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NO_X EMISSIONS MODELING IN BIOMASS COMBUSTION GRATE FURNACES

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Abstract. A new flamelet combustion model is developed for the modeling of NO_x emissions in biomass grate furnaces. The model describes the combustion chemistry using premixed flamelets. The chemical system is mapped on two controlling variables: the mixture fraction and a reaction progress variable. The species mass fractions and temperature are tabulated as functions of the controlling variables in a pre-processing step to speed up the numerical calculations. The turbulence-chemistry interaction is described by an assumed shape PDF approach. Transport equations are solved for mean and variance of mixture fraction and progress variable. For the accurate prediction of NO formation, an extra transport equation is solved for the mean NO mass fraction. The model is validated for a well documented flame, Sandia Flame D. Good agreement between predictions and experimental data is found. The model is also applied to a 2D biomass grate furnace. The preliminary results are encouraging.

Keywords: biomass combustion, grate furnace, flamelet modeling, NO_x emissions.

1 Introduction

Grate furnaces are a popular conversion method for biomass combustion. These furnaces have a considerable exhaust of NO_x, originating from the nitrogen present in biomass fuels. As NO_x compounds are harmful to the environment, governments continue to lower their emission limits. Therefore, research is done into the reduction of NO_x exhaust. To optimize the design of biomass combustion furnaces for NO_x emission reduction, numerical models can be used. The requirements to these models are twofold: the model has to be sufficiently detailed to predict the NO_x production accurately and the calculation time of the model must be within reasonable limits to be able to calculate the emission levels for different design parameters and operating conditions. Standard approaches of combustion modeling include the Eddy Dissipation Concept model (EDC) and the (diffusion) flamelet model. The problem with the first model is the crude implementation of turbulence-chemistry interactions and the long computational time in case of using a detailed reaction mechanism. The second model can not handle partially premixed conditions. The model proposed in this paper is based on a (premixed) flamelet-PDF (probability density function) approach. The combustion system is described by premixed flamelets, the advance of chemical reaction being monitored by a reaction progress variable. The turbulence-chemistry interaction is accounted for with an assumed shape PDF approach. This combustion model benefits from the low calculation time and memory usage of a flamelet model and is thought to improve the accuracy of gas-phase species and temperature predictions due to the use of a reaction progress variable.

2 Description of the combustion model

As already mentioned in the introduction, in this paper a new flamelet model is presented. The model is intended for the simulation of the gas-phase combustion in biomass grate furnaces. The model works as follows. A database is calculated using the flamelet generated manifold (FGM) chemical reduction method [6], developed in the Combustion Technology Group at Eindhoven University of Technology (TUE). The chemistry is described by a detailed reaction mechanism. A number of premixed flamelets covering the flammability range are computed using the CHEM1D code [4], developed in the same research group. A progress variable is defined, to monitor the advance of the chemical reaction in the gaseous system. The species mass fractions, the temperature, the density and the species chemical source terms are tabulated as functions of the mixture fraction and the progress variable (the last two are therefore called controlling variables). The resulting laminar database is PDF-averaged using an assumed shape function. The calculation of the turbulent database, which serves as a look-up table, is done in a pre-processing step to speed up the simulations. During a simulation, turbulent transport equations for the mean and variance of mixture fraction and the progress variable are solved, making use of the tabulated density and progress variable source term. A transport equation for the NO mass fraction is also solved to predict the NO formation. At the end of the simulation, the species mass fractions and the temperature corresponding to the values of the controlling variables in every point of the computational domain are retrieved from the tables and thus the complete structure of the combustion system is made available.

