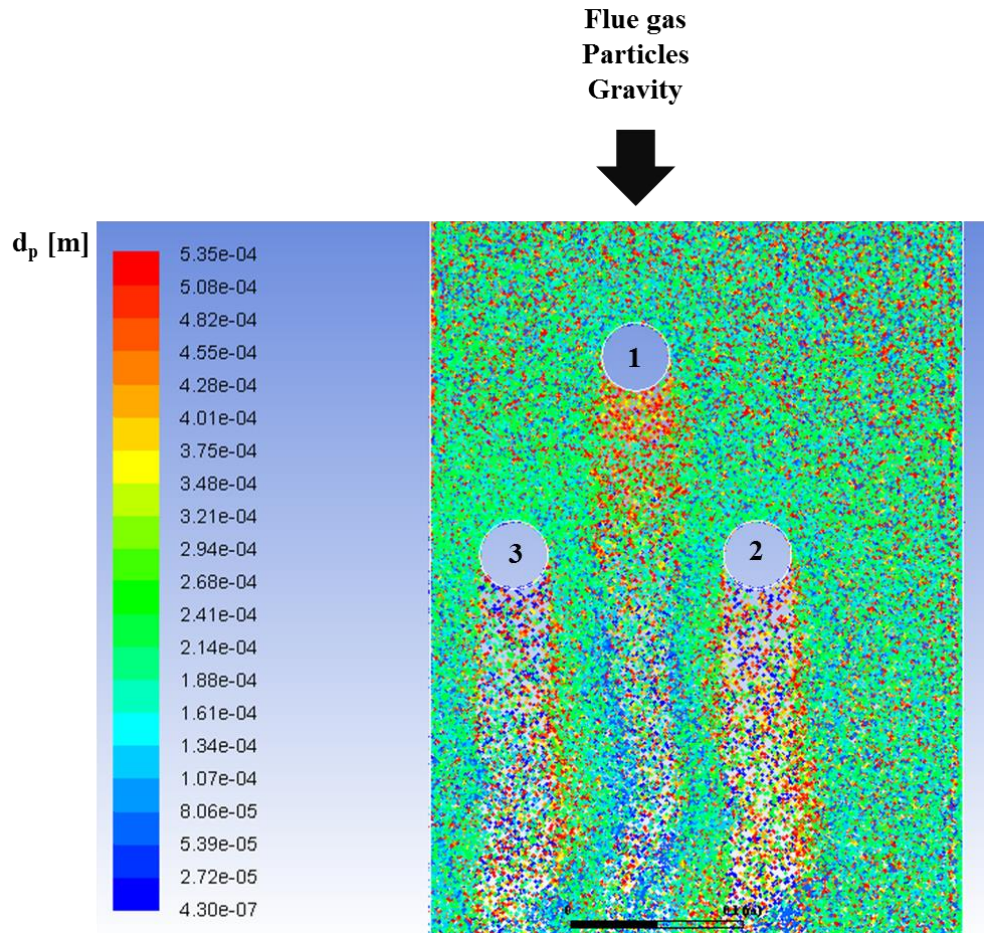


Figure B-7: Tracking of ash particles around the probes ($d_t = 39$ mm) using the 2nd configuration in the presence of the bend ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

Table B-4: Deposition fluxes on different zones around probes in the 1st configuration in the presence of the bend ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s).

	PROBE 1	PROBE 2	PROBE 3
UPSTREAM	7.85	10.58	9.03
SIDES	0.45	0.24	0.30
DOWNSTREAM	0.06	0.002	0.003
TOTAL	3.37	4.43	3.81

Table B-5: Deposition fluxes on different zones around probes in the 1st configuration in the absence of the bend ($d_{min}= 0.43\text{ }\mu\text{m}$, $d_{mean}= 68\text{ }\mu\text{m}$, $d_{max}= 535\text{ }\mu\text{m}$, polydispersion parameter $n= 1.07$, $U_0 = 2\text{ m/s}$).

	PROBE 1	PROBE 2	PROBE 3
UPSTREAM	7.53	10.23	8.70
SIDES	0.39	0.29	0.40
DOWNSTREAM	0.19	0.03	0.06
TOTAL	3.25	4.29	3.70

Table B-6: Deposition fluxes on different zones around probes in the 2nd configuration in the presence of the bend ($d_{min}= 0.43\text{ }\mu\text{m}$, $d_{mean}= 68\text{ }\mu\text{m}$, $d_{max}= 535\text{ }\mu\text{m}$, polydispersion parameter $n= 1.07$, $U_0 = 2\text{ m/s}$).

	PROBE 1	PROBE 2	PROBE 3
UPSTREAM	8.20	11.50	11.78
SIDES	0.21	0.20	0.44
DOWNSTREAM	0.11	0.001	0.01
TOTAL	3.48	4.81	4.99

Table B-7: Deposition fluxes on different zones around probes in the 2nd configuration in the absence of the bend ($d_{min}= 0.43\text{ }\mu\text{m}$, $d_{mean}= 68\text{ }\mu\text{m}$, $d_{max}= 535\text{ }\mu\text{m}$, polydispersion parameter $n= 1.07$, $U_0 = 2\text{ m/s}$).

	PROBE 1	PROBE 2	PROBE 3
UPSTREAM	9.48	12.12	12.58
SIDES	0.31	0.34	0.65
DOWNSTREAM	0.26	0.10	0.22
TOTAL	4.05	5.10	5.41

Appendix C

In this Appendix, the major and minor gas components detected in all the experiments are reported in Figure C-1 to Figure C-8 for comparison with the composition reported in Chapter 6 (section 6.2).

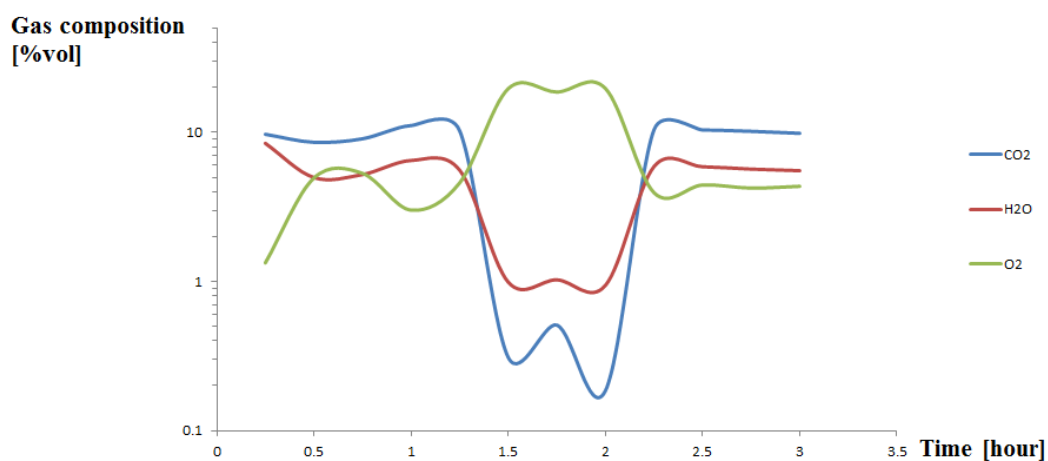


Figure C-1: Major gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (1st experiment).

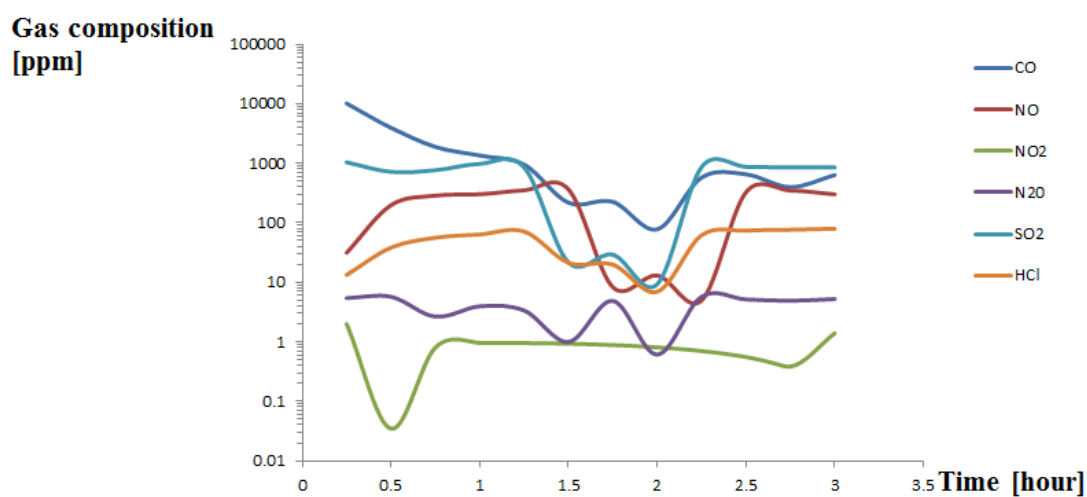


Figure C-2: Minor gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (1st experiment).

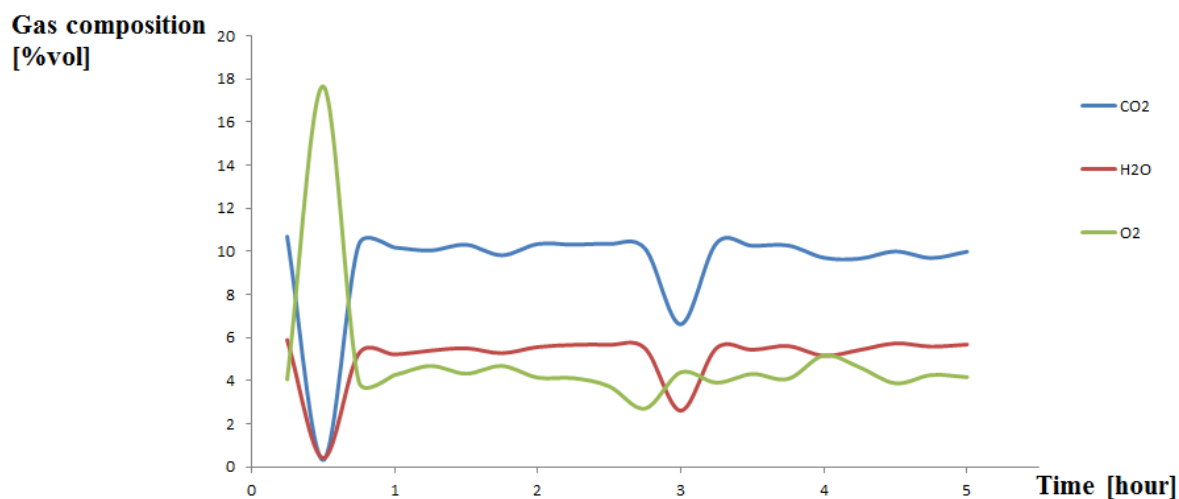


Figure C-3: Major gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (2nd experiment).

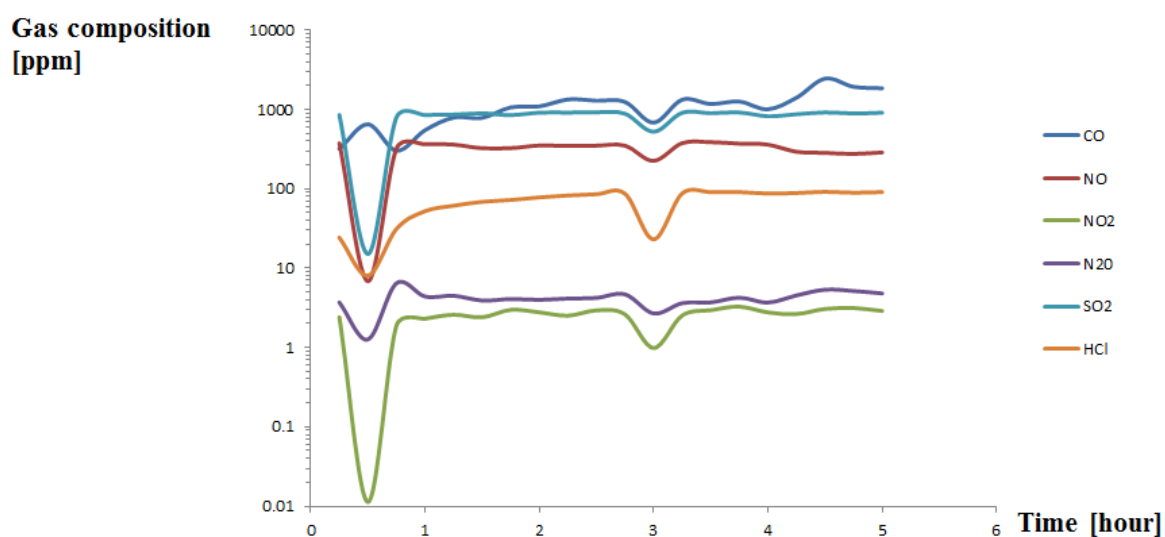


Figure C-4: Minor gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (2nd experiment).

