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Numerical simulations of staged biomass grate fired combustion with an emphasis on NO_x emissions

Mette Bugge^{a*}, Øyvind Skreiberg^a, Nils Erland L. Haugen^a, Per Carlsson^a,
Ehsan Houshfar^b, Terese Løvås^c

^aSINTEF Energy Research, Kolbjørn Hejes vei 1A, NO-7465 Trondheim, Norway

^bEnergos AS, Kvenildmyra 5, NO-7072 Trondheim, Norway

^cNorwegian University of Science and Technology, Kolbjørn Hejes vei 1B, NO-7491 Trondheim, Norway

Abstract

In the present paper NO_x emissions from biomass combustion was studied, with the objective to demonstrate the applicability of stationary computational fluid dynamics 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 NO_x formation is the fuel NO_x mechanism. The formation of fuel NO_x is very complex and sensitive to fuel composition and combustion conditions. And hence, accurate predictions of fuel NO_x formation from biomass combustion rely heavily on the use of chemical kinetics with sufficient level of details. In the present work we use computational fluid dynamics together with three gas phase reaction mechanisms; one detailed mechanism consisting of 81 species and 1401 reactions, and two skeletal mechanisms with 49 and 36 species respectively. Using the detailed mechanism (81 species), the results show a high NO_x reduction at a primary excess air ratio of 0.8, comparable to the NO_x emission reduction level achieved in the corresponding experiment, demonstrating both the validity of the model and the potential of NO_x reduction by staged air combustion.

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Keywords: Biomass; combustion; CFD simulations; NO_x 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 simulations can provide useful information in parts of combustion devices where optical access and measurements are impossible. In addition, modifications can rather inexpensively be investigated. Normally, only a simplified description of the gas phase chemistry is

* Corresponding author. Tel.: +47 472 78 241; fax: +47 73 59 28 89.
E-mail address: Mette.Bugge@sintef.no.

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 NO_x formation is the fuel NO_x mechanism [1]. The formation of fuel NO_x is very complex and sensitive to both fuel composition and combustion conditions. And hence, accurate predictions of fuel NO_x formation from biomass combustion rely heavily on the use of chemical kinetics with sufficient level of details. The objective of this work is to demonstrate the applicability of stationary CFD simulations, including detailed gas phase chemistry, to a multi-fuel lab-scale grate fired reactor using biomass as fuel. Recently, gas phase reaction mechanisms were developed for biomass combustion [2], and were used in this study. Only a few papers have been published where a similar approach has been used to study NO_x formation in biomass applications [3][4]. Most previous CFD studies predicting NO_x emissions from biomass combustion applications rely on a simplified description of the gas phase chemistry, like Miltner et al. [5], or NO_x is post-processed from the main combustion results (e.g. Scharler et al. [6]). One weakness of the latter approach is that many of the fuel NO_x reaction steps depend on radical concentrations formed mainly from hydrocarbon reactions, which make decoupled fuel-N chemistry and hydrocarbon chemistry inaccurate.

2. The modelling approach

2.1. General

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 was used for the simulations. FLUENT 15 is a general-purpose CFD code, which is based on finite volumes, and 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 CFD simulations in this work were performed using the realizable k - ϵ turbulence model and the Eddy Dissipation Concept (EDC) by Magnussen [7][8] for turbulent combustion coupling in conjunction with three different reaction mechanisms developed for biomass combustion [2]. The detailed reaction mechanism includes 81 species, while the two skeletal mechanisms reduced from the detailed one include 49 and 36 species, respectively. The discrete ordinates method (DO) in conjunction with the Moss & Brookes soot model [9] was used to model radiative heat transfer. Acetylene and ethylene (C₂H₂ and C₂H₄) was used as soot precursors in the Moss & Brookes model. The physical models used were described in more detail in previous work [10].