3 Construction of look-up tables for numerical simulations

Following the description given in the previous section, the detailed chemical system is mapped on two controlling variables: the mixture fraction (*Z*) and a reaction progress variable (*c*). The mixture fraction describes the mixing of the species and enthalpy, while the progress variable follows the advance of the chemical reaction. Hence, the species mass fractions, temperature, density and species chemical source terms become functions of *Z* and *c*. The mixture fraction is defined according to [2] as:

$$Z = \frac{Y^* - Y^*_{ox}}{Y^*_{fu} - Y^*_{ox}}, \quad Y^* = 0.5\frac{Y_H}{M_H} + 2.0\frac{Y_C}{M_C} \tag{1}$$

where Y_{H} and Y_{C} are the element mass fractions for H and C, respectively and M_{H}, M_{C} are their molar masses. Y^* is a combined element mass fraction. Y^*_{ox} and Y^*_{fu} are the values of Y^* corresponding to the oxidizer and fuel streams, respectively. Following Eq. (1), *Z* varies between 0 in the oxidizer stream and 1 in the fuel stream. The progress variable is defined as:

$$c = \frac{Y_{CO_2} - Y^{\min}_{CO_2}}{Y^{\max}_{CO_2} - Y^{\min}_{CO_2}} \tag{2}$$

where Y_{CO_2} is the mass fraction of CO_2, which varies between $Y_{CO_2}^{\min}$ in the unburned mixture and $Y_{CO_2}^{\max}$ in the burned (equilibrium) gas.

The species mass fractions, temperature, density and chemical source terms present in the laminar database correspond to laminar premixed flamelets with mixture fraction values spanning the flammability range (depending on the fuel type) and progress variable values from 0 (reactants) to 1 (products).

In turbulent reactive flows, the chemical species and temperature fluctuate in time and space. As a result, any variable can be decomposed in its mean and fluctuation. In Reynolds-averaged Navier Stokes (RANS) simulations, only the means of the variables are computed. Therefore, a method to obtain a turbulent database (containing the means of species, temperature, etc) from the laminar data is needed. In this work, the mean variables are calculated by PDF-averaging their laminar values with an assumed shape PDF function. The Favre-average $\tilde{\phi}$ of a variable ϕ which stands for species mass fractions (Y_i), temperature (T), density (ρ) and species chemical source terms (S_i) is calculated as:

$$\tilde{\phi} = \int_0^1 \int_0^1 \phi(Z,c)\,\tilde{P}(Z,c)\,dZdc \qquad (3)$$

where $\tilde{P}(Z,c)$ is the joint PDF of Z and c. Using the common assumption of the statistical independence of Z and c, the joint PDF can be computed as the product of the marginal PDFs. For these PDFs, a β shape function is assumed. The marginal PDFs are determined by the mean and the variance of the corresponding controlling variable.

4 Turbulent transport equations for controlling variables

In the present combustion model, transport equations for the mean and variances of the mixture fraction and the progress variable and the mean mass fraction of NO are solved. They read:

$$\nabla\left(\bar{\rho}\tilde{u}\tilde{Z}\right) - \nabla\left(\left(\bar{\rho}D + \frac{\mu_T}{Sc_T}\right)\nabla\tilde{Z}\right) = 0\,, \qquad (4)$$

$$\nabla\left(\bar{\rho}\tilde{u}\tilde{c}\right) - \nabla\left(\left(\bar{\rho}D + \frac{\mu_T}{Sc_T}\right)\nabla\tilde{c}\right) = \bar{S}_c\,, \qquad (5)$$

$$\nabla\left(\bar{\rho}\tilde{u}\widetilde{Z''^2}\right) - \nabla\left(\left(\bar{\rho}D + \frac{\mu_T}{Sc_T}\right)\nabla\widetilde{Z''^2}\right) = 2C_1\frac{\mu_T}{Sc_T}\left(\nabla\tilde{Z}\right)^2 - C_2\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\widetilde{Z''^2}\,, \qquad (6)$$

$$\nabla\left(\bar{\rho}\tilde{u}\overline{c''^2}\right)-\nabla\left(\left(\bar{\rho}D+\frac{\mu_T}{Sc_T}\right)\nabla\overline{c''^2}\right)=2C_1\frac{\mu_T}{Sc_T}\left(\nabla\tilde{c}\right)^2-C_2\bar{\rho}\frac{\tilde{\varepsilon}}{\tilde{k}}\overline{c''^2}+2\overline{c''S_c}\,, \tag{7}$$

$$\nabla\left(\bar{\rho}\tilde{u}\tilde{Y}_{NO}\right)-\nabla\left(\left(\bar{\rho}D+\frac{\mu_T}{Sc_T}\right)\nabla\tilde{Y}_{NO}\right)=\bar{S}_{NO}\,. \tag{8}$$