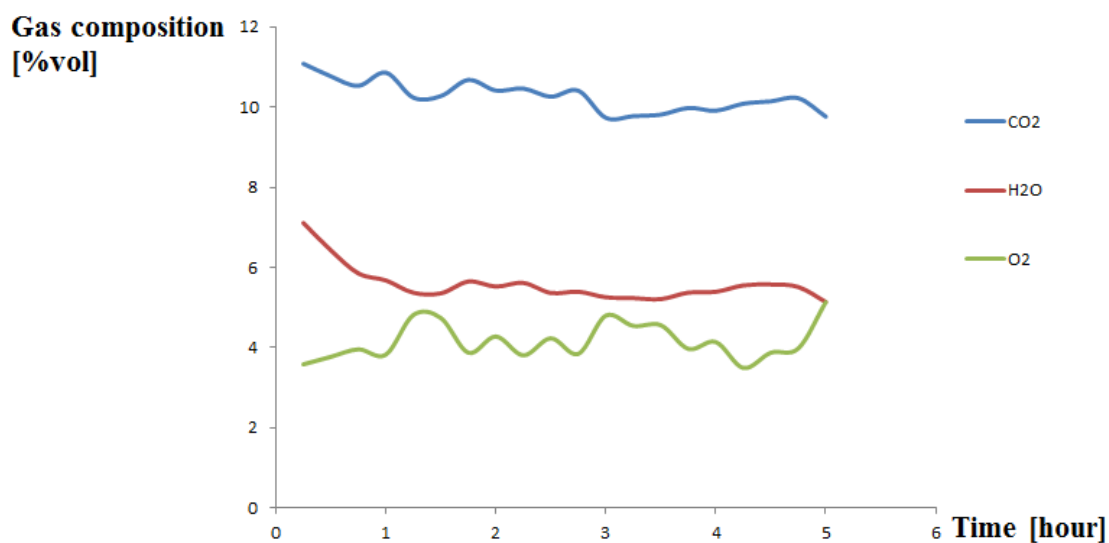


Figure C-5: Major gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (3rd experiment).

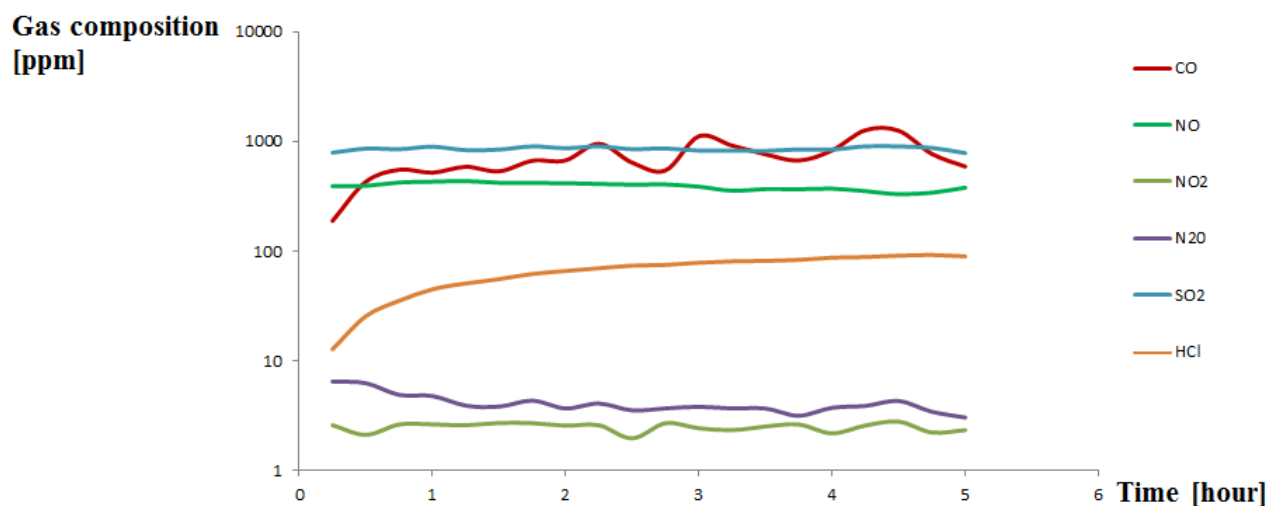


Figure C-6: Minor gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (3rd experiment).

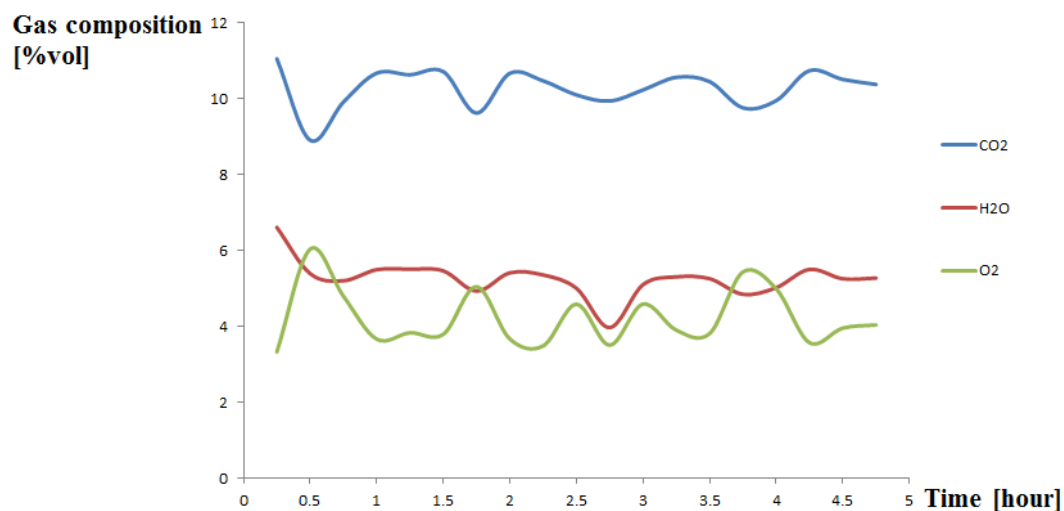


Figure C-7: Major gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (4th experiment).

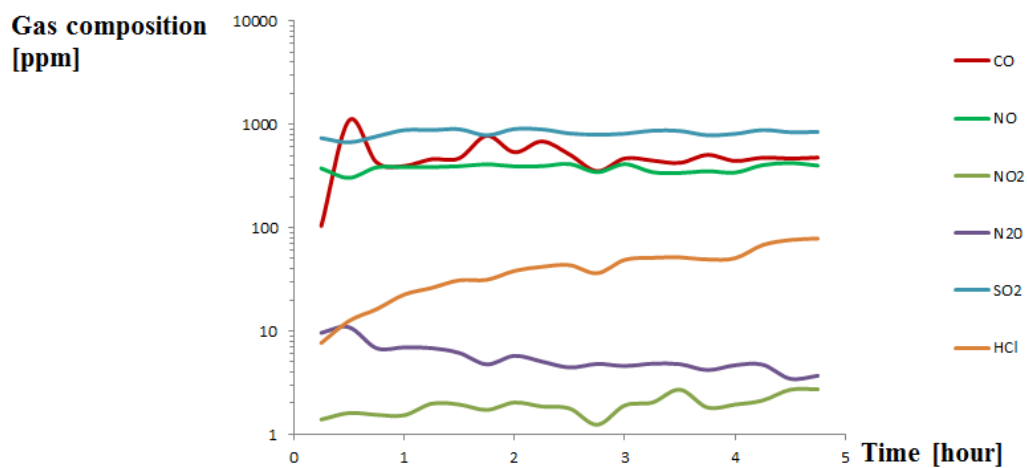


Figure C-8: Minor gas components from combustion of pulverised Daw Mill-12 wt.% Miscanthus (4th experiment).

Appendix D

In this Appendix, examples of SEM images are reported. Some of them have been taken for ash particle size measurements (Figure D-1) (using the software Image J) to identify a distribution of ash particles deposited around the probes (only for the second experiment in section 6.3.2).

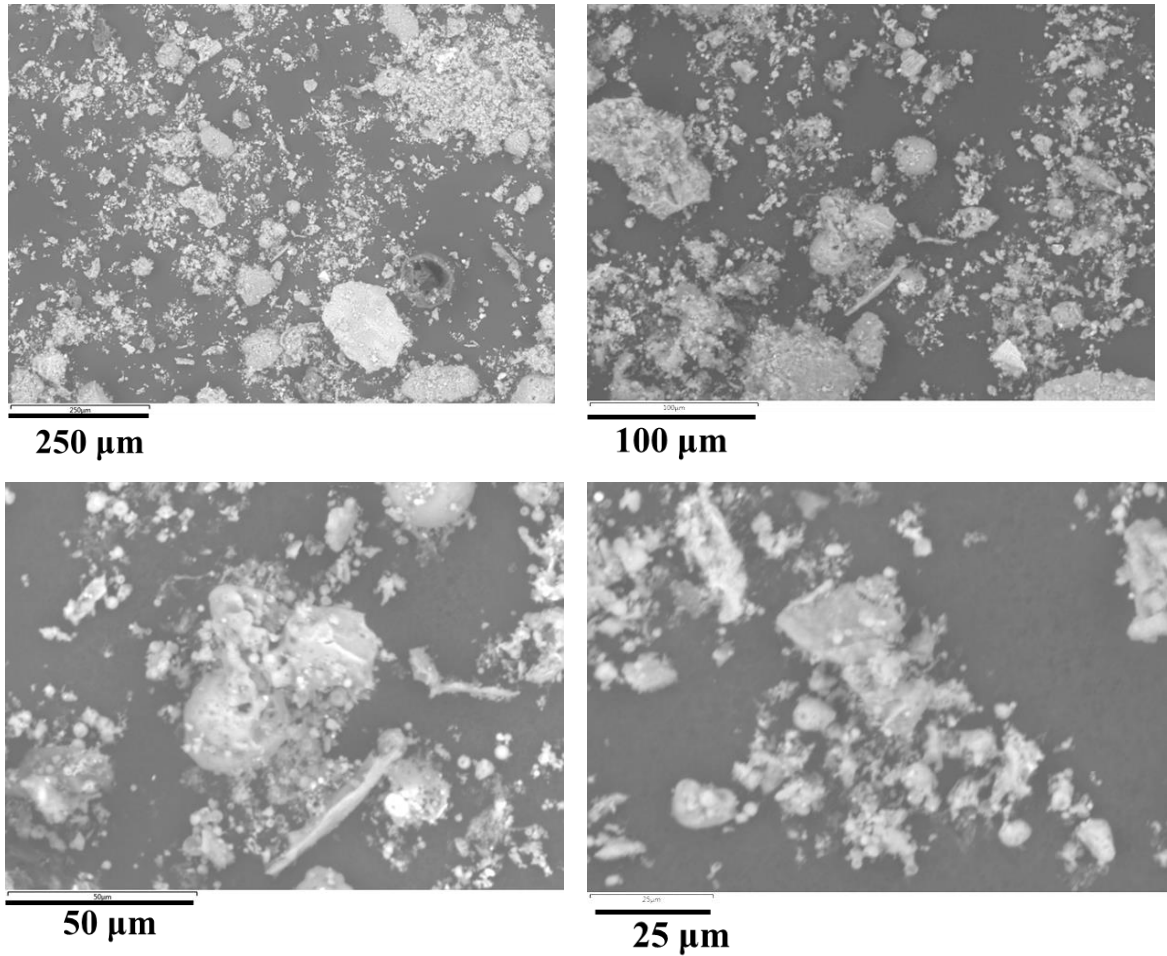


Figure D-1: Example of SEM images taken at different magnification to measure ash particle sizes with Image J (2nd experiment, probe 1 top and right).

Moreover, examples of SEM images of ash samples collected from the ports in the combustor rig and after the ash analysis tests are in Figure D-2.

