CFD modelling of NOx emissions from wood stoves

Mette Bugge, Øyvind Skreiberg, Nils Erland L. Haugen, Morten Seljeskog
SINTEF Energy Research
Kolbjørn Hejesvei 1A, Trondheim, Norway
Mette.Bugge@sintef.no, Oyvind.Skreiberg@sintef.no, Nils.E.Haugen@sintef.no,
Morten.Seljeskog@sintef.no

ABSTRACT

The present paper addresses NOx emissions from wood stoves through a CFD modeling approach. The most significant route for NOx formation in traditional biomass combustion applications is the fuel NOx mechanism. The formation of fuel NOx is very complex and sensitive to fuel composition and combustion conditions. Thus, accurate predictions of fuel NOx formation in wood stoves, which constitute a wide range of compositions and states, 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 [2][3] for turbulent combustion in conjunction with a detailed chemical reaction mechanism and two skeletal mechanisms recently developed for biomass combustion [4].

This work is a step in the development of a numerical tool required to study concept improvements with respect to NOx emissions from wood stoves.

KEYWORDS: Wood, combustion, NOx emissions, CFD, reaction mechanism

1   INTRODUCTION

Today small-scale wood combustion in wood stoves accounts for half of the bioenergy use in Norway, and the use of wood logs in small-scale units and pellets in pellet stoves is expected to increase substantially towards 2020. The national goal is to increase the energy conversion from these units by 8 TWh within 2020 [1]. This means that the energy conversion in these units has to be almost doubled compared with today. This calls for an increased effort with respect to emission reduction, both gaseous emissions due to incomplete combustion, particulates and NOx.

The present paper addresses NOx emissions from wood stoves through a CFD modeling approach. The most significant route for NOx formation in traditional biomass combustion applications is the fuel NOx mechanism. The formation of fuel NOx is very complex and sensitive to fuel composition and combustion conditions. Thus, accurate predictions of fuel NOx formation in wood stoves, which constitute a wide range of compositions and states, rely heavily on the use of chemical kinetics with sufficient level of details. CFD modelling of wood stoves have been published by very few [5][6][7][8][9], for stationary conditions and with considerable simplifications especially when it comes to gas phase chemistry.

In 2009 Scharler et al. [5] wrote a paper on CFD simulations of a commercial wood stove, where the simulations were used to optimize the stove by increasing the thermal efficiency at the same time as the emissions of CO and fine particulates were decreased. They used the realizable k-e turbulence model and the eddy dissipation model with finite rate kinetics for the turbulence-combustion coupling. An extended version of a global 3-step methane mechanism was used for the gas phase chemical kinetics.

Scharler et al. (2011) [6] demonstrate how CFD can be used to develop, among other applications, wood stoves. They use a 3-step methane mechanism coupled with EDM for the homogeneous chemistry. The simulations are stationary and post processing with EDC is used in order to obtain predictions for NOx emissions.

Bugge et al. [10] demonstrate the use of the Eddy Dissipation Concept (EDC) for turbulent combustion in conjunction with a skeletal mechanism with 36 species developed for biomass combustion for prediction of NOx emissions from woodstoves.

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 in this work were performed using the realizable k-ε turbulence model and the Eddy Dissipation Concept (EDC) by Magnussen [2][3] for turbulent combustion in conjunction with chemical reactions from three different reaction mechanisms developed for biomass combustion [4]. The detailed reaction mechanism includes 81 species, while the two skeletal mechanisms reduced from the detailed one includes 49 and 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 [10].

2.3   Geometry and boundary conditions

The wood stove chosen is a 5 kW natural draught wood log stove. The total combustion chamber volume is $0.0266 m^3$, and the wood amount is 2 kg based on the Norwegian standard NS 3058/3059. Primary air is injected through slots at the bottom of the stove, secondary air through 13 holes from the backside of the stove and flushing air is injected vertically through a slot above the front glass window.

The model is 3-dimensional and in full scale. As the stove is symmetrical, a symmetry boundary is defined through the vertical center plane, which means that the model includes one half of the stove. The geometry has been gridded with the ANSYS meshing platform (AMP). The mesh consists of approximately 256 000 tetrahedral elements.

The wood logs are represented as volumes. The thermochemical conversion of the solid fuel is not included in the CFD-calculations. The volatiles are released from the outer surfaces of the wood pile.

Wood-log combustion is a batch process including drying, pyrolysis, gasification, char combustion as well as combustion of the gas components. The release of volatiles from the wood log is time

dependent with respect to mass flow and gas composition, and the driving force for the decomposition of the solid fuel is the heat flux to the wood log. A model for the gas release is developed and implemented.

The gas composition and flow is based on Norway spruce, a wood consumption of 1.5 kg/h and the specific 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.

