CFD simulations of staged biomass grate fired combustion with an emphasis on NOx emissions

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ABSTRACT

The present paper addresses NOx emissions from biomass combustion, and the objective is to demonstrate the applicability of stationary CFD simulations, including a detailed representation of the gas phase chemistry, to a multi-fuel lab-scale grate fired reactor using biomass as fuel.

In biomass combustion applications, the most significant route for NOx formation is the fuel NOx mechanism. The formation of fuel NOx is very complex and sensitive to fuel composition and combustion conditions. And hence, accurate predictions of fuel NOx formation from biomass combustion rely heavily on the use of chemical kinetics with sufficient level of details. The computational fluid dynamics (CFD) simulations in this work were performed using the realizable k-ε turbulence model and the Eddy Dissipation Concept (EDC) by Magnussen [1][2] for turbulent combustion in conjunction with a detailed chemical reaction mechanism and one skeletal mechanisms recently developed for biomass combustion [3].

The results give a significant NOx reduction at a primary excess air ratio of 0.8, showing the potential of NOx reduction by staged air combustion.

KEYWORDS: Biomass, combustion, CFD simulations, NOx emissions, reaction mechanism.

1   INTRODUCTION

Computational Fluid Dynamics (CFD) is a very useful tool to study flow and mixing behaviour, combustion and emissions from furnaces. CFD computations can provide useful information in parts of combustion devices and furnaces where optical access and measurements are impossible. In addition, modifications and possible improvements can rather inexpensively be investigated. Normally, only a simplified description of the gas phase chemistry is used in simulations involving combustion. Such simplified descriptions, e.g. one-step reaction chemistry, are tuned to match combustion characteristics at certain conditions; hence, the accuracy may drop dramatically outside the valid state and composition

window. Thus, by adopting a simplified treatment of the chemical processes, the possibility to capture ignition and extinction together with pollutant formation and reduction is very limited. For many applications it is therefore important to use detailed chemical kinetics.

In biomass combustion applications, the most significant route for NOx formation is the fuel NOx mechanism. The formation of fuel NOx is very complex and sensitive to fuel composition and combustion conditions. And, hence, accurate predictions of fuel NOx formation from biomass combustion rely heavily on the use of chemical kinetics with sufficient level of details. The computational fluid dynamics (CFD) simulations in this work were performed using the realizable k-ε turbulence model and the Eddy Dissipation Concept (EDC) by Magnussen [1][2] for turbulent combustion in conjunction with a detailed chemical reaction mechanism and one skeletal mechanism recently developed for biomass combustion [3].

The objective of this work is to demonstrate the applicability of stationary CFD simulations, including a detailed representation of the gas phase chemistry, to a multi-fuel lab-scale grate fired reactor using biomass as fuel.

2   THE MODELLING APPROACH

2.1   General

Computational Fluid Dynamics (CFD) is the analysis of systems involving fluid flow by means of computer-based simulations. These systems may also involve heat transfer and associated phenomena such as chemical reactions. CFD simulations are based upon a numerical solution of the basic equations of the fluid dynamics; conservation of mass, momentum, and energy, together with mathematical sub-models. The equations can be solved time-dependent and in three-dimensions. Comprehensive modelling of combustion in general requires simulation of turbulent fluid dynamics, chemical kinetics as well as their interactions.

In the current study, the ANSYS FLUENT software is used for the calculations. FLUENT 15 is a general-purpose CFD code, which is based on finite volumes. When using the finite volume method, the region of interest is divided into small sub-regions called control volumes. The equations are discretized and solved iteratively, providing the value of each variable (velocity, temperature, mass fractions etc.) for each control volume throughout the calculation domain. A description of the CFD tool can be found on the ANSYS website (www.ansys.com), and a short description of the various models used is given in the section below.