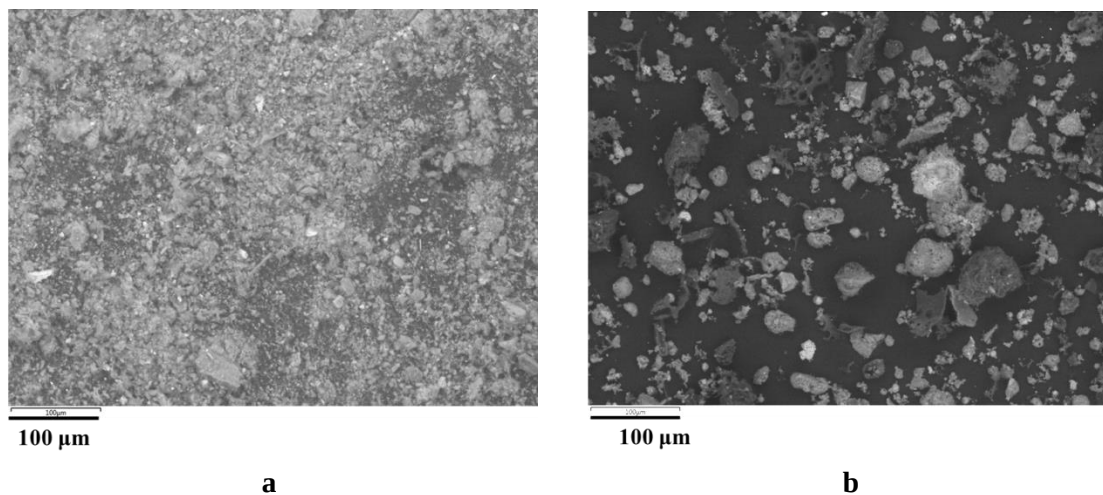


Figure D-2: a) Example of SEM image of ash obtained from one of the ash content tests (section 5.4.1); b) example of SEM image of fly ash collected from port 1 (4th experiment).

Appendix E

This Appendix compleates the information provided in section 5.7. The main steps followed during the experiments of Daw Mill-12 wt.% Miscanthus combustion in the pulverised combustion rig at Cranfield have been summarised as follows:

- 1) Assemble the deposition probes and place them in the combustor
- 2) Fix the probes' thermocouples (air in and out, probe front and back)
- 3) Start the combustor and warm it up overnight:
 - Extraction fan, compressed air and cooling pump ON
 - N₂ valve ON (this was used for the feeding system and for the view ports)
 - Set the control panel
 - Open condenser bypass
 - Enable rig fans
 - Set air rotameters
 - Open natural gas valves
 - Check feeder valve is closed, open MB (main burner) and PILOT inlet valves on the top of the combustor
 - Make sure the pressure is negative (> 100 Pa) varying the ID fan
 - Light the FB combustor
 - Light the PF combustor with PILOT and MB gas
 - Once the flame can be seen in the combustor, set the MB to 30 L/min
 - Check the flame from the view ports and keep an eye on all the rotameters
 - Start recording FTIR and Piccolo data
 - Check at least one hour after lighting and adjust rotameters if necessary. Some reference values at this stage are: O₂~ 8% , P~ 200 Pa
 - Set the air flow rate for the ceramic probes (30 L/min for example). Check that the air pressure is 4 bar

The main values to set the rig up are in Table E-1.

Table E-1: Main parameters used to set the rig up. Abbreviations: ID= induced draft; FD= forced draft; MB= main burner; FBP= fluidised bed primary air; FBS= fluidised bed secondary air; FB= fluidised bed.

P [Pa]	ID [Hz]	FD [Hz]	MB [L/min]	PILOT AIR [L/min]	FBP [L/min]	FBS [L/min]	FB [L/min]
>100	15	25	30	120	400	800	16

4) Warm the combustor up the morning after:

- Increase slowly FD from 25 to 35 Hz and adjust PILOT AIR, FBP, FBS rotameters
- Adjust MB to get ~ 5% O₂
- Open condenser valves and close bypass
- Increase/decrease ID fan slowly to achieve P> 100 Pa
- In this stage T should be up to 850°C
- Open condenser drain valve and cyclone valve

The main reference parameters at this stage are in Table E-2.

Table E-2: Main parameters used to warm the rig up. Abbreviations: ID= induced draft; FD= forced draft; MB= main burner; FBP= fluidised bed primary air; FBS= fluidised bed secondary air; FB= fluidised bed.

P [Pa]	ID [Hz]	FD [Hz]	MB [L/min]	PILOT AIR [L/min]	FBP [L/min]	FBS [L/min]	FB [L/min]
~200-300	↑↓(~19)	35	35	120	600	2000	16

5) Start feeding solid fuel:

- When $T_{flame\ up\ right} \sim 800^{\circ}C$, set the gas off and start feeding the solid fuel
- Turn MB and Pilot OFF
- Maintain P~ 100 Pa using ID fan
- If in the combustor there is no flame, relight again with PILOT and MB gas
- Set rotameters (MB= 0, PILOT AIR= 100, FBP= 750, FBS= 1600, FB= 0)
- Adjust FBS air up/down or fuel feed rate to achieve O₂~ 4% (use FTIR to check)
- Check that T≥ 800 °C. Every time FBS is changed, PILOT AIR and FBP will change as a consequence, adjust them and keep an eye on P

- Adjust air flow rate to keep the probe temperatures constant
- 6) Cool down overnight:
- Stop feeding solid fuel
 - ID= 15, FD= 25
 - Air ports: (PILOT AIR= 30, FBP= 200, FBS= 0)
 - Close gas valves
 - Open bypass and close condenser valves
 - Check that the flame is extinguished
 - Close condenser drain and cyclone valves
 - Set air flow rate of the probes to ~ 30 L/min
- 7) Switch off:
- Check water ($T \sim 40$ °C or < 100 °C) and gas temperature ($T_{\text{upright}} \sim 100$ °C)
 - Extraction fan, compressed air and cooling pump OFF
 - Main control panel OFF
 - N₂ valve off
 - Once the combustor cools down, the probes can be extracted for ash collection and analysis

Appendix F

In this Appendix, additional simulations run at the beginning of the PhD or to study specific aspects (e.g. ash particle diameters, different geometries, probe configurations, etc.) have been reported. This material supports the results in Chapter 4 and Chapter 7.

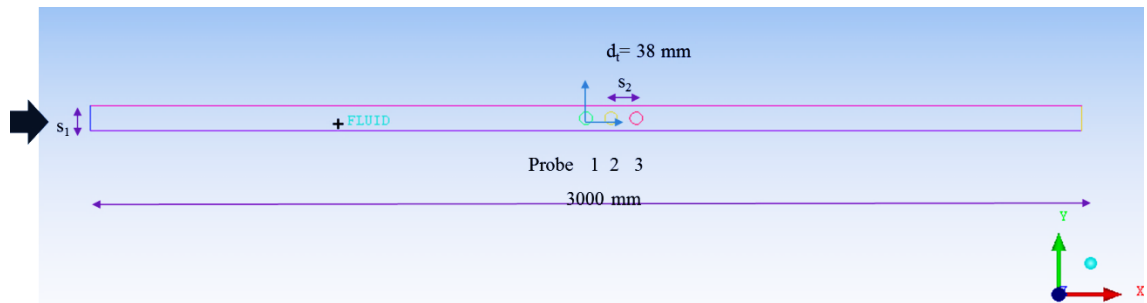
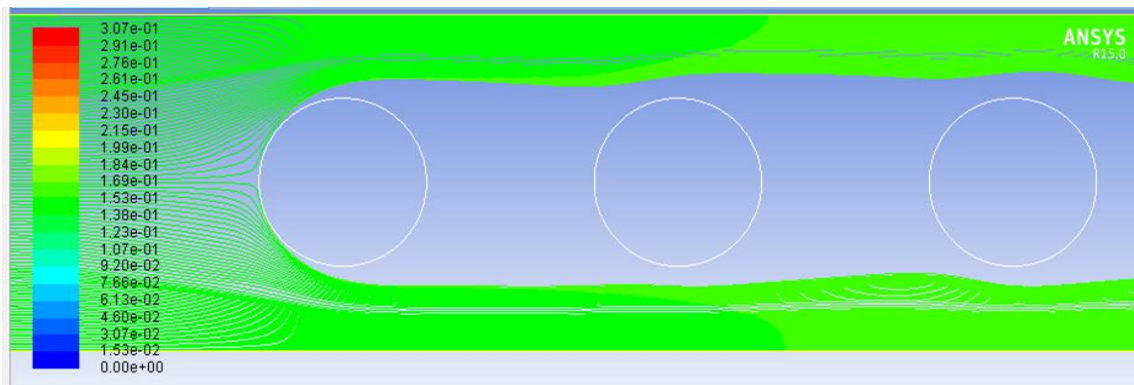
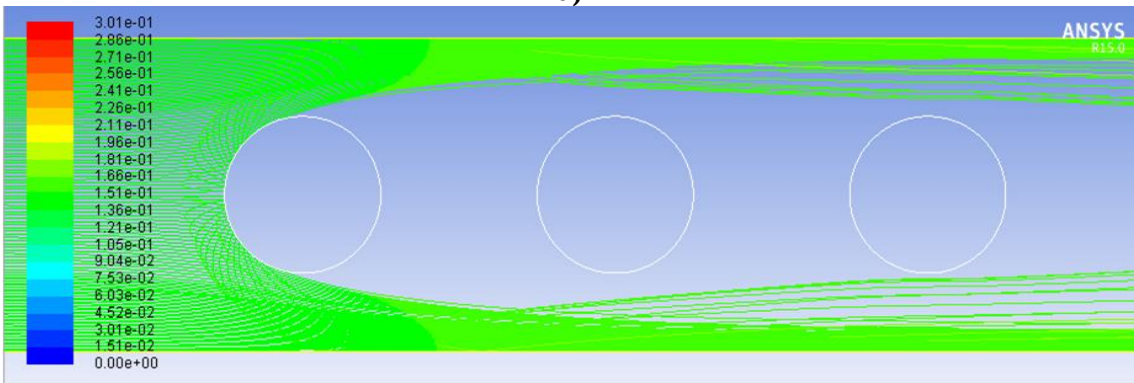


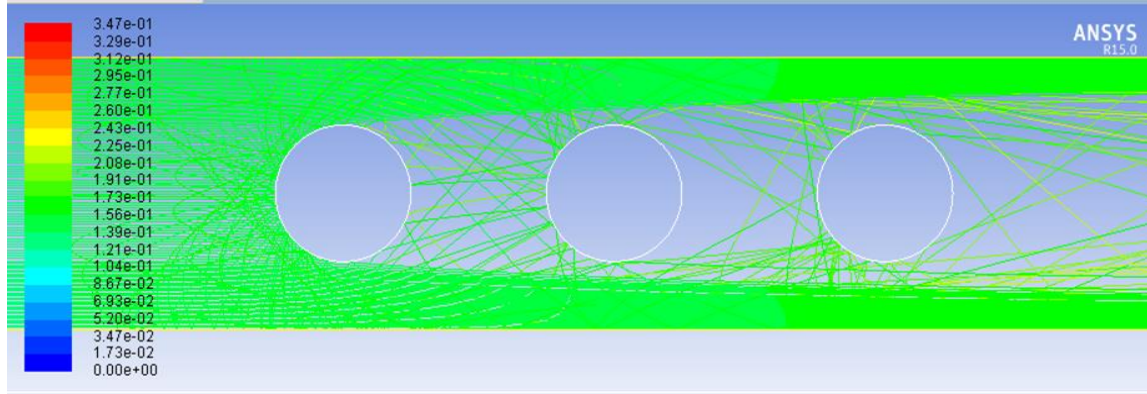
Figure F-1: 2D geometry from (Waclawiak and Kalisz, 2014) ($d_t = 38$ mm, $s_1/d_t = 2$, $s_2/d_t = 2$).



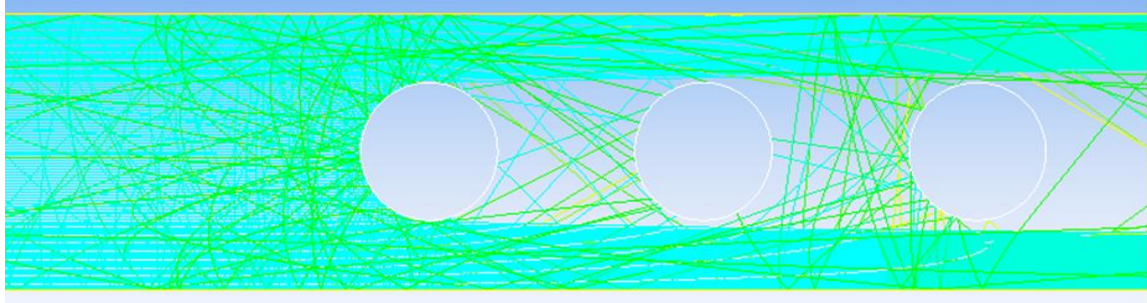
a)



b)



c)



d)

Figure F-2: Ash particle trajectories around probes ($d_t = 38$ mm, $U_0 = 10$ m/s, $\mu_g = 46 \cdot 10^{-6}$ Pa·s, $\rho_g = 0.245$ kg/m³, $\rho_p = 2200$ kg/m³, $k-\varepsilon$ standard, a) $d_p = 10$ μ m, b) $d_p = 40$ μ m, c) $d_p = 100$ μ m, d) $d_p = 200$ μ m).

