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Predicting NOx emissions from wood stoves using detailed chemistry and computational fluid dynamics

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Abstract

The present paper addresses NO_x emissions from wood stoves through a computational fluid dynamics (CFD) modeling approach. The most significant route for NO_x formation in traditional biomass combustion applications is the fuel NO_x mechanism. The formation of fuel NO_x is very complex and sensitive to fuel composition and combustion conditions. Thus, accurate predictions of fuel NO_x 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. In the present work we use CFD 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 to predict NO_x emissions from wood stoves. The results show that; using the detailed mechanism as reference the 49-specie reaction mechanism predict similar results whilst the 36-specie mechanism overpredicts the total amount of fixed nitrogen emissions (NO, NO_2, N_2O, HCN, NH_3) whilst underpredicting NO_x emissions. Furthermore, the results indicate that even in these small-scale applications, air staging can be used to reduce the NO_x emissions.

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Keywords: Wood; combustion; NO_x 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

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compared with today. This calls for an increased effort with respect to emission reduction, both gaseous emissions due to incomplete combustion, particulates and NO_x.

The present paper addresses NO_x emissions from wood stoves through a CFD (Computational Fluid Dynamics) modeling approach. The most significant route for NO_x formation in traditional biomass combustion applications is the fuel NO_x mechanism [2]. The formation of fuel NO_x is complex and sensitive to both fuel composition and combustion conditions. Thus, accurate predictions of fuel NO_x 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. Considering previous work there are only a limited number (compared with, for example, large scale boilers) of available CFD modeling studies of wood stoves [3-7]. These are also limited to stationary conditions and using considerable simplifications when it comes to gas phase chemistry. Previous wood stove CFD studies including detailed gas phase chemistry have not been found in the open literature.

Scharler et al. [3] used CFD to optimize a commercial wood stove by increasing the thermal efficiency whilst decreasing the emissions of CO and fine particulates. The realizable k-ε model was used to predict turbulence and the eddy dissipation model (EDM) combined with limiting finite rate chemistry was used for the turbulence-combustion coupling. A global 3-step reaction mechanism developed for methane combustion was used as gas phase reaction mechanism. In a later study, Scharler et al. [4] demonstrated how CFD can be used to develop, among other applications, wood stoves. In their study a 3-step methane mechanism was coupled with EDM for the homogeneous chemistry. The simulations were stationary and post processing with EDC was used in order to obtain predictions for NO_x emissions.

Bugge et al. [8] demonstrated 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 NO_x emissions from wood stoves.

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 15 software was 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. 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 [9], [10] for turbulent combustion coupling in conjunction with three different reaction mechanisms developed for biomass combustion [11]. The detailed reaction mechanism includes 81 species (1401 reactions), while the two skeletal mechanisms

reduced from the detailed one include 49 and 36 species. The discrete ordinates method (DO) in conjunction with the Moss & Brookes soot model [12] was used to model radiative heat transfer. Acetylene and ethylene (C_2H_2 and C_2H_4) was used as soot precursors in the Moss & Brookes model, similar to the work performed in [8] were the physical models are described in more detail.

2.3. Geometry and boundary conditions

The wood stove modeled in this study was a 5 kW natural draft wood log stove. The stove has a total combustion chamber volume of 0.0266 m^3, with a wood amount of 2 kg based on the Norwegian standard NS 3058/3059. In the stove, primary air was injected through slots at the bottom, secondary air through 13 holes at the back wall of the stove and flushing air was injected vertically through a slot above the front glass window.

The computational model describing the stove was 3-dimensional and in full scale. As the stove is symmetrical, a symmetric boundary condition was applied through the vertical center plane. The geometry was spatially discretized with the ANSYS meshing platform using 256 000 tetrahedral elements. In the computational grid the wood logs were represented as volumes which were not internally discretized. Hence, the thermochemical conversion of the solid fuel was not included in the CFD-model. Instead, as a representation 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 was based on Norway spruce, a wood consumption of 1.5 kg/h and a specific excess air ratio (λ_p). 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 the 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 inlet temperature of the volatiles was set to 773K.

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

The mass flow rate of volatiles released from the wood logs will be 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 were 1/0.25/0.375 respectively. The stove has cast iron walls, an insulated combustion chamber and a front glass window. In this work all the walls were treated identical, as isothermal walls with a temperature of 673K, and hence the radiation heat loss through the front glass window was neglected.