2.2   Physical models

The computational fluid dynamics (CFD) simulations were performed using the realizable k-ε turbulence model and the Eddy Dissipation Concept (EDC) by Magnussen [1][2] for turbulent combustion in conjunction with chemical reactions from two different reaction mechanisms developed for biomass combustion [3]. The detailed reaction mechanism includes 81 species, while the skeletal mechanism reduced from the detailed one includes 36 species. In this work the discrete ordinates method (DO) is used to model the radiative transfer, and the soot model chosen is the Moss & Brookes model with the soot precursors acetylene and ethylene (C_2H_2 and C_2H_4). The physical models used are described in more detail in previous work [4].

2.3   Geometry and boundary conditions

The objective of this work is to study combustion of biomass in a grate fired lab-scale multi-fuel reactor (Figure 1). The reactor is located in the SINTEF Energy Research laboratory. The reactor has an electrically heated ceramic inner tube with a diameter of 100 mm and a length of 2 m. The reaction section located above the grate is 1.6 m long. The reactor is fitted with a unique two-level grate system, as shown in Figure 1, which allows for two-stage fuel burning. There are rotating blades on each level that moves the unburned fuel particles on the grates, from the upper grate to the lower grate and from the

lower grate to the ash bin through a slot in the grates. Air can be fed to the reactor at two levels; below the lower grate and at a level above the second grate. A more detailed description of the reactor can be found in a recent study by Khalil et al. [5].

Experiments studying the effect of excess air ratio on NOx emissions were performed by Houshfar et al. [6] for staged and non-staged air combustion. The experiments were carried out using 6-mm-diameter pellets of demolition wood fed to the reactor at a set rate. Their experiments carried out at 1123 K were selected as a basis for comparison in this numerical study.

In the simulations the geometry model includes the 1.6 m high reaction section above the grate. The model is 3-dimensional and in full scale. The geometry has been gridded with the ANSYS meshing Platform (AMP). The mesh consists of approximately 202 100 hexahedral elements.
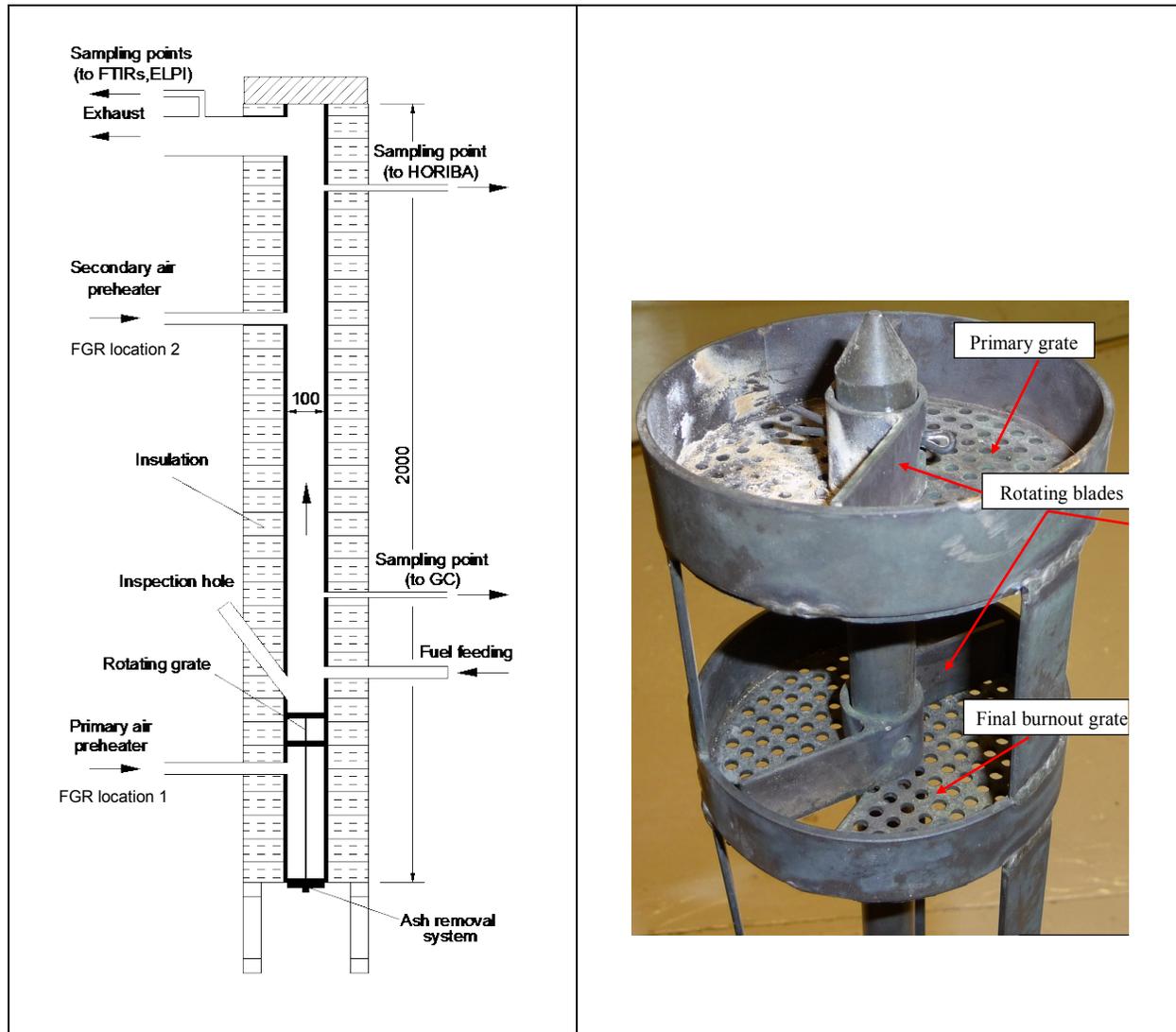
Figure 1:   Left: Schematic drawing of the multi-fuel reactor of SINTEF Energy Research.
             Right: The two-level grate system