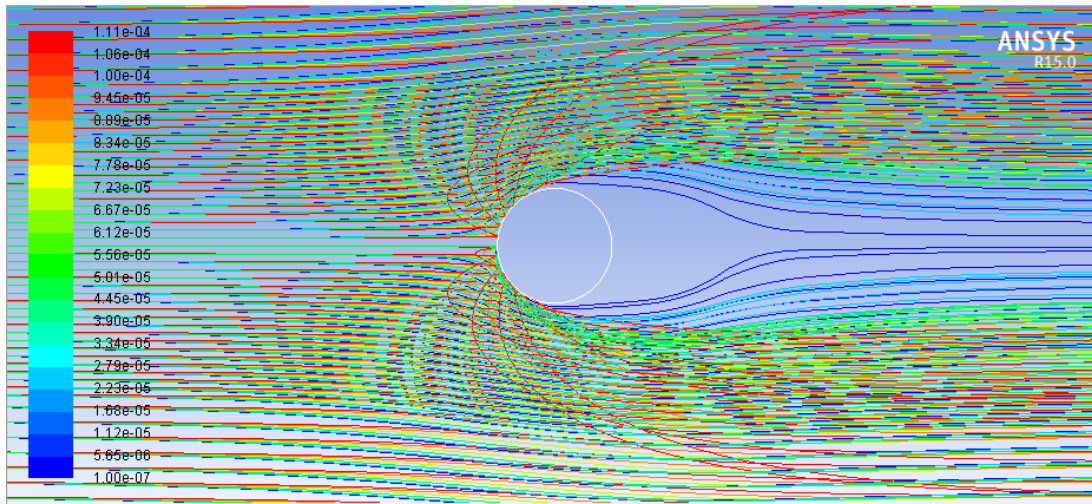


Figure F-3: Ash particle trajectories without turbulent dispersion ($d_{min} = 0.1$ μ m, $d_{mean} = 40$ μ m, $d_{max} = 200$ μ m, $n = 0.8$) around probe (geometry from (Weber et al., 2013)) ($d_t = 38$ mm, $U_0 = 10$ m/s, $\mu_g = 46 \cdot 10^{-6}$ Pa·s, $\rho_g = 0.245$ kg/m³, $\rho_p = 2200$ kg/m³, $k-\varepsilon$ standard).

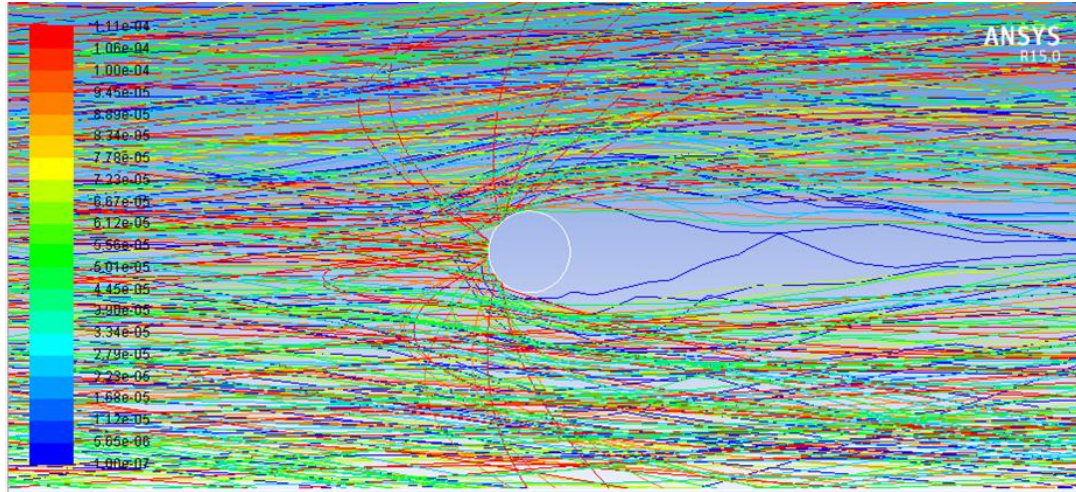


Figure F-4: Ash particle trajectories with turbulent dispersion ($d_{min}=0.1\text{ }\mu\text{m}$, $d_{mean}=40\text{ }\mu\text{m}$, $d_{max}=200\text{ }\mu\text{m}$, $n=0.8$) around probe (geometry from (Weber et al., 2013)) ($d_t=38\text{ mm}$, $U_0=10\text{ m/s}$, $\mu_g=46\text{ }10^{-6}\text{ Pa}\cdot\text{s}$, $\rho_g=0.245\text{ kg/m}^3$, $\rho_p=2200\text{ kg/m}^3$, number of tries=1, number of particles tracked= 582, $k-\varepsilon$ standard).

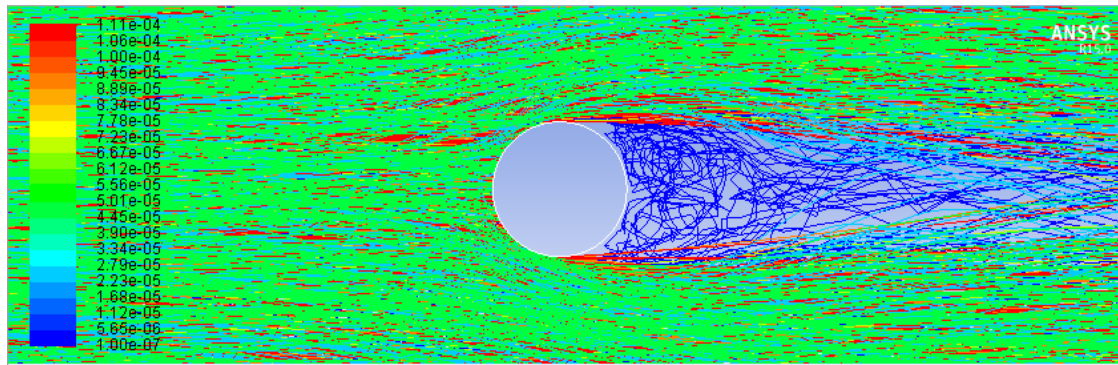


Figure F-5: Ash particle trajectories with turbulent dispersion ($d_{min}=0.1\text{ }\mu\text{m}$, $d_{mean}=40\text{ }\mu\text{m}$, $d_{max}=200\text{ }\mu\text{m}$, $n=0.8$) around probe (geometry from (Weber et al., 2013)) ($d_t=38\text{ mm}$, $U_0=10\text{ m/s}$, $\mu_g=46\text{ }10^{-6}\text{ Pa}\cdot\text{s}$, $\rho_g=0.245\text{ kg/m}^3$, $\rho_p=2200\text{ kg/m}^3$, number of tries=10, number of particles tracked= 5820, $k-\varepsilon$ standard).

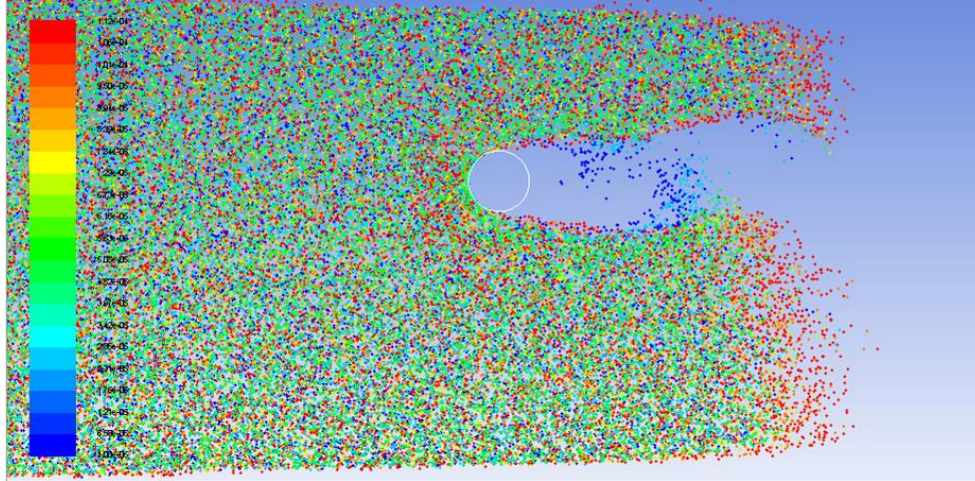


Figure F-6: Ash particle tracking ($d_{min}=1\text{ }\mu\text{m}$, $d_{mean}=40\text{ }\mu\text{m}$, $d_{max}=112\text{ }\mu\text{m}$, $n=0.8$) around probe 2 (Cranfield rig) ($d_t=39\text{ mm}$, $U_0=4\text{ m/s}$, $\mu_g=46\text{ }10^{-6}\text{ Pa}\cdot\text{s}$, $\rho_g=0.345\text{ kg/m}^3$, $\rho_p=2200\text{ kg/m}^3$, $k-\omega\text{ SST}$, $t=0.365\text{ s}$).

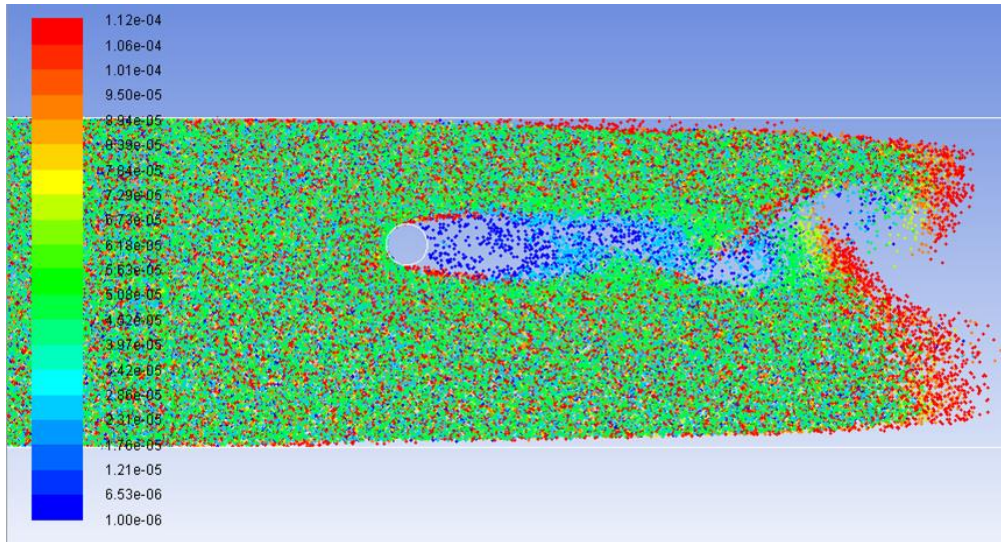


Figure F-7: Ash particle tracking ($d_{min}=1\text{ }\mu\text{m}$, $d_{mean}=40\text{ }\mu\text{m}$, $d_{max}=112\text{ }\mu\text{m}$, $n=0.8$) around probe 2 (Cranfield rig) ($d_t=39\text{ mm}$, $U_0=4\text{ m/s}$, $\mu_g=46\text{ }10^{-6}\text{ Pa}\cdot\text{s}$, $\rho_g=0.345\text{ kg/m}^3$, $\rho_p=2200\text{ kg/m}^3$, $k-\omega\text{ SST}$, $t=0.43\text{ s}$).

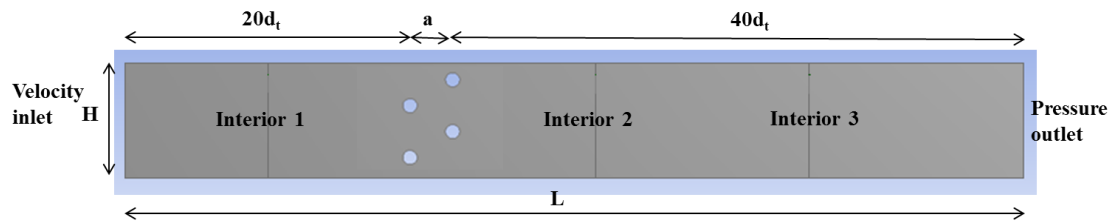


Figure F-8: 2D geometry and boundary conditions around probes in the combustor rig at Cranfield (tube diameter $d_t = 39$ mm) ($L = 2453.54$ mm, $H = 305.054$ mm, $a = 113.538$ mm).

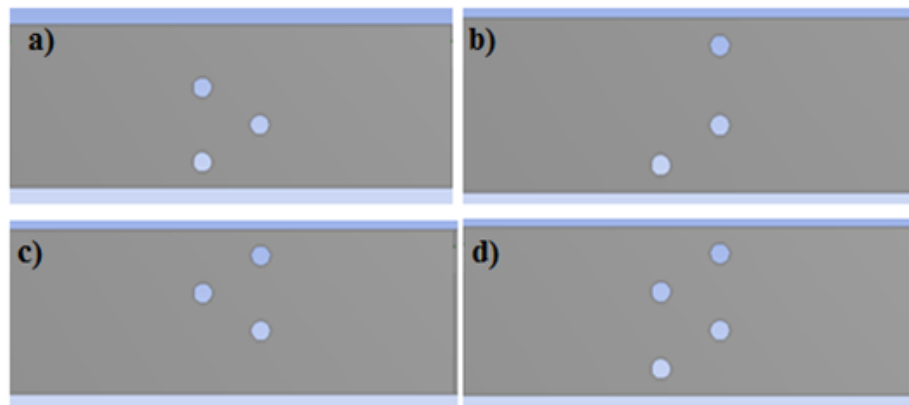


Figure F-9: Different probes' configuration (tube diameter $d_t = 39$ mm).