2.3. Geometry and boundary conditions

The grate fired lab-scale multi-fuel reactor studied in the present work 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, which allows for two-stage fuel burning. There are rotating blades on each level that move 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 (Figure 1). Khalil et al. [11] have given a more detailed description of the reactor. Experiments studying the effect of excess air ratio on NO_x emissions were performed by Houshfar et al. [12] for staged and non-staged air combustion 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.

The geometry model used in the simulations included the 1.6 m high reaction section above the grate. The model was 3-dimensional and in full scale. The mesh consisted of approximately 202 100 hexahedral elements. The thermochemical conversion of the solid fuel was not included in the CFD simulations. A pyrolysis gas/air mixture was injected through an inlet boundary defined at the level of the upper grate. The gas composition and flow were based on demolition wood, a fuel feeding rate of 400 g/hr and a primary excess air ratio (λ_p) of 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

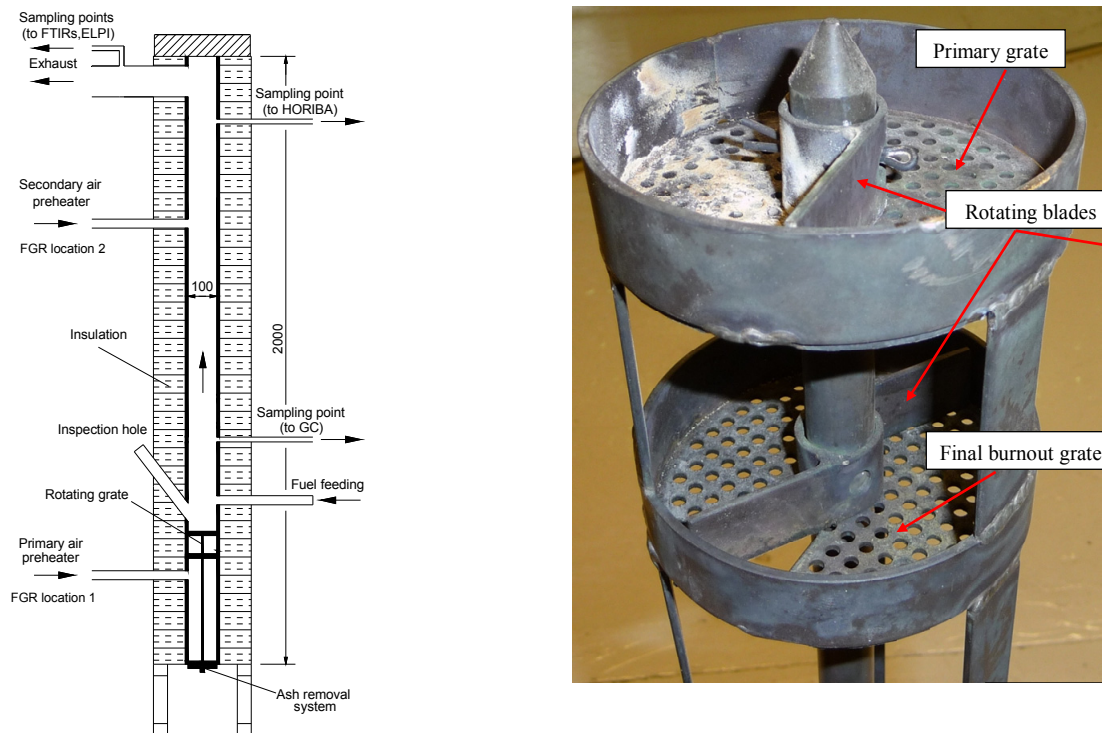


Figure 1 Left: Schematic drawing of the multi-fuel reactor of SINTEF Energy Research
Right: The two-level grate system

simulations, was also taken into account. Table 1 shows the composition of the fuel gas/air mixture based on a λ_p of 0.8. The gas temperature is 1123 K. The secondary air was injected through an inlet with a diameter of 35 mm, located 417.5 mm above the upper grate, and at a temperature of 1123 K. Total excess air ratio was 1.6, while the λ_p was 0.8, thus 50% of the air was fed at each stage.