The thermochemical conversion of the solid fuel is not included in the CFD-calculations. An inlet boundary is defined at the level of the upper grate, and a pyrolysis gas/air mixture is flowing into the

reaction section. The gas composition and flow is based on demolition wood, a fuel feeding rate of 400 g/hr and the specific primary excess air ratio (λ_p=0.8). The gas composition has been optimized towards satisfying available relevant pyrolysis gas compositions and char gasification while maintaining the elemental balances for the solid fuel. The fact that burnout of the char will occur at the lower grate below the inlet boundary in the simulations is also taken into account. Table 1 shows the composition of the fuel gas/air mixture based on a primary excess air ratio of 0.8. The gas temperature is 1123 K.

The secondary air is injected through an inlet with a diameter of 35 mm, located 417.5 mm above the upper grate. The secondary air temperature is 1123 K. Total excess air ratio is 1.6, while the primary excess air ratio is 0.8, which means that 50% of the air is fed at each stage.

The electrical heating elements serve to maintain a constant wall temperature. In the model the solid walls are specified as isothermal with a wall temperature of 1123 K.

Table 1 : Composition of fuel gas/air mixture for primary excess air ratio (λ_p) of 0.8.

	wt %	g
CO_2	13.8483	275.79
H_2O	5.3929	107.40
O_2	9.9429	198.01
N_2	60.7130	1209.10
CO	6.3018	125.50
H_2	0.2561	5.10
CH_4	1.3307	26.50
C_2H_2	0.0552	1.10
C_2H_4	0.5825	11.60
C_2H_6	0.3113	6.20
NO	0.0151	0.30
HCN	0.1105	2.20
NH_3	0.1054	2.10
Ar	1.0344	20.60
Total gas	100.0000	1991.50
Ash		8.70
Total		2000.20

3   RESULTS AND DISCUSSION

3.1   Simulations with master mechanism (81 species)

Figure 2 (upper right) shows the mean temperature and the mass flow rate of carbon in CO along the reactor length. The simulations show that the majority of the fuel conversion occurs in the primary zone, as expected. The final burn-out occurs when the secondary air is injected, giving elevated temperatures also in the secondary zone (Figure 2). The highest temperatures in the secondary zone are 1300-1400 K. The simulated mean outlet temperature is 1130 K, which corresponds well with the experimental results.

The mass flow rates [kg/s] of nitrogen in selected species along the reactor length are shown in Figure 2 (lower left). It can be seen that NO is produced in the primary zone. In the secondary zone there is a net reduction of HCN, NH_3 and NO, and it can be mentioned that there is a minor increase in NO_2 and N_2O.