In Eqs. (4)-(8), $\bar{\rho}$ is the mean density, $\tilde{u}$ is the mean velocity vector, $\tilde{Z}$ is the mean mixture fraction, D is the molecular diffusion coefficient, μ_T is the turbulent viscosity, Sc_T is the turbulent Schmidt number, $\tilde{c}$ is the mean progress variable, $\bar{S}_c$ is the mean chemical source term of c, $\overline{Z''^2}$ is the variance of the mixture fraction, C_1 and C_2 are modeling constants, $\tilde{k}$ is the mean turbulent kinetic energy, $\tilde{\varepsilon}$ is the mean dissipation rate, $\overline{c''^2}$ is the variance of c, $\tilde{Y}_{NO}$ is the mean mass fraction of NO and $\bar{S}_{NO}$ is the mean chemical source term of NO. The values of constants Sc_T and C_2 are 0.85 and 2.0, respectively. As for C_1, it was given the value 1.2155 for the transport equation of $\overline{Z''^2}$ (Eq. (6)), in accordance with FLUENT manual recommendation and 1.0 for the transport equation of $\overline{c''^2}$ (Eq. (7)). More details about this flamelet combustion model can be found in [7].

5 Validation of the combustion model

The model was validated using a well documented flame: Sandia Flame D. This is a turbulent piloted flame, the fuel consisting of a mixture of CH_4 (25 % vol.) and air (75 % vol.). The flame is surrounded by a pilot that produces the same equilibrium composition as a CH_4/air flame with an equivalence ratio of 0.77. The bulk velocities of the fuel jet, pilot and air co-flow are 49.6, 11.4 and 0.9 m/s, respectively. The operating conditions are 293 K and 0.993 atm. The configuration of Sandia Flame D, used to build the computational domain, is shown in Figure 1.

A structured numerical grid consisting of 40,000 cells, refined in the region of fuel inlet and along the symmetry axis was used. The inlet profiles of velocity, turbulent kinetic energy and dissipation rate are taken from [1]. The inlet boundary conditions for $\tilde{Z}$, $\tilde{c}$ and $\tilde{Y}_{NO}$ are given in Table 1. Note that, in this simulation, the progress variable c was taken equal to the mass fraction of CO_2 and not with its normalized value, as given by Eq. (2). The variances of the combustion scalars $\overline{Z''^2}$ and $\overline{c''^2}$ are considered 0 at the inlets.

Table 1: Inlet conditions for $\tilde{Z}$, $\tilde{c}$ and $\tilde{Y}_{NO}$.

Inlet	$\tilde{Z}$	$\tilde{c}$	$\tilde{Y}_{NO}$
Fuel	1	0	0
Pilot	0.27	0.1098	$4.8\cdot10^{-6}$
Air	0	0	0

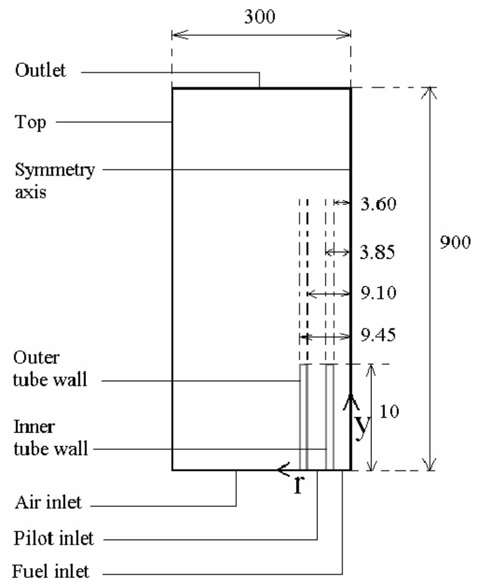


Figure 1: Configuration of Sandia Flame D. Courtesy of H.A.J.A. van Kuijk [5].