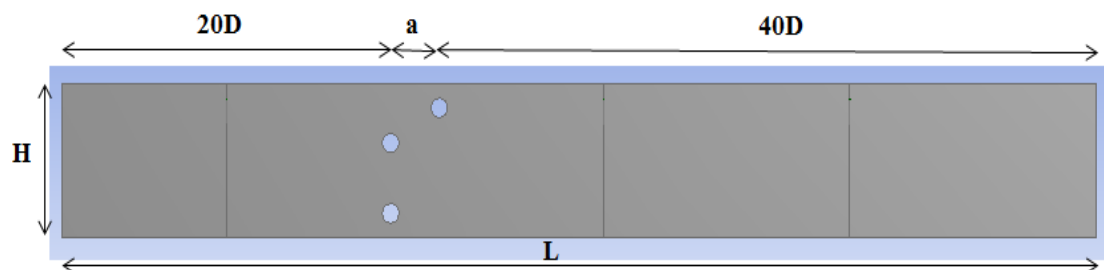


Figure F-10: Different probes' configuration ($d_t = 39$ mm, $L = 2453.54$ mm, $H = 305.054$ mm, $a = 113.538$ mm).

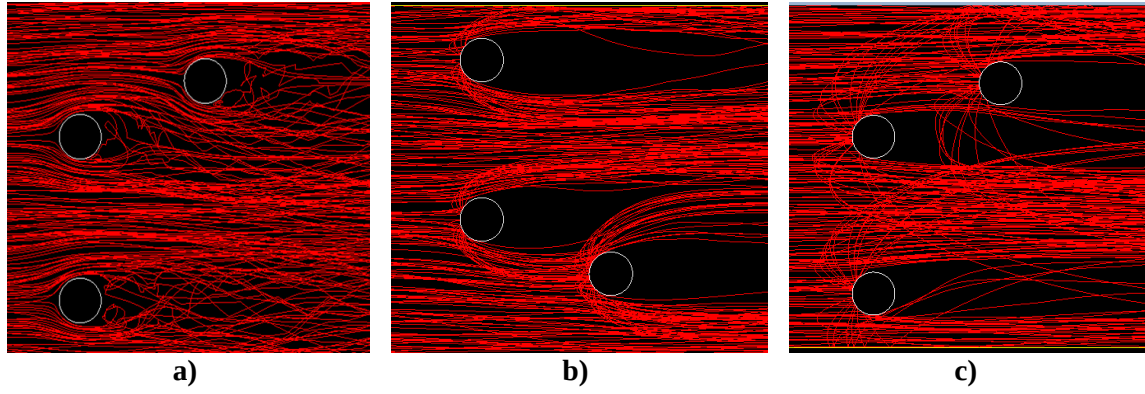


Figure F-11: Ash particle trajectories (a) $d_p = 1 \mu\text{m}$, b) $d_p = 50 \mu\text{m}$, c) $d_p = 100 \mu\text{m}$) ($d_t = 39 \text{ mm}$, $U_0 = 4 \text{ m/s}$, $\mu_g = 46 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$, $\rho_g = 0.345 \text{ kg/m}^3$, $\rho_p = 2200 \text{ kg/m}^3$, $k-\omega$ SST).

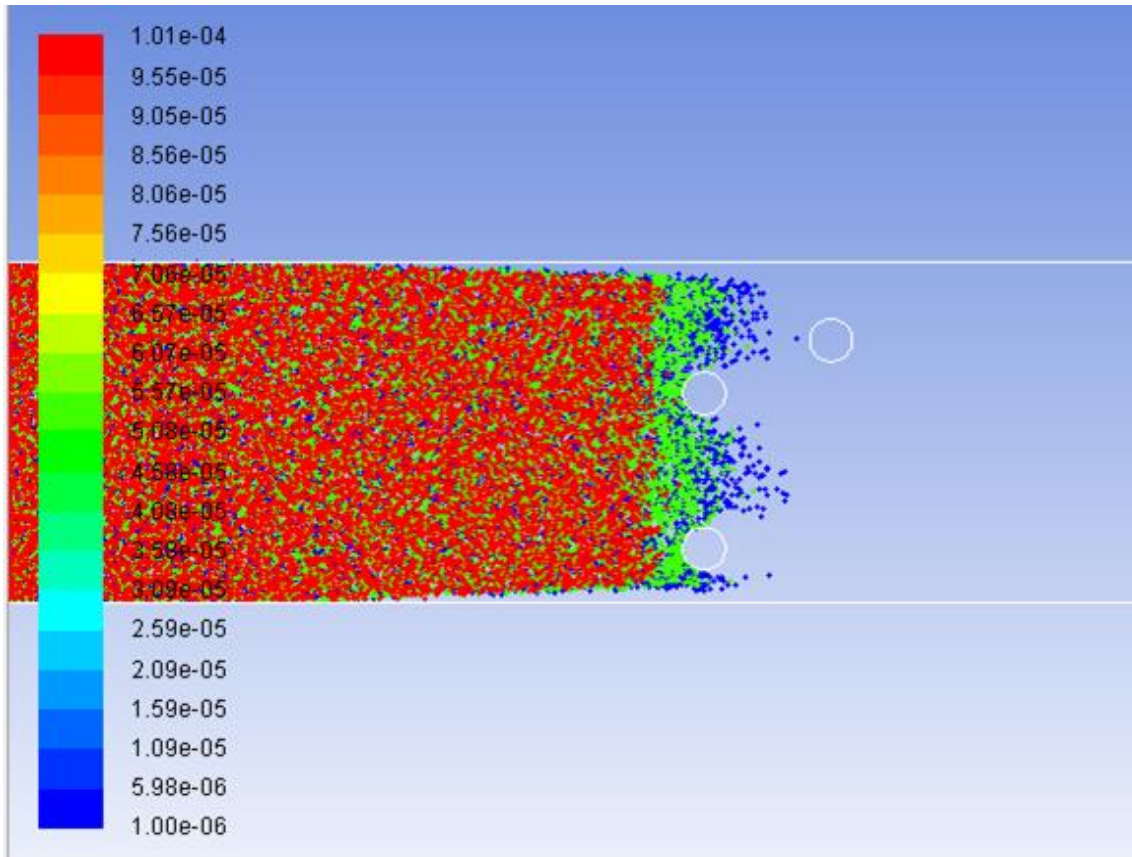


Figure F-12: Ash particle tracking ($d_{min} = 1 \mu\text{m}$, $d_{mean} = 40 \mu\text{m}$, $d_{max} = 100 \mu\text{m}$, $n = 0.8$) ($d_t = 39 \text{ mm}$, $U_0 = 4 \text{ m/s}$, $\mu_g = 46 \cdot 10^{-6} \text{ Pa}\cdot\text{s}$, $\rho_g = 0.345 \text{ kg/m}^3$, $\rho_p = 2200 \text{ kg/m}^3$, $k-\omega$ SST, $t = 0.2 \text{ s}$).

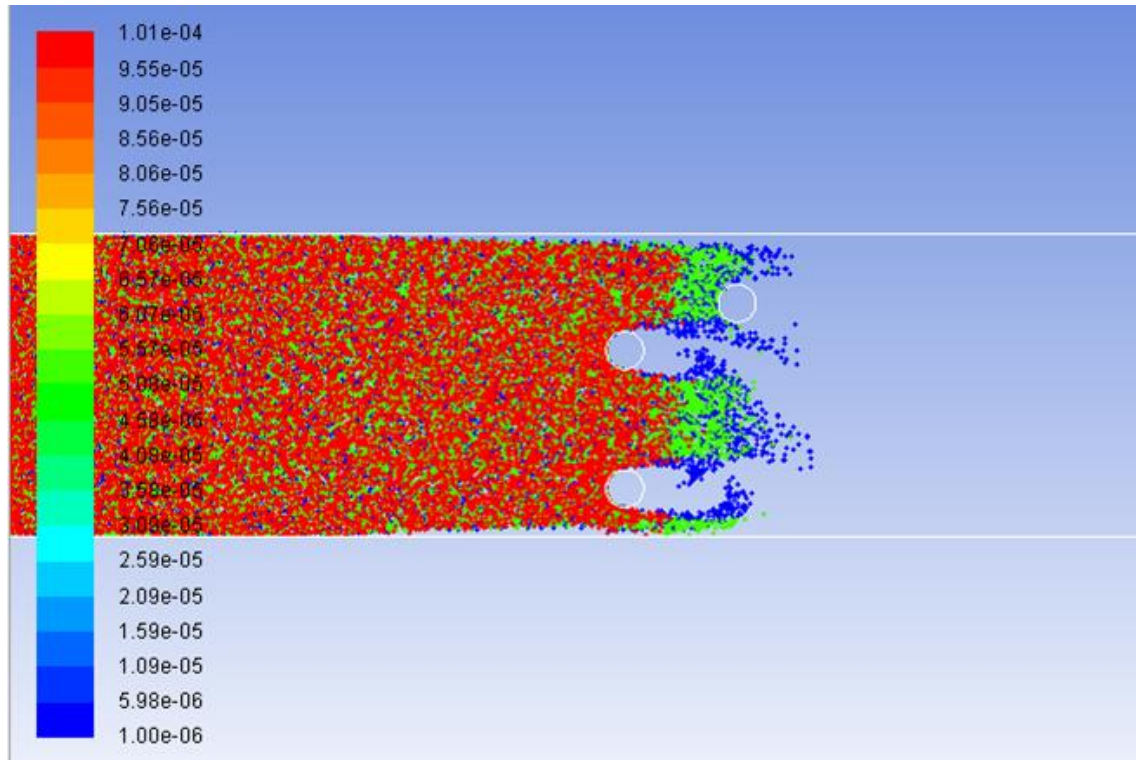


Figure F-13: Ash particle tracking ($d_{min}=1\text{ }\mu\text{m}$, $d_{mean}=40\text{ }\mu\text{m}$, $d_{max}=100\text{ }\mu\text{m}$, $n=0.8$) ($d_t=39\text{ mm}$, $U_0=4\text{ m/s}$, $\mu_g=46\text{ }10^{-6}\text{ Pa}\cdot\text{s}$, $\rho_g=0.345\text{ kg/m}^3$, $\rho_p=2200\text{ kg/m}^3$, $k-\omega\text{ SST}$, $t=0.227\text{ s}$).

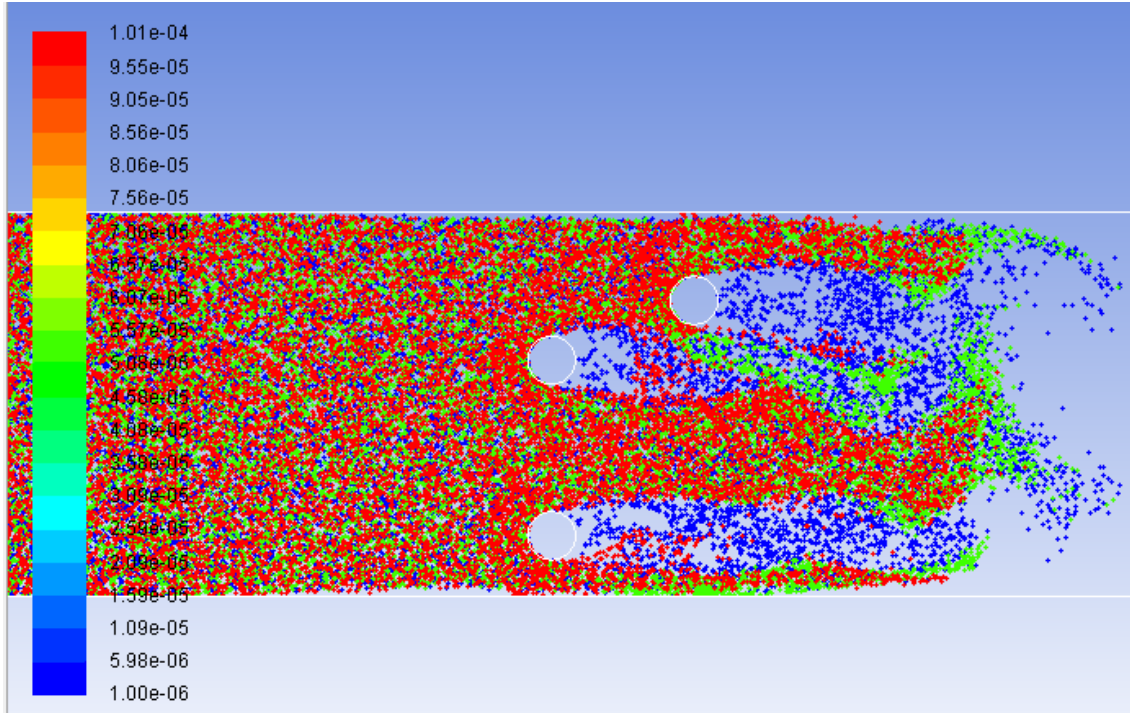


Figure F-14 Figure F-15: Ash particle tracking ($d_{min}=1\text{ }\mu\text{m}$, $d_{mean}=40\text{ }\mu\text{m}$, $d_{max}=100\text{ }\mu\text{m}$, $n=0.8$) ($d_t=39\text{ mm}$, $U_0=4\text{ m/s}$, $\mu_g=46\text{ }10^{-6}\text{ Pa}\cdot\text{s}$, $\rho_g=0.345\text{ kg/m}^3$, $\rho_p=2200\text{ kg/m}^3$, $k-\omega$ SST, $t=0.28\text{ s}$).