The TFN (total fixed nitrogen)/Fuel-N ratio at the outlet are compared in Figure 3. Four assumptions are used for the TFN ratio; in A0 only the nitrogen in NO is included, while in A3 the TFN includes all the major nitrogen species NO_2, N_2O, HCN and NH_3 in addition to NO. The two other assumptions are A1 including NO, HCN and NH_3, and A2 including NO, NO_2 and N_2O.

According to the simulations, there is a reduction in total fixed nitrogen (TFN) found in all the major nitrogen components; NO, HCN and NH_3, NO_2 and N_2O, from the fuel gas (at the inlet) to the sample surface (z=0.4 m) before the secondary air injection level, and a further reduction towards the flue gas outlet. At the outlet the TFN/Fuel-N ratio is 0.175 (see Figure 3), i.e. a high NOx reduction level is achieved, comparable to the NOx emission reduction level achieved in the corresponding experiment. Nearly 98% of the TFN is the contribution from NO, the remaining is mainly NO_2. This means that the major part of the fuel-nitrogen is converted to molecular nitrogen instead of NOx.

Removing the nitrogen components (NO, HCN and NH$_3$) from the fuel gas, prevents the formation of fuel NOx and allows to check the contribution from the other NOx formation mechanisms to the NOx emission level. As the temperatures are below 1700K, the production of thermal NOx is negligible. The predicted emissions of NOx, which then will be prompt NOx, is 1.3% of the base case level. When including all the major nitrogen components it increases to 1.5%. Hence, prompt NOx formation is negligible compared to the fuel NOx formation.
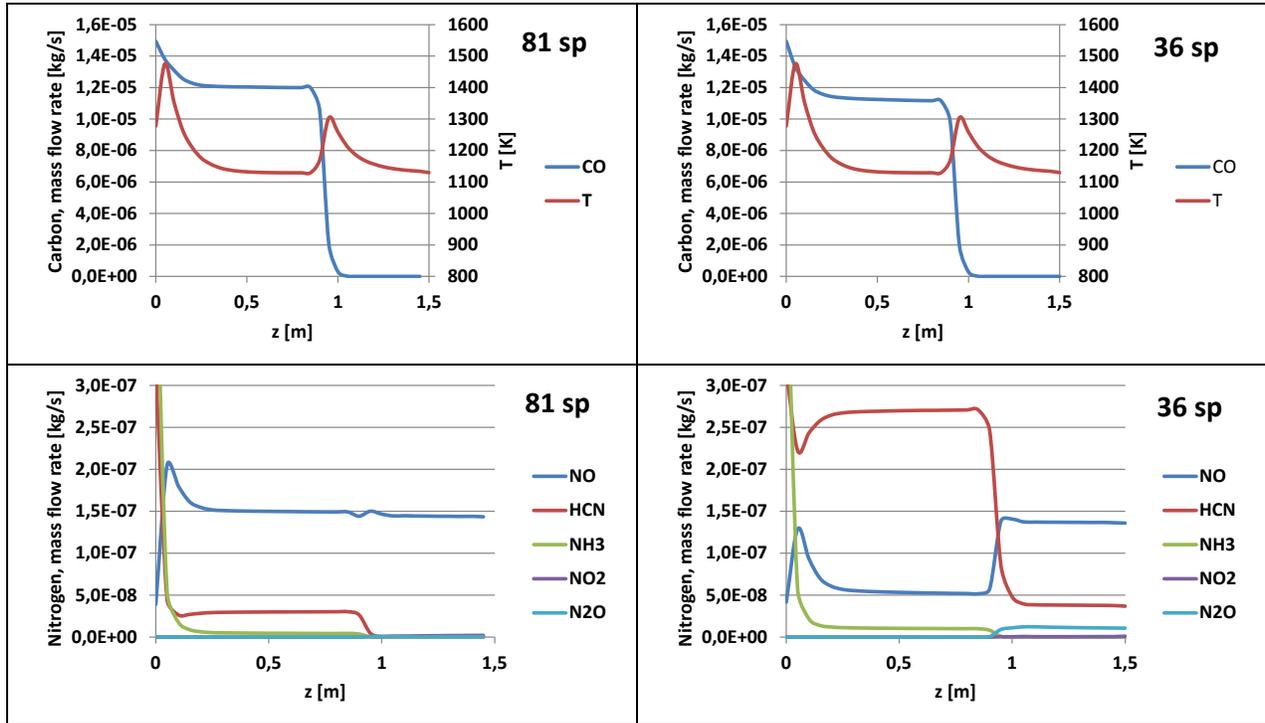
Figure 2: Mean temperature [K] and mass flow rate of selected species [kg/s] along the reactor length. Left: 81 species mechanism, Right: 36 species mechanism
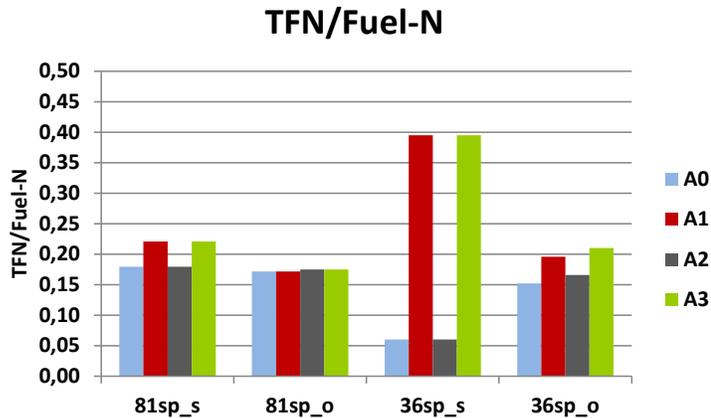
Figure 3: TFN/Fuel-N ratio at the sample surface (s) and the outlet (o) for the two reaction mechanisms, 81 (left) and 36 (right) species.
A0-N in NO, A1-N in NO/HCN/NH$_3$, A2-N in NO/NO$_2$/N$_2$O, A3- N in NO/NO$_2$/N$_2$O/HCN/NH$_3$