Table 1 shows the composition of the fuel gas/primary air mixture based on a primary excess air ratio of 0.8. The amount of primary air injected through the slots corresponds to the excess oxygen in this composition. Increasing the primary excess air ratio will only change the mass of oxygen (O_2) and nitrogen (N_2), diluting the fuel gas. The mass of the combustible components will remain unchanged while the mass flow of primary air injected through the bottom slots will increase. The gas temperature is set to 773K.
The mass flow of volatiles released from the wood logs is determined by the heat flux from the combustion zone which means that the surfaces that are most visible to the flames will have the highest release. In this work the relative ratio between the release velocity for the top, side and end surfaces of the wood pile are 1/0.25/0.375.

The stove has cast iron walls, an insulated combustion chamber and a front glass window. In this work all the walls are treated identical, as isothermal walls with temperature 673K, and hence the radiation heat loss through the front glass window is neglected. In this initial work this is regarded as justifiable assumptions.

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

Specie	wt%	g
CO_2	4.1016	286.2761
H_2O	7.0759	493.8693
CO	12.5715	877.4385
H_2	0.2609	18.2101
CH_4	1.3293	92.7789
C_2H_2	0.0539	3.7646
C_2H_4	0.5811	40.5602
C_2H_6	0.3114	21.7374
NO	0.0011	0.0735
HCN	0.0075	0.5215
NH_3	0.0072	0.5055
O_2	13.3430	931.2863
N_2	59.3434	4141.9418
Ar	1.0122	70.6486
Tot gas	100.0000	6979.6123
Ash		4.9200
Total		6984.5323

In the base case, the total excess air ratio is 1.6, the fraction of primary/secondary/flushing air is 0.5/0.4/0.1, and the air temperatures used are 300, 373 and 623K, respectively. Simulations with two skeletal mechanisms are carried out and compared with the results for the detailed mechanism they originate from. The effect of air distribution on the NOx emission level is also studied.

3   RESULTS AND DISCUSSION

3.1   Effect of reaction mechanism for the base case

The fuel gas is released from the outer surfaces of the wood pile. The major part is released from the top surface, and the fuel conversion occurs mainly above the wood pile where the secondary air is injected, but also to an extent where the fuel gas from the side and end faces meets the primary air. As shown in Figure 1 the simulations give elevated temperatures in these areas. The maximum temperature is 1600K. The mean outlet temperature obtained in the simulations is 910 K. The three reaction mechanisms used give similar results for the temperature field.
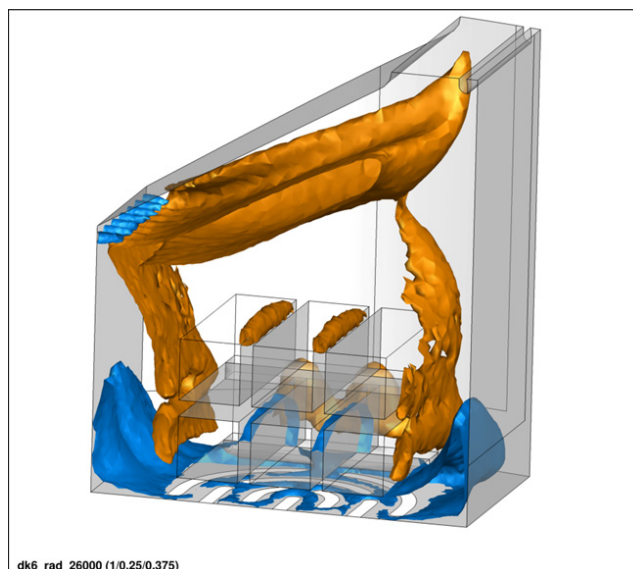
Figure 1: Iso-surfaces for temperatures of 600 and 1100K for base case

When it comes to NOx emissions, there are some variations in the predicted results for the three mechanisms. The TFN (total fixed nitrogen)/Fuel-N ratio at the outlet are compared in Figure 2. 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.
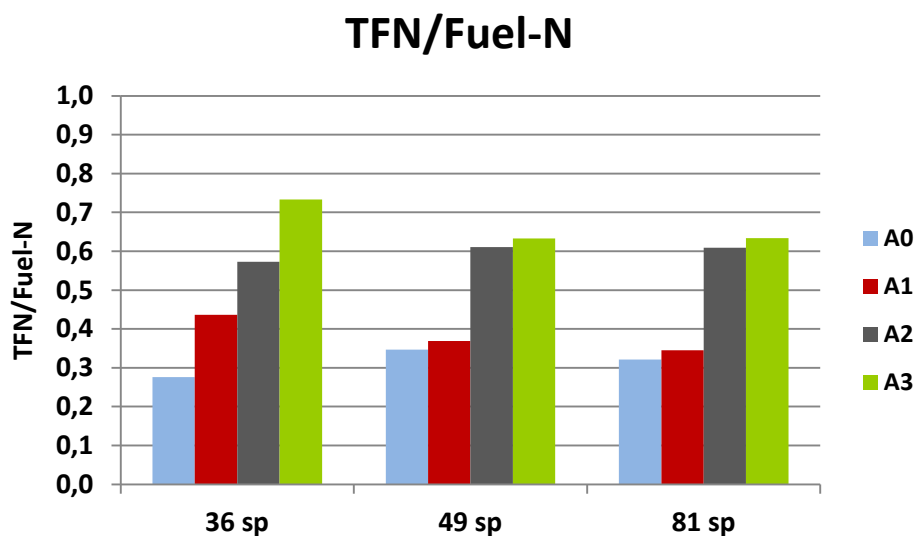