Table F-1: Predicted deposition fluxes due to the stickiness of the surface around probe 1 ($d_t=39\text{ mm}$) using the 1st probes' configuration ($d_{min}=0.43\text{ }\mu\text{m}$, $d_{mean}=68\text{ }\mu\text{m}$, $d_{max}=535\text{ }\mu\text{m}$, polydispersion parameter $n=1.07$, $U_0=2\text{ m/s}$) at Na_2SO_4 [1 ppm] and different probe surface temperatures.

T [K]	Deposition flux [$\text{mg/cm}^2\text{ hr}$]			
	Upstream	Side	Downstream	Total
773	$2.45\text{ }10^{-3}$	$9.13\text{ }10^{-5}$	$2.13\text{ }10^{-4}$	$1.09\text{ }10^{-3}$
873	$2.22\text{ }10^{-3}$	$6.85\text{ }10^{-5}$	$7.35\text{ }10^{-5}$	$9.52\text{ }10^{-4}$
973	$2.10\text{ }10^{-3}$	$5.16\text{ }10^{-5}$	$4.96\text{ }10^{-5}$	$8.89\text{ }10^{-4}$

Table F-2: Predicted deposition fluxes due to the stickiness of the surface around probe 2 ($d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at Na_2SO_4 [1 ppm] and different probe surface temperatures.

Deposition flux [$\text{mg}/\text{cm}^2 \text{ hr}$]				
T [K]	Upstream	Side	Downstream	Total
773	$2.74 \cdot 10^{-3}$	$1.06 \cdot 10^{-4}$	$1.21 \cdot 10^{-4}$	$1.19 \cdot 10^{-3}$
873	$2.53 \cdot 10^{-3}$	$4.96 \cdot 10^{-5}$	$3.41 \cdot 10^{-5}$	$1.06 \cdot 10^{-3}$
973	$2.55 \cdot 10^{-3}$	$5.19 \cdot 10^{-5}$	$5.24 \cdot 10^{-5}$	$1.07 \cdot 10^{-3}$

Table F-3: Predicted deposition fluxes due to the stickiness of the surface around probe 3 ($d_t = 39$ mm) using the 1st probes' configuration ($d_{min} = 0.43$ μm , $d_{mean} = 68$ μm , $d_{max} = 535$ μm , polydispersion parameter $n = 1.07$, $U_0 = 2$ m/s) at Na_2SO_4 [1 ppm] and different probe surface temperatures.

Deposition flux [$\text{mg}/\text{cm}^2 \text{ hr}$]				
T [K]	Upstream	Side	Downstream	Total
773	$2.44 \cdot 10^{-3}$	$6.34 \cdot 10^{-5}$	$4.49 \cdot 10^{-4}$	$1.15 \cdot 10^{-3}$
873	$2.30 \cdot 10^{-3}$	$5.42 \cdot 10^{-5}$	$5.88 \cdot 10^{-5}$	$9.76 \cdot 10^{-4}$
973	$2.24 \cdot 10^{-3}$	$6.17 \cdot 10^{-5}$	$8.93 \cdot 10^{-6}$	$9.38 \cdot 10^{-4}$

Appendix G

The main formula used for heat transfer calculations are reported in this Appendix and were taken from (Incropera and De Witt, 2006) (Figure G-1, Figure G-2 and Table G-1). These were used for heat transfer calculations and deposit temperature predictions in section 3.9 and in Chapter 4 and 7.

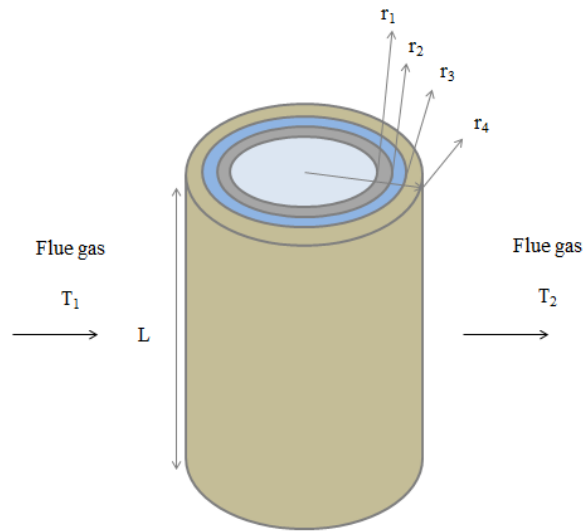


Figure G-1: Schematic of air cooled ceramic probe used in the rig at Cranfield.

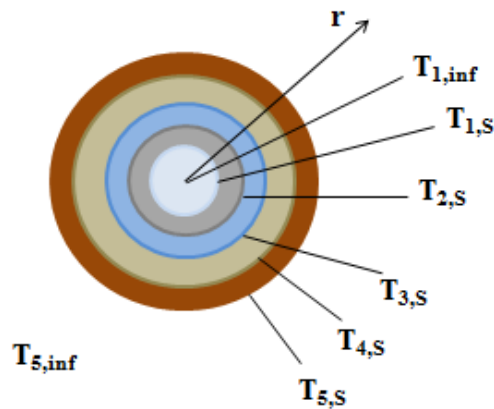


Figure G-2: Schematic of temperature around probe with deposit.

Table G-1: Thermal resistances formula.

Thermal Resistance	Heat transfer
$R_1 = \frac{1}{h_1 A_1}$	Convection (air inlet)
$R_2 = \frac{\ln(\frac{r_2}{r_1})}{2\pi k L}$	Conduction (stainless steel)
$R_3 = \frac{1}{h_3 A_3}$	Convection (air outlet)
$R_4 = \frac{\ln(\frac{r_4}{r_3})}{2\pi k L}$	Conduction (probe)
$R_5 = \frac{\ln(\frac{r_5}{r_4})}{2\pi k L}$	Conduction (deposit)
$R_6 = \frac{1}{h_6 A_5}$	Convection (flue gas)
$R_7 = \frac{1}{h_r A_5}$	Radiation

CALCULATIONS:

1) CONVECTION (AIR INLET)

- At $T_{1,INF}$ and $P_{AIR,IN}$ find all the air properties
- Calculate Reynolds number and check if it is laminar or turbulent

If it is laminar:

$$Nu \sim 4 \quad (G-1)$$

$$h_i = Nu_i \frac{k_i}{L} \quad (G-2)$$

Where:

Nu = Nusselt number (ratio of convection to pure conduction heat transfer)

h_i = convective heat transfer coefficient [W/(m² K)]

k_i = material thermal conductivity [W/m K]

L = characteristic length [m]

If it is turbulent, the Dittus-Boelter equation can be applied (Equation (G-3)).

$$Nu = 0.023 Re_D^{0.8} Pr^n \quad (G-3)$$

Where:

Pr = Prandtl number (ratio of the momentum and thermal diffusivities) $= \frac{c_p \mu}{k} = \frac{\nu}{\alpha}$

$$\frac{\nu}{\alpha} = \frac{\text{momentum diffusivity}}{\text{thermal diffusivity}} = \frac{\mu/\rho}{k/\rho c_p}$$

$n = 0.4$ if the fluid is being heated which means that the wall is at a higher temperature than the entering fluid ($T_s > T_m$) with T_s surface temperature and $T_m = \frac{T_{in} + T_{out}}{2}$

$n = 0.3$ if the fluid is being cooled ($T_s < T_m$)

All the physical properties used in the Dittus-Boelter correlation must be evaluated at the average bulk temperature of the fluid T_m . This is the arithmetic average of the bulk average temperatures at the entrance and the exit. The usual recommendation is to use the Dittus-Boelter correlation for $Re > 10000$, but it is used even at lower Reynolds numbers as long as the flow is turbulent, because it is a simple correlation to use.

The Dittus-Boelter equation (for turbulent flow) is easy to solve but is less accurate when there is a large temperature difference across the fluid. It is tailored to smooth tubes and its use for rough tubes (most commercial applications) is cautioned. The Dittus-Boelter equation is valid for:

$$0.6 \leq Pr \leq 160, Re_D \geq 10\,000, \frac{L}{D} \geq 10$$

2) CONVECTION (AIR OUT)

- At $T_{2,OUT}$ and $P_{AIR,OUT}$ find all the air properties
- Calculate Reynolds number
- Calculate the convection heat transfer coefficient according to the previous point (AIR INLET)

3) CONVECTION FLUE GAS (OUTSIDE)

- At $T_f = \frac{T_s + T_{inf}}{2}$ and $P_{FLUE\ GAS}$ find all the air properties
- Calculate Nusselt number using Churchill and Bernstein equation (Equation (G-4)) (it is a single comprehensive equation that covers the entire range of Re_D and a wide range of Pr . This equation is recommended for $Re_D Pr \geq 0.2$)
- Calculate the convection heat transfer coefficient

$$\overline{Nu_D} = 0.3 + \frac{0.62 Re_D^{1/2} Pr^{1/3}}{[1 + (\frac{0.4}{Pr})^{2/3}]^{1/4}} [1 + (\frac{Re_D}{282000})^{5/8}]^{4/5} \quad (G-4)$$

4) CONDUCTION (METAL, CERAMIC AND DEPOSIT)

Calculate the conduction heat transfer coefficient using the material thermal conductivity.

$$h_i = \frac{k}{r_o \ln(\frac{r_o}{r_i})} \quad (G-5)$$

With: r_o outer and r_i inner radius [m], k material thermal conductivity [W/m K].

5) RADIATION

$$h_r = \varepsilon \sigma (T_s + T_{surr})(T_s^2 + T_{surr}^2) \quad (G-6)$$

ε = radiative property of the surface (emissivity)

σ = Stefan Boltzmann = $5.67 \cdot 10^{-8} \text{ W/(m}^2 \text{ K}^4)$

T_s = surface temperature [K]

T_{surr} = surrounding temperature [K]

Appendix H

This Appendix contains the pictures of the paper presented during the Poster presentation at the Heat Exchanger Fouling and Cleaning XII Conference – Madrid, 11-16 June 2017 (as highlighted in section 1.4).

PREDICTING DEPOSITION ONTO SUPERHEATER TUBES IN BIOMASS AND COAL-FIRED COMBUSTION SYSTEMS

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ABSTRACT

The formation of deposits on superheaters and reheaters in biomass and coal-fired combustion systems is associated with increased fireside corrosion damage and reduced heat transfer.

This paper reports the development of predictive models for deposition on such heat exchanger tubes using computational fluid dynamics. Initial calculations have used the simplifications of a two-dimensional geometry and an air flow with inert spherical “ash” particles. An Eulerian model has been used to describe the continuous phase and a Lagrangian model for particle trajectories. Particles with different diameters have been injected to study their trajectories and impaction locations. In addition, the effect of flue gas turbulence has been investigated. These models have been extended by adding a vapour deposition process. Finally, a grid motion code has been incorporated to allow the prediction of the thickness and shape of the deposits on tubes. These predictions have been compared to results in the existing literature.

INTRODUCTION

Generating electricity from coal-fired combustion systems is currently the world’s dominant form of power production (IEO, 2016). Predictions of worldwide energy demands for the next 35 years suggest that there will be a steadily increasing demand (IEO, 2016). To meet this need, it is predicted that the level of coal-fired power will stabilise, but that there will be a steady increase in the amount of electricity generated using renewable sources and from natural gas fired systems. At present, the biomass combustion systems are the dominant form of renewable power generation (IEO, 2016). However, both coal- and biomass-fired combustion systems have outstanding challenges in their operation, including deposition onto heat exchanger tubes and corrosion of those tubes. Such issues are expected to become more significant as steam system operating temperatures and pressures are increased in order to improve energy conversion efficiencies (Nicol, 2013).