The electrical heating elements serve to maintain a constant wall temperature, and the solid walls were specified as isothermal with a temperature of 1123 K.

3. Results and discussion

3.1. Simulations with master mechanism (81 species) models

Figure 3 (upper) shows the mean temperature and the mass flow rate of carbon in CO along the reactor length. The simulations showed that the majority of the fuel conversion occurred in the primary zone, as expected. The final burn-out occurred when the secondary air was injected, giving elevated temperatures also in the secondary zone. The highest temperatures in this zone were 1300–1400 K. The simulated mean outlet temperature was 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 3 (lower left). NO was produced in the primary zone. In the secondary zone there was a net reduction of HCN, NH₃ and NO, and it can be mentioned that there was a minor increase in NO₂ and N₂O.

The TFN (total fixed nitrogen)/Fuel-N ratio at the outlet are compared in Figure 2. Four assumptions were used for the TFN; in A0 only the nitrogen in NO was included, while in A3 the TFN included all the major nitrogen species NO₂, N₂O, HCN and NH₃ in addition to NO. The two other assumptions are A1 including NO, HCN and NH₃, and A2 including NO, NO₂ and N₂O.

According to the simulations, there was a reduction in TFN found in all the major nitrogen components; NO, HCN and NH₃, NO₂ and N₂O, 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 was 0.175 (Figure 2), i.e. a high NO_x reduction level was achieved, comparable to the NO_x emission reduction level achieved in the corresponding experiment. Nearly 98% of the TFN was the contribution from NO, the remaining was mainly NO₂. This means that the major part of the fuel-nitrogen was converted to molecular nitrogen instead of NO_x.

Removing the nitrogen components (NO, HCN and NH₃) from the fuel gas, prevented the formation of fuel NO_x and allowed to check the contribution from the other NO_x formation mechanisms to the NO_x emission level. As the temperatures were below 1700 K, the production of thermal NO_x was negligible. The predicted emissions of NO_x, which then will be prompt NO_x, were 1.3% of the base case level. Including all the major nitrogen components it increased to 1.5%. Hence, prompt NO_x formation was negligible compared to fuel NO_x formation.

Table 1 Composition of fuel gas/air mixture for λ_p of 0.8.

Specie	wt%
CO ₂	13.8483
H ₂ O	5.3929
O ₂	9.9429
N ₂	60.7130
CO	6.3018
H ₂	0.2561
CH ₄	1.3307
C ₂ H ₂	0.0552
C ₂ H ₄	0.5825
C ₂ H ₆	0.3113
NO	0.0151
HCN	0.1105
NH ₃	0.1054
Ar	1.0344
Tot gas	100.0000

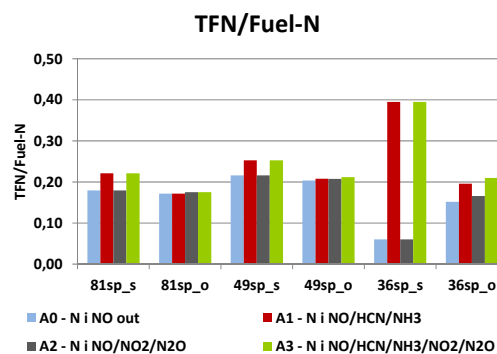


Figure 2 TFN/Fuel-N ratio at the sample surface (s) and the outlet (o) for the three reaction mechanisms, 81 (left), 49 (middle) and 36 (right) species

3.2. Simulations with skeletal mechanisms (36 and 49 species)

Simulation results for the skeletal mechanisms are compared with the full detailed mechanism in Figure 2 and Figure 3. The mean temperatures along the reactor length corresponded well. The predicted CO concentration before the injection of secondary air was slightly lower for the 36 species mechanism, while for the 49 species one it corresponded well with the detailed mechanism.