The present model was implemented in the FLUENT flow solver to simulate the Sandia Flame D. For the construction of the database, the GRI-Mech3.0 reaction mechanism [3] was used. The realizable k-ε model was employed for turbulence modeling.

Figures 2a-h present a selection of the simulation results. All the figures show profiles along the centerline, the axial coordinate (*y*) being divided through the diameter of the fuel nozzle (*d* = 7.2 mm). The predictions are compared with measurements reported in [9].

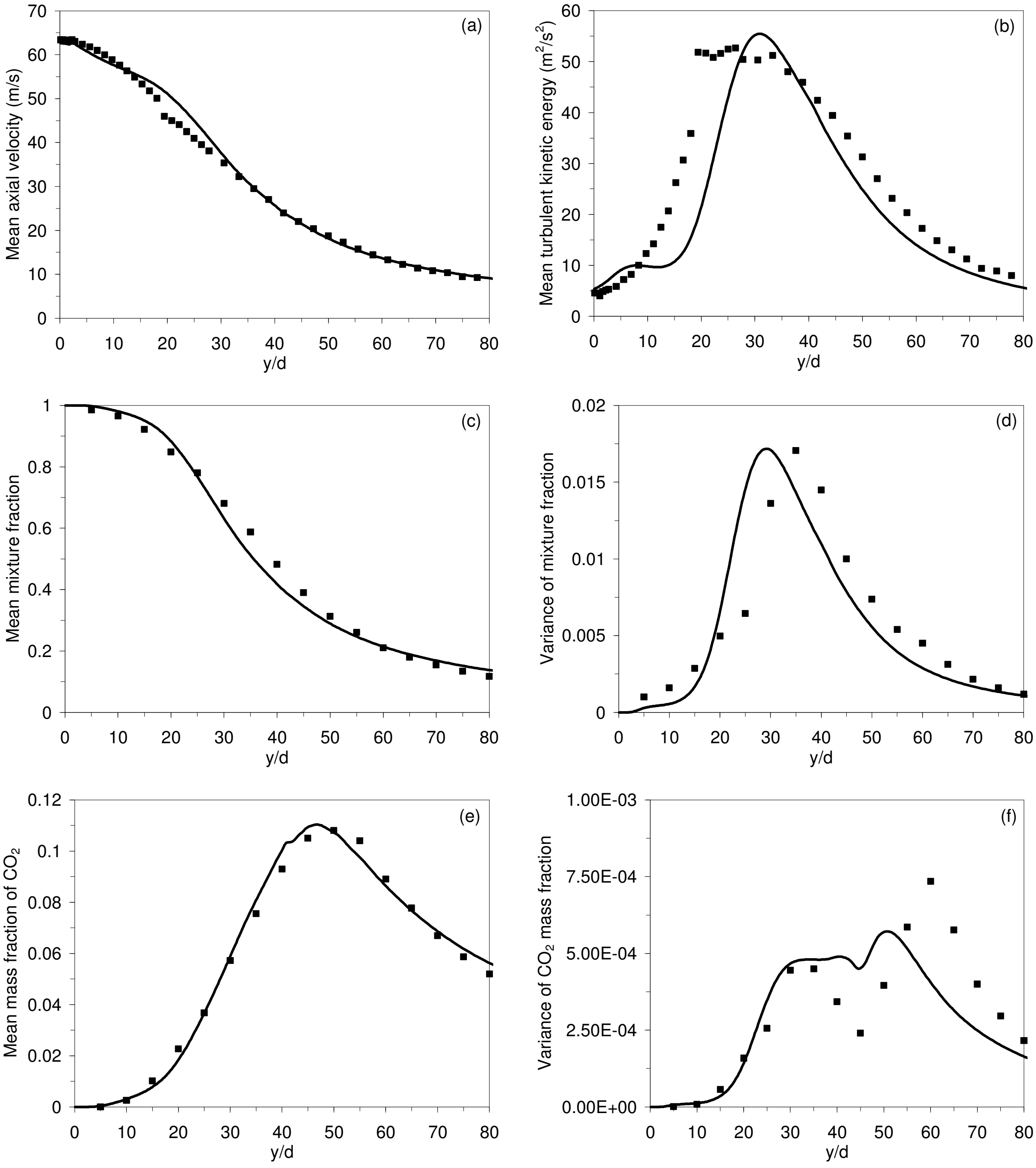
In Figures 2a and b the flow variables $\tilde{u}$ and $\tilde{k}$ are plotted. It can be noticed that the axial velocity is generally well predicted. As for the turbulent kinetic energy, the predictions are close to measurements for y/d greater than 35. However, the simulations under-predict k in the interval y/d = 10 – 30. The plateau between y/d = 20 and y/d = 35 cannot be predicted as well.