The formation of deposits on heat exchangers, also known as fouling and slagging, is recognized to be one of the most serious problems since the formation of insulating layers on tube surfaces can reduce boiler thermal efficiency (Nunes et al., 2016), and the corrosion damage caused by such deposits results in increased maintenance costs through

reduced tube life and increasing risk of unexpected tube failures (Simms et al, 2013).

During the combustion of coal and biomass, extraneous and inherent mineral matter leads to the formation of larger and finer solid ash particles, respectively (Tomeczek and Waclawiak, 2009). In addition, the decomposition of minerals and coal produces vapours able to condense homogeneously in the gas phase or heterogeneously on solid particles and on heat exchanger deposit surfaces (Magda, 2012).

Inertial impaction is considered to be the main deposition mechanism for solid ash particles ($dp > 10 \mu\text{m}$) impacting mainly on the upstream sides of tubes. Smaller particles can also hit the downstream sides of tubes as a consequence of the eddy impaction ($dp < 10 \mu\text{m}$), thermophoresis and brownian diffusion ($dp < 1 \mu\text{m}$) (Tomeczek and Waclawiak, 2009). Thermophoresis depends on the temperature gradient from the bulk gas to the surface and so its contribution to deposition is stronger during the initial stages of deposit formation when the surface is clean (as the surface temperature increases as the deposit layer grows because of the reduced heat transfer). In addition, vapour condensation can occur, if the partial pressures of the gaseous contaminants are high enough compared to the cooled tube surface, and can enhance the growth of the deposit by creating a sticky layer on the tube surfaces. In addition to that, some chemical reactions in the gas phase or in the deposit layer can increase the accumulation. However, the variability of coal and biomass fuels has made predictions of deposition fluxes and deposit compositions on heat exchanger surfaces challenging.

The variety and multidisciplinary of this subject has made its study more difficult (Pérez et al., 2017). Therefore, a common approach to developing predictive models is to make simplifications. In recent years progress with the power of computers means that computational fluid dynamics (CFD) now represents one of the best tools to study deposition onto heat exchangers as it enables calculation of both gas behaviour and particle trajectories, as well as enabling the prediction of deposit location around tubes and deposition fluxes.

In previous works, the deposition has been studied according to several criteria based on the physical properties of particles and surfaces (e.g., Waclawiak and Kalisz, 2011). Some of these demonstrated that particles are more

likely to deposit onto a sticky, or fouled, surface rather than a clean surface. However, such a modelling approach needs to be developed further to enable the combination of different deposition mechanisms in a simulated combustion environment, and validation of the various parts of the model with experimental data.

This paper reports research targeted at investigating the prediction of deposition on heat exchanger tubes using a CFD model developed in Fluent combined with User Defined Functions (i.e. UDFs). It focuses on the effects of particular input variable on the model predictions, including deposition of dry or sticky particles onto dry or sticky surfaces. In addition, it reports the effects of incorporating grid motion code to allow the prediction of the thickness and shape of the deposits on tubes, and their comparison to existing literature data.

MODEL DEVELOPMENT

Computational domain

The computational domain was simplified to a two-dimensional geometry. The gas entered at the left boundary, flowed across the tube (diameter $d_t = 38$ mm) and exited at the right boundary of the computational domain, as a typical external flow scenario (Fig. 1).

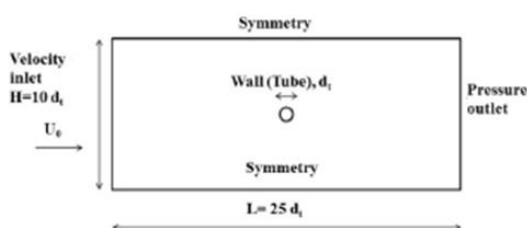


Fig. 1 Geometry and boundary conditions.

This domain was divided into an array of cells to solve the equations for the motion of the flue gases and particles. Firstly, a structured mesh (using quadrilateral cells) was created in order to get better convergence and a higher resolution. Later, an unstructured mesh (using triangular cells) was generated (Fig. 2) to enable study the grid movement. In fact, the UDF for grid motion with remeshing option only works with triangular meshes (Waclawski and Kalisz 2011; Garc Pérez 2016). However, the triangular mesh can reduce the accuracy of other predictions.

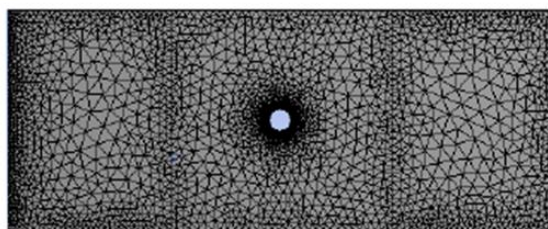


Fig. 2 Mesh used for CFD modelling.

Model assumptions

This work is aimed at developing a model to predict deposition flux and location. For these initial trials the flue gas was approximated to air and ash particles are assumed to be inert spheres ($\rho_p = 2200$ kg/m³, $C_{p,p} = 923$ J/kg K). Both the gas and particles enter the domain with the same velocity ($U_0 = 10$ m/s) and a temperature of 1273 K (giving gas properties of $\rho_g = 0.245$ kg/m³, $C_{p,g} = 1203$ J/kg K, $k_g = 0.077921$ W/m K, $\mu_g = 46 \cdot 10^{-6}$ kg/m s (Yang et al., 2016)). The tube surface temperature was fixed at 700 K. The Reynolds number was calculated using the appropriate flue gas properties and the tube diameter. Its value ($Re \approx 2024$) is such that the von Kármán vortex trail is turbulent, the Reynolds Averaged Navier-Stokes (RANS) approach was used for studying the flow and the turbulent model $k-\epsilon$ was chosen (using the default values in FLUENT as a starting point) and, at the inlet, the gas was assumed to have a turbulent intensity of 10% (Waclawski and Kalisz, 2014).

Initially, simulations were run for the fluid without any particles. These simulations were then used as the fluid field initial condition for the transient simulations with particles.

Particle trajectories

The particle trajectory model was developed using an Euler-Lagrange approach enabling the Discrete Phase Model DPM in Fluent®. The Eulerian model describes the continuous phase and the Lagrangian model is used to describe particle trajectories. Fluent® predicts the trajectory of a discrete phase particle by integrating the force balance on the particle. Here, particle inertia is balanced with the forces acting on the particle and can be written for the x direction in Cartesian coordinates as:

$$\frac{du_p}{dt} = F_D(u_g - u_p) + \frac{g_x(\rho_p - \rho_g)}{\rho_p} + F_x \quad (1)$$

where: $F_D(u_g - u_p)$ is the drag force per unit particle mass; g_x is the gravitational force; F_x the additional force term (e.g. Brownian, Thermophoretic, Lift force etc); u_g is the fluid phase velocity; u_p is the particle velocity; ρ_g is the fluid density; and, ρ_p is the density of the particle. Particles were assumed to be perfectly spherical and inert. The particles were injected at the inlet boundary where 90 cell faces were used. Eq. (1) was used including the force of

gravity acting with the same directions of the flue gas. However, the effect of the additional forces was neglected.

The dispersion of particles due to the turbulence in the gaseous fluid was included, using the Discrete Random Walk (i.e. DRW) and the Random Eddy Lifetime with time scale constant 0.15. In fact, with these options, it is possible to predict small particles trajectories and see their impaction on the downstream faces of the tubes. This effect would not be detected in absence of turbulence (Lee et al., 2014; Tomeczek and Wacławski, 2009). This option is also another way of increasing the number of injected particles. The trajectories were calculated for a series of different particle diameters, with three examples given in Fig. 3.

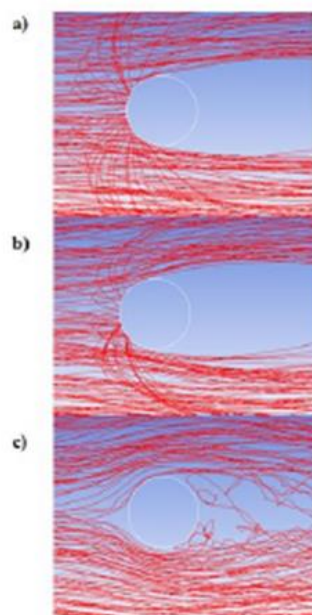


Fig. 3 Trajectories of particles with different diameters: a) 150 μm , b) 50 μm , c) 0.5 μm .

As indicated by some previous papers (e.g., Baxter, 1993; Lee et al., 2014; Wacławski and Kalisz, 2012), inertial impaction is the main process by which particles are transported to the surface. This is the most important particle deposition mechanism for particles larger than 10 μm whose impaction occurs mainly close to the cylinder stagnation point where they can hit the surface and rebound off because of their higher kinetic energy and mass. In contrast, small particles do not have enough inertia to overcome the drag force and tend to follow the flue gas streamlines to the downstream side of the tube where they can deposit because of the Eddy impaction, and the Thermophoretic and Brownian Forces.

Deposition models

The range of mechanisms and species involved in the deposit growth make this process complicated. At the beginning, when the probe is clean, only vapours and fine particles in a sticky condition create the first deposit layer. After that, inertial impaction increases the initial deposit and its build-up. This process can be strongly enhanced by some chemical reactions, in the deposit layer or in the gas phase, which can lead to eutectic mixes with lower melting points (Zhou et al., 2007).

The increasing deposit thickness reduces the heat transfer through to the cooling fluid inside the tube (effectively adding an external insulating layer) and, as a consequence, the temperature of the deposit surface increases. Therefore, the thermophoretic and condensation contributions will decrease as they are based on the temperature gradient between the flue gas and the deposit surface (but by different functions).

For this study, the deposition modelling required the calculation of the flux of particles deposited ($\text{kg}/\text{m}^2 \text{ s}$) which was dependent on the total flux of particles that hit the tube surface. In fact, for these calculations the deposition efficiency could be considered as the product between the impaction and the sticking efficiency as defined in Fig. 4.



Fig. 4 Particle deposition efficiency.

The probability of a particle sticking on the surface after hitting is a function of the particle and surface properties (i.e., stickiness, roughness), impact angle and particle impaction velocity.

This deposition is a complex phenomenon which needs to take into account all the mechanisms and components involved to be studied (Khodier et al., 2012). In some previous papers (Subbarao and Rindt, 2016; Wacławski and Kalisz, 2011) it was defined the “dry impaction”, better known as powdery deposition (mainly due to dry ash particles impacting on a clean surface), and “wet impaction” (due to vapour condensation and sticky particles). In fact, as outlined above, not only ash particles but also vapours can deposit on the tube surfaces.

The model to predict the deposition was developed using the DEFINE_DPM_EROSION procedure in Fluent®. This procedure has been widely used in this field to calculate the deposition flux as is able to calculate both the

impact angle between the particle path and the face and the flow rate of the particle stream as it hits the face (in kg/s) ("ANSYS FLUENT 12.0 UDF Manual," 2009). The deposition flux can be calculated with Eq. 2 as a function of the fouling probability P_f , the mass flow rate m_p of particulate matter striking the deposition surface A and the impact angle γ (Fig. 5).

$$m_{dep,A} = P_f \frac{dm_p}{dA} \sin(\gamma) \quad (2)$$

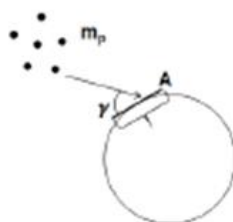


Fig. 5 Parameters for particle impact on tube.

If the tube surface is clean and the particle is dry, the deposition is due to a force balance that involves the particle and tube material properties, Van der Waals force and the gravity force. According to this model, the inertial impaction is the main deposition mechanism and the capture depends on the values of three different forces: the normal elastic rebound force $F_{s,n}$, Van der Waals adhesion force $F_{v,w}$ and the normal component of gravity F_G (Fig. 6). In Fluent® the default value of gravity is zero but it has been included in this study because it can influence the deposit location and its flux according to the flue gas direction (Lee et al., 2014; Waclawski, 2010).

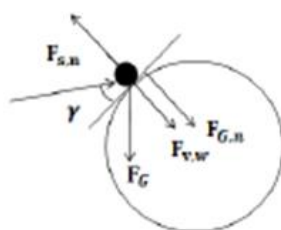


Fig. 6 Parameters for powdery deposition model.

$$F_{s,n} = K d_p^2 w_p^{1.2} \quad (3)$$

$$F_{v,w} = \frac{B d_p}{6 \delta^2} \quad (4)$$

$$F_G = \frac{1}{6} \pi d_p^3 \rho_p g \quad (5)$$

where: K is a constant depending on elasticity of particle and deposition surface, B is molecular interaction constant, δ is the distance between particle and deposition surface, g is the gravitational acceleration.