For the 36 species case a much lower reduction of HCN in the primary zone was predicted compared to the full detailed mechanism, resulting in also a higher HCN concentration at the reactor outlet. Some NO was produced early in the primary zone, and in the secondary zone not all of the remaining HCN but all of the NH₃ were converted to NO, while in the base case all HCN and NH₃ were reduced in the primary zone and there was also a slight net reduction of NO in the secondary zone. For the 49 species case HCN was close to the full detailed mechanism in the primary zone, while NO was slightly overpredicted.

Figure 2 shows that compared to the full detailed mechanism NO at the sample surface was significantly underpredicted for the 36 species case and slightly overpredicted for the 49 species case, while TFN/Fuel-N at the sample surface was significantly overpredicted for the 36 species case mainly due to the overprediction of HCN and slightly overpredicted for the 49 species case due to the slight overprediction of NO. The trends were the same at the outlet, however the deviation was reduced. The TFN/Fuel-N at the outlet was overpredicted by about 20% for both the 36 and the 49 species case, however, in the 36 species case a significant part of the TFN was HCN, while primarily NO in the 49 species case. Hence, the 49 species skeletal mechanism overall captured the kinetics of the full detailed mechanism much better than the 36 species skeletal mechanism.

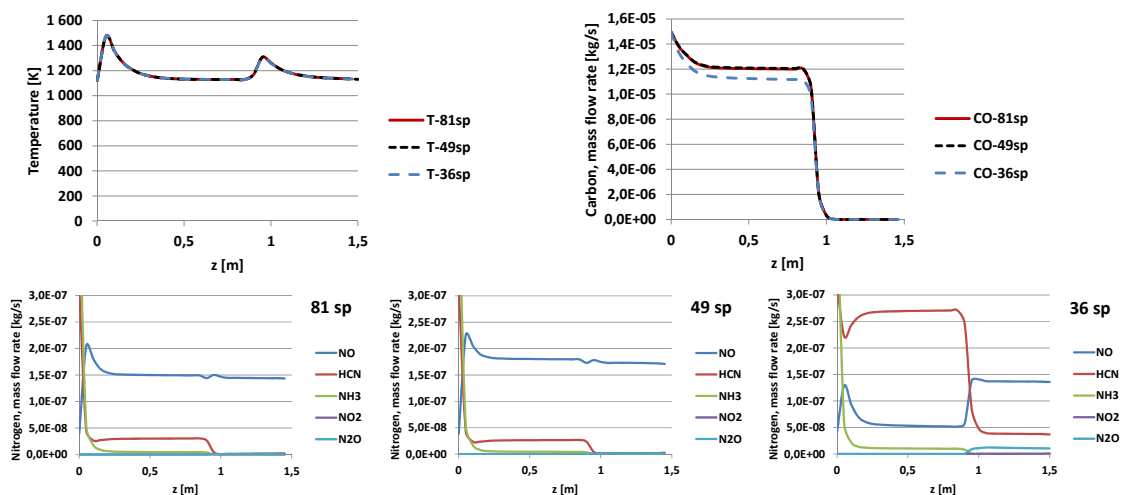


Figure 3 Upper: Mean temperature [K] and mass flow rate of selected species [kg/s] along the reactor length.
Lower left: 81 species mechanism, Lower middle: 49 species mechanism, Lower right: 36 species mechanism

4. Conclusion

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

There were deviations in the prediction of the concentrations of the nitrogen components especially in the primary zone for the three chemical mechanisms compared. The 36 species skeletal mechanism overpredicted the concentration of HCN and underpredicted the concentration of NO in the primary zone, as well as overpredicted the prompt NO_x contribution, while the 49 species skeletal mechanism slightly overpredicted the NO in the primary zone. Both skeletal mechanisms overpredicted by about 20% the TFN content at the reactor outlet. However, the 49 species skeletal mechanism captured the kinetics of the full detailed mechanism much better than the 36 species one at reducing conditions, in the primary zone.

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Biography

Mette Bugge, MSc, Mech Eng from The Norwegian University of Science and Technology. Since 1991 research scientist at SINTEF Energy Research, Trondheim, Norway. Main research topics; Combustion of gas/solid fuels, NO_x formation/reduction, CFD.