3.2 Simulations with skeletal mechanism (36 species)

Figure 2 and Figure 3 show results from the simulations with the skeletal mechanism compared with the full detailed mechanism. It can be seen that the mean temperatures along the reactor correspond well, while the predicted CO concentration before the injection of secondary air is slightly lower for the skeletal mechanism.

For the 36 species case a much lower reduction of HCN in the primary zone is predicted compared to the full detailed mechanism, resulting in also a higher HCN concentration at the reactor outlet than for the base case. Some NO is produced early in the primary zone, and in the secondary zone only some of the remaining HCN but all of the NH_3 are converted to NO, while in the base case all HCN and NH_3 is reduced in the primary zone and there is also a slight net reduction of NO in the secondary zone. Figure 3 shows that compared to the full detailed mechanism NO at the sample surface is underpredicted, while TFN/Fuel-N at the sample surface is significantly overpredicted mainly due to the overprediction of HCN. The trend is the same at the outlet, however the deviation is reduced. The TFN/Fuel-N at the outlet is overpredicted by 20%.

Removing the nitrogen components (NO, HCN and NH_3) from the fuel gas, investigating the prompt NO contribution, shows that the skeletal mechanism predicts a significantly higher NO value than the 81 species mechanism. The prompt NO contribution is overpredicted 20 times compared to the full detailed mechanism.

4 CONCLUSION

Using the full detailed mechanism (81 species), the results give a high NOx reduction at a primary excess air ratio of 0.8, comparable to the NOx emission reduction level achieved in the corresponding experiment, showing the potential of NOx reduction by staged air combustion.

There are deviations in prediction of the concentrations of the nitrogen components in the primary zone for the two chemical mechanisms compared. The skeletal mechanism overpredicts the concentration of HCN and underpredicts the concentration of NO in the primary zone, as well as overpredicts the prompt NOx contribution, indicating that an improved or less reduced skeletal mechanism is needed.

5 ACKNOWLEDGEMENTS

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