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

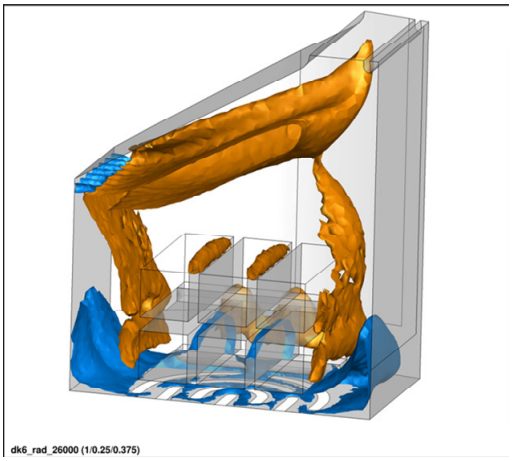

Figure 1 Iso-surfaces for temperatures of 600 (blue color) and 1100K (orange color)

When it comes to NO_x 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 definitions 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.

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 overprediction of HCN, while the NO emissions are underpredicted. And hence, the 49 species mechanism could be used for prediction of NO_x emissions from wood stoves, while the 36 species mechanism is less suitable for the current problem.

Løvås et al. [11] 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 NO_x 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 1).

3.2. The effect of air distribution

Previous studies [13][14] have shown that air staging could be an efficient method to reduce NO_x 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 excess air 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 excess air 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 for all the primary excess air ratios studied, with the largest reduction for a primary excess air ratio of 0.8.

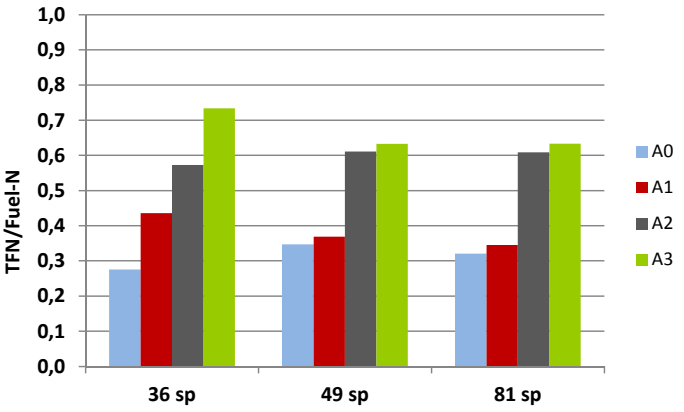

Figure 2 TFN/Fuel-N ratio at the outlet for the three reaction mechanisms, 36, 49 and 81 species.
A0-N in NO, A1-N in $NO/HCN/NH_3$, A2-N in $NO/NO_2/N_2O$,
A3- N in $NO/NO_2/N_2O/HCN/NH_3$

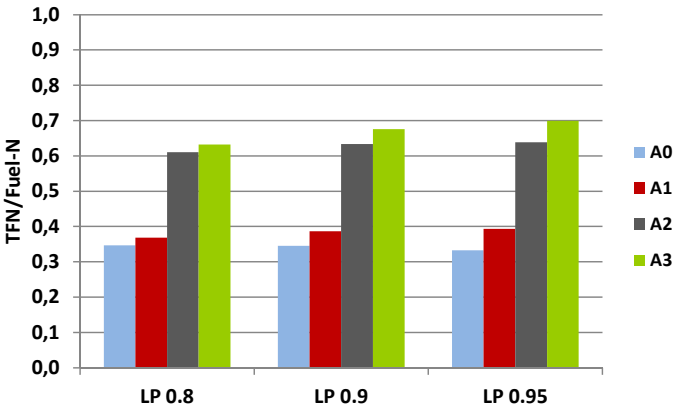

Figure 3 TFN/Fuel-N ratio at the outlet for different air distributions.
A0-N in NO, A1-N in $NO/HCN/NH_3$, A2-N in $NO/NO_2/N_2O$,
A3- N in $NO/NO_2/N_2O/HCN/NH_3$

4. Conclusions

The simulations show that the skeletal mechanism with 49 species predicts results that correspond well with the detailed reaction mechanism and which give TFN/Fuel-N ratios comparable with measured results while the one with 36 species overpredicts the NO_x formation at the conditions in this study, with relatively low temperatures in a significant part of the domain. The results give a significant NO_x reduction at a primary excess air ratio of 0.8, showing the potential of NO_x reduction by staged air combustion. Further work will expand the modelling approach, including time-dependent simulations, as well as focus on corresponding time-dependent experimental verification.

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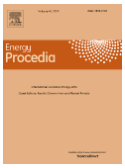

Biography

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