Figures 2c and d show the mean and the variance of Z. The prediction of $\tilde{Z}$ agree quite well with the measurements. The shape of $\overline{Z''^2}$ is also close to experiments, but the position of its maximum value is moved to the left.

In Figures 2e and f, the mean and the variance of CO_2 mass fraction are depicted, respectively. The mass fraction of CO_2 was chosen for representation because the progress variable *c* is based on it. It can be seen that the mean of CO_2 mass fraction is well predicted both qualitatively and quantitatively. As for the variance, it is well predicted for y/d < 35, but further away from the inlet the model fails to predict the magnitude of the minimum and maximum of the variance. However, the shape of the variance is reasonable guessed.

The axial temperature profile is given in Figure 2g. It can be noticed that the simulation result is close to the experiments. Nevertheless, at the top of the profile, the predicted temperature curve presents a wiggle. A similar distortion of the predicted profile is noticeable also in the mean mass fraction of CO_2 from Figure 2e. The source of this wiggle is presently a subject of investigation.

The mean mass fraction on NO is shown in Figure 2h. The shape of the axial NO profile is well predicted by the present combustion model. The maximum value is only slightly under-predicted, within 10 % of the measured data.



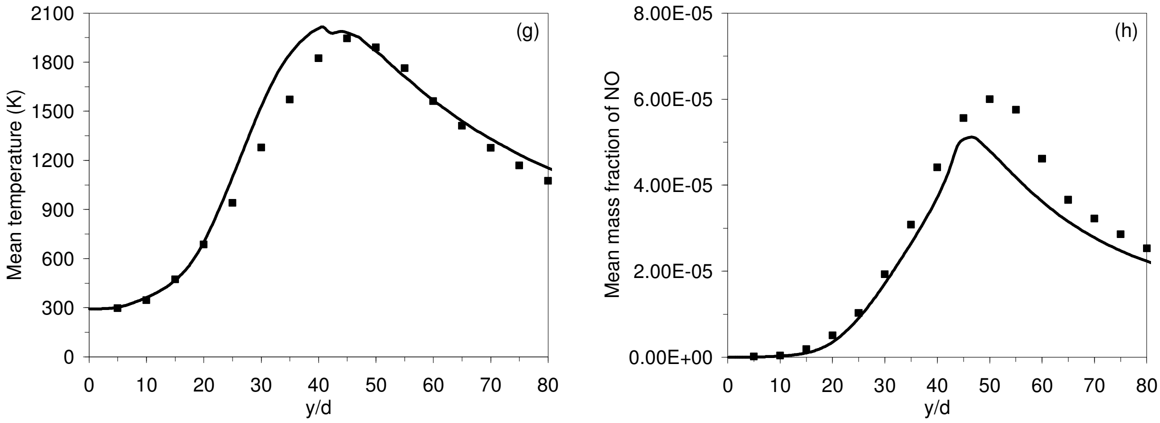


Figure 2: Axial profiles, as given by predictions (solid lines) and measurements (symbols) of (a) mean axial velocity, (b) mean turbulent kinetic energy, (c) mean mixture fraction, (d) variance of mixture fraction, (e) mean mass fraction of CO_2, (f) variance of CO_2 mass fraction, (g) mean temperature and (h) mean mass fraction of NO, for the Sandia Flame D.