Figure 2: TFN/Fuel-N ratio at the outlet for the three reaction mechanisms, 36, 49 and 81 species. A0-N in NO, A1-N in NO/HCN/NH_3, A2-N in NO/NO_2/N_2O, A3- N in NO/NO_2/N_2O/HCN/NH_3

It can be seen that the results for the 49 species mechanism correspond well with the detailed reaction mechanism (81 species). For the A3 and A2 assumption, the results are nearly identical (less than 0.5% deviation), while the NO emission is slightly overpredicted for the skeletal mechanism (~8%).

The results for the 36 species mechanism are less satisfactory. In this scenario the A3 assumption, emission of the major nitrogen species, is overpredicted with approximately 16% compared to the detailed mechanism. This is mainly due to the over estimation of HCN, while the NO emissions are

underpredicted. And hence, the 49 species mechanism could be used for prediction of NOx emissions from woodstoves, while the 36 species mechanism is less suitable for the current problem.

Løvås et al. [4] found that the gas concentrations predicted with the 36 species mechanism were in agreement with the master mechanism (81 species) at higher temperatures (1073K), but the NOx concentrations could be overpredicted at lower temperatures (873K). Gas concentrations predicted with the 49 species mechanism corresponded well with the master mechanism also at lower temperatures. In the present CFD study the temperatures are lower than 1073K in a significant part of the domain (Figure 2).

3.2   The effect of air distribution

Previous studies [11][12] have shown that air staging could be an efficient method to reduce NOx emissions. Even if the present wood stove is not a classic air staged scenario as the mixing of fuel gas and primary air is far from complete before the secondary air is injected, some effect could be expected.

The effect of air injection and distribution are studied. Simulations with primary air excess ratio of 0.8, 0.9 and 0.95 have been carried out. The total excess air ratio is 1.6 in all scenarios, and the ratio between flushing and secondary air is kept constant (1/4).

According to the simulations the NO emissions are nearly the same for the three scenarios (Figure 3). However, comparing the values of total fixed nitrogen (TFN) including NO_2, N_2O, HCN and NH_3 in addition to NO, the emissions (A3) are increasing when the primary air excess ratio increase, due to an increase in both the emissions of HCN+NH_3 as well as the emissions of NO_2+N_2O. The simulations show a significant reduction in TFN, with the largest reduction for a primary excess ratio of 0.8.
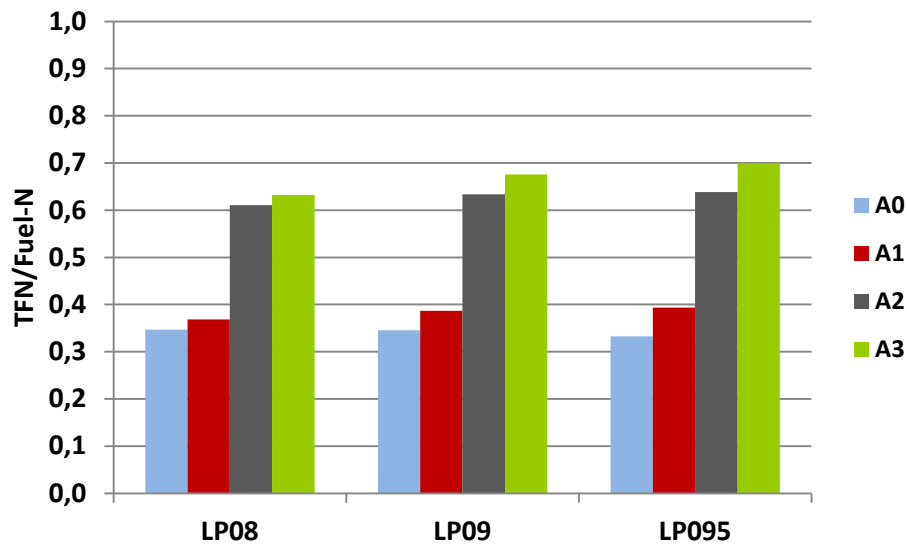

Figure 3: TFN/Fuel-N ratio at the outlet for different air distributions.
A0-N in NO, A1-N in NO/HCN/NH_3, A2-N in NO/NO_2/N_2O, A3- N in NO/NO_2/N_2O/HCN/NH_3

4   CONCLUSIONS

The simulations show that the skeletal mechanism with 49 species predicts results that correspond well with the detailed reaction mechanism while the one with 36 species overpredicts the NOx formation at the conditions in this study, with relatively low temperatures in a significant part of the domain. 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.

5   ACKNOWLEDGEMENTS

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