In this case, the probability of deposition P_f can be calculated as follows:

$$P_f = 0 \text{ if } F_{s,n} > (F_{v,w} \pm F_{G,n}) \quad (6)$$

$$1 \text{ if } F_{s,n} \leq (F_{v,w} \pm F_{G,n}) \quad (7)$$

This model, from Zaniczyszczych (1992) and widely used by other authors, explains that the contact between particles and surface generates some microscopic deformations. However, particle deposition will occur only if the rebounding force is lower than the sum of the Van der Waals and gravitational forces. Similar approach has been used by other authors where the deposition criteria were based on the particle energy and velocity (El-Batsh, 2001; Weber et al., 2013).

The model was applied to different particle diameters confirming that the deposition occurs mainly on the upstream side of the tube for bigger particles (Fig. 7) and the deposition location is strongly affected by the energy and the impact angle of particles. In fact, a correlation between Fig. 3a and Fig. 7a shows that bigger particles have more energy to bound and rebound off the tube surface. Contrarily, smaller particle diameters are able to deposit also on the downstream part of the tube as shown in Fig. 7 and in previous works (Lee et al., 2014).

In addition to this, a further development of the calculations for deposition onto heat exchanger tubes involves the particle and surface stickiness. This stickiness can be the result of vapour condensation and/or chemical reactions. According to this development, the deposition rate can be calculated by including in Eq. 2 the total probability depending on the properties (in particular the sticking probability) of both surface and particles (Kær et al., 2006; Schulze et al., 2011).

$$P_{tot} = P_w(1 - P_p) + P_p(1 - P_w) + P_w P_p \quad (8)$$

where: P_w is the wall stickiness probability and P_p is the particle stickiness probability. The particle stickiness probability is related to the particle composition and properties. Deposition criteria based on the viscosity and softening temperature values have been used previously (e.g., Beckmann et al., 2016).

However, for this paper, only the tube surface stickiness, due to the condensation of alkali vapours, was included, therefore $P_p = 0$ and Eq. (8) can be simplified as follows in Eq. (9).

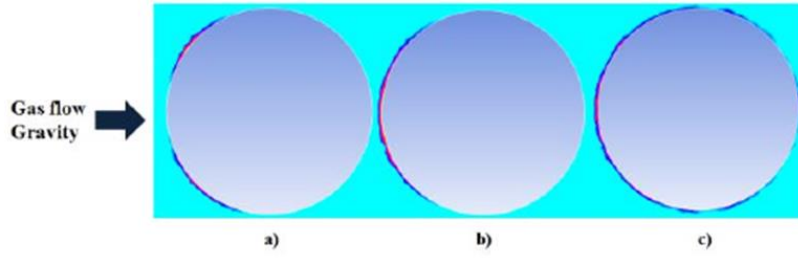


Fig. 7 Distribution of deposition locations around a tube for particles with diameters of: a) 150 μm , b) 50 μm , c) 0.5 μm .

$$P_{\text{tot}} = P_w \quad (9)$$

In this paper, for simplicity in initial condensation calculations, Na_2SO_4 at concentration of 1 vppm was considered to be the only vapour present. The temperature gradient between the gas and the tube leads to vapour condensation on the surface creating a sticky layer able to enhance the particle deposition (Fig. 8).

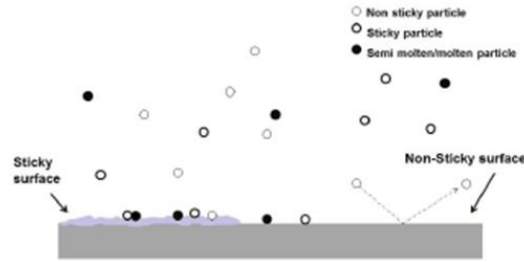


Fig. 8 Sticking of particles from a hot gas stream onto a cooled surface.

The probability can be calculated as it follows:

$$P_w = S m_{c,A} \quad (10)$$

where: S has the inverse units to flux and can be experimentally estimated on the basis of the final deposit (Tomeczek and Waclawski, 2009).

The flux of the condensable vapour i -th can be calculated using Eq. 11 (Tomeczek and Waclawski, 2009):

$$m_{c,A,i} = \beta_i \frac{p_i - p_{s,i}}{p} \rho_g \quad (11)$$

where: $m_{c,A,i}$ is the deposition flux and β_i is the mass transfer coefficient of the i th component defined as (Incropera et al., 2002):

$$\beta_i = \frac{Sh D_i}{d_t} \quad (12)$$

where: D_i is the diffusion coefficient of the i th component through the flue gases (Green and Perry, 2008), Sh is the dimensionless Sherwood number used in mass-transfer operation, p_i is the partial pressure of i -th gaseous component, p is the gas pressure and ρ_g is the gas density.

The saturation pressure of the i -th gaseous component at surface temperature, $p_{s,i}$, is calculated according to the following formula (Tomeczek and Waclawski, 2009):

$$\frac{p_{s,i}}{p_n} = \exp \left(A_i - \frac{B_i}{T + C_i} \right) \quad (13)$$

where: A , B and C are given constants in Tab. 1, $p_n = 10^5$ Pa and T is the tube temperature.

Table 1. Constants A_i , B_i , C_i used in Eq. (13) (Tomeczek and Waclawski, 2009)

Component	A	B	C	T [K]
Na_2SO_4	15.03	37 452.4	0	1 150-1 800
K_2SO_4	18.08	39 449.6	0	1 150-1 800
KCl	11.01	17 132	-122.7	1 094-1 680
NaCl	11.68	19 315	-82.6	1 138-1 738

Predictions from the resulting model are shown in Fig. 9, and compared to predictions from the dry deposition model for the same particle size. This confirms the qualitative description above that if the surface becomes sticky because of the vapour condensation, then the bigger particles (e.g. 150 μm) hitting close to the centre of the upstream tube face will stick rather than rebound off as it happens if the surface is clean.

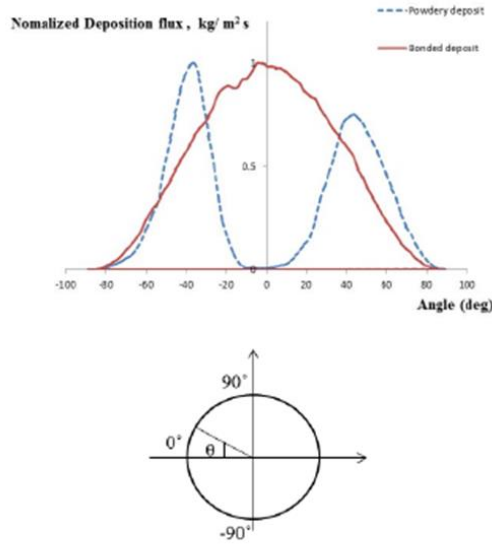


Fig. 9 Variation of deposition location between a “dry” and a sticky surface for $d_p=150 \mu\text{m}$.

A further stage in the model development has been to also include the contribution of the vapour deposition flux to the total deposition (Eq. 14). This combines both the contribution of the deposition of particles onto a sticky surface and the condensation flux itself.

$$m_{\text{tot}} = S m_{cA} \frac{dm_p}{dA} \sin(\gamma) + m_{cA} \quad (14)$$

The deposition flux calculated from this was higher than for just a sticky surface, but there was no change in the deposition location (i.e., compared to the solid line in Fig. 9).

Deposit shape and thickness

The shape of the deposit can be modelled in Fluent® using the DEFINE_GRID_MOTION procedure which allows the grid nodes to be moved in response to the deposition flux calculated using DEFINE_DPM_EROSION (Pérez et al., 2015). The thickness of the deposit at each node (j^{th}) of the cylinder face can be calculated from the deposition flux, its density and the time step Eq. (15). These values can then be used in the DEFINE_GRID_MOTION procedure to update the node coordinates on each face of the cylinder at each time step. One drawback of dynamic meshes is the necessity of using a triangular (unstructured mesh) that implies less accuracy in the results.

$$t_j = \frac{(m_{\text{dep},A})_j}{\rho_{\text{dep}}} \Delta t \quad (15)$$

where: t_j is the deposition thickness at node j , ρ_{dep} is the deposit density and Δt is the time step.

The deposition thickness at each node of the cylinder t_j is used to update the node coordinates. The direction of accretion is computed considering the angle θ normal to each face defined as in Eq. (16):

$$\theta = \tan^{-1} \left(\frac{Y_p}{X_p} \right) \quad (16)$$

As is shown in Fig. 10 and by Eq. (17) and (18), the new coordinates of each node can be calculated using the thickness and the direction of accretions:

$$X'_p = X_p + t_j \cos \theta \quad (17)$$

$$Y'_p = Y_p + t_j \sin \theta \quad (18)$$

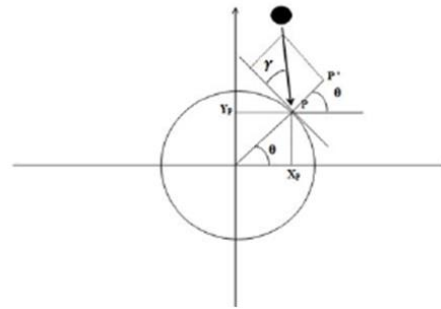


Fig. 10 Calculation of new node coordinates.

For this paper, this calculation method has been used to predict the deposit shape when assuming $150 \mu\text{m}$ diameter particles and vapour deposition. As indicated by the previous prediction (Fig. 10), the deposition takes place on the upstream side of the tube (Fig. 11).

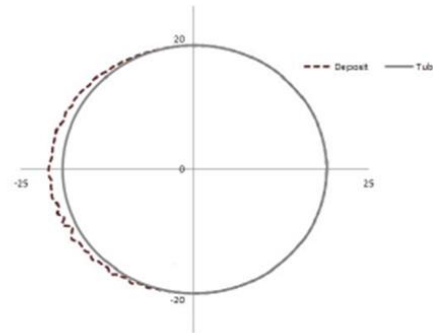


Fig. 11 Calculated deposit shape for combined particle ($d_p=150 \mu\text{m}$) and vapour deposition.

GENERAL DISCUSSION

The deposition on heat exchanger has been studied using a CFD model developed in FLUENT. The software can simulate the trajectories of particles with different diameters but, in order to model the deposit accretion and its shape, UDFs must be included. Previous models from the literature have been applied and the influence of having a sticky surface due to vapour condensation on particle deposition has been highlighted. Moreover, the combined effects of ash particle deposition and vapour condensation have been included aiming for a more realistic model. The shape of the deposit has been simulated displacing the cylinder coordinates according to the increasing deposit thickness. In order to do that, the triangular mesh was necessary and the neighbouring faces overlap was confirmed to be one of the biggest issues leading to a "negative volume" error which does not allow completion of the simulation.

CONCLUSIONS

In this work, preliminary CFD and coding studies are reported for the development of a model for the deposition of particles and condensation of vapour phase species onto heat exchangers. The Fluent® CFD programme, enhanced with UDFs, was used to carry out initial calculations investigating the sensitivity of particle and vapour deposition on tube surfaces to assumptions about particle sizes and potential particle and vapour deposition mechanisms. For the purposes of the particle deposition calculations, the geometry was simplified to 2D, the flowing gas stream was assumed to be air and the particles were inert spheres. An Eulerian model was used to describe the continuous phase and a Lagrangian model was used to describe the particle trajectories.

The sensitivity of deposition flux and its location around the tube were calculated using the DEFINE_DPM_EROSION procedure for different particle diameters and deposition criteria. In addition, the results of these calculations were used to predict deposit shapes and thicknesses using the DEFINE_GRID_MOTION procedure.

Future studies will be carried out to generate data from combusting coal and biomass fuels (e.g., gas compositions, ash particle distributions, ash and deposits compositions, and the effect of deposits on heat transfer) under well controlled conditions to generate data to enable optimisation and validation of this model.

NOMENCLATURE

A	surface area, m ²
C _p	specific heat, J/kg K
D	diffusion coefficient of the ith component through the flue gases, m ² /s
d	diameter, m
F _D	drag force, N
F _G	gravity force, N
F _{s,n}	normal elastic rebound force, N
F _{v,w}	Van der Waals adhesion force, N
g	gravitational acceleration, m/s ²
k	thermal conductivity, W/m K

m	deposition flux, kg/m ² s
p	total pressure, Pa
P	probability, dimensionless
Re	Reynolds number, dimensionless
Sh	Sherwood number, dimensionless
T	temperature, K
t	deposit thickness, m
u	velocity, m/s
w	perpendicular component of impact velocity, m/s
x	direction, dimensionless
β	mass transfer of the ith component, m/s
γ	impaction angle, rad
Δt	time step, s
θ	angle normal to each face, rad
μ	viscosity, Pa s
ρ	density, kg/m ³

Subscript

A	area
c	condensation
dep	deposition
f	fouling
g	gas
i	i-th component
imp	impaction
j	j-th node
n	normal
p	particle
s	saturation
stick	sticking
t	tube
tot	total
w	wall

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