6 Application of the combustion model on a 2D grate furnace

As shown in the previous section, the flamelet model was validated by comparing model predictions with measurements for a diffusion methane flame, the Sandia Flame D. The next step is to test the model for the combustion of gaseous fuel originating from the biomass gasification/combustion on a grate.

Thus, in cooperation with Graz University of Technology (TU-Graz), the model was applied to a biomass combustion grate furnace for the prediction of combustion and NO_x emissions [8]. A 2D geometry together with appropriate boundary conditions for such a furnace was supplied by TU-Graz. This was used to test the present flamelet model by TUE. Two inlets have been set: one at the grate, where the primary air is mixed with the biomass gasification/combustion products and the other one corresponding to the secondary air that is added to complete the combustion process. However, the recirculation gases which are usually introduced for temperature control in the furnace in order to prevent ash slagging or sintering and to reduce the NO_x emissions have not been considered in the present stage of the simulations. This is because including recirculation gases at low temperature (200 °C) in the simulation requests the use of an enthalpy variable. This additional variable is still not present in the model but it will be added in the near future. At the fuel bed, profiles of velocity, species mass fractions and temperature have been supplied by TU-Graz. They result from the gasification/combustion of a biomass fuel on the grate when blowing air from bellow the grate. A fuel and an oxidizer are defined, which are mixed by using the mixture fraction to generate an approximation of the species profiles provided by TU-Graz. They are given in Table 2. This way, the only profiles needed for the simulation at the furnace inlet are those of the velocity and the mixture fraction. The new defined fuel and oxidizer are used to construct first a laminar database and then a turbulent database, following the procedure described in section 3. A detailed reaction scheme dedicated to biomass combustion was used: the SKG03 reaction mechanism [10]. During a simulation, transport equations for the mean and variance of the mixture fraction and progress variable and the mean mass fraction of NO are solved. The density and the chemical source terms are taken from the look-up table containing the turbulent database. At the end of the simulation, the species mass fractions and the temperature are retrieved from the database. The simulations were performed with the FLUENT flow solver using the realizable k-ε model for turbulence modeling.

Table 2: Composition of fuel and oxidizer streams.

Species (mole fractions)	Fuel	Oxidizer
CO	0.095	-
H_2	0.068	-
CH_4	0.016	-
CO_2	0.120	-
H_2O	0.140	-
NO	$4 \cdot 10^{-5}$	-
NH_3	$50.3 \cdot 10^{-5}$	-
N_2	0.561	0.79
O_2	-	0.21
Temperature (K)	1386	361
Stoichiometric mixture fraction	0.63	

Figures 3a-c show the 2D profiles of mixture fraction, temperature and NO mass fraction, as predicted by the current flamelet model. In Figure 3a, at the bottom line of the furnace, the distribution of the mixture fraction on the grate can be seen. The mixture fraction is 1 somewhere in the middle of the grate, where only gaseous fuel is present, and 0 at the sides of the grate, where only air is present. In between, there are mixtures of fuel and air with mixture fractions between 0 and 1. This distribution of the mixture fraction on the grate is a result of different degrees of biomass conversion to gasification and combustion products along the grate when blowing air from below the grate, through the fuel bed. Later on, the streams with different mixture fractions coming from the grate mix with each other and start to burn, leading to a more homogeneous mixture with rising temperature (see also Figure 3b). After the first turn in the furnace, the main flow meets the secondary air flows (4 tiny flows in a row in Figure 3a), which dilute the mixture and insure the complete combustion of the fuel still present in the mixture. This results in more temperature increase, as indicated by the red colored areas in Figure 3b. Figure 3c shows that the NO is formed where the combustion takes place. This is indicated by the high temperature zones in the furnace (see Figure 3b). It should be noted that the results presented in Figures 3a-c are preliminary and they are included here to illustrate the application of the present flamelet model to a biomass combustion furnace. However, before the numerical results can be compared with measurements, the combustion model has to be improved by adding an extra enthalpy variable. This will take into account the heat loss and to allow the inclusion of the recirculated gases. It is expected that both consideration of the heat loss in the furnace and the recirculated gases addition will have an important effect on the temperature and NO mass fraction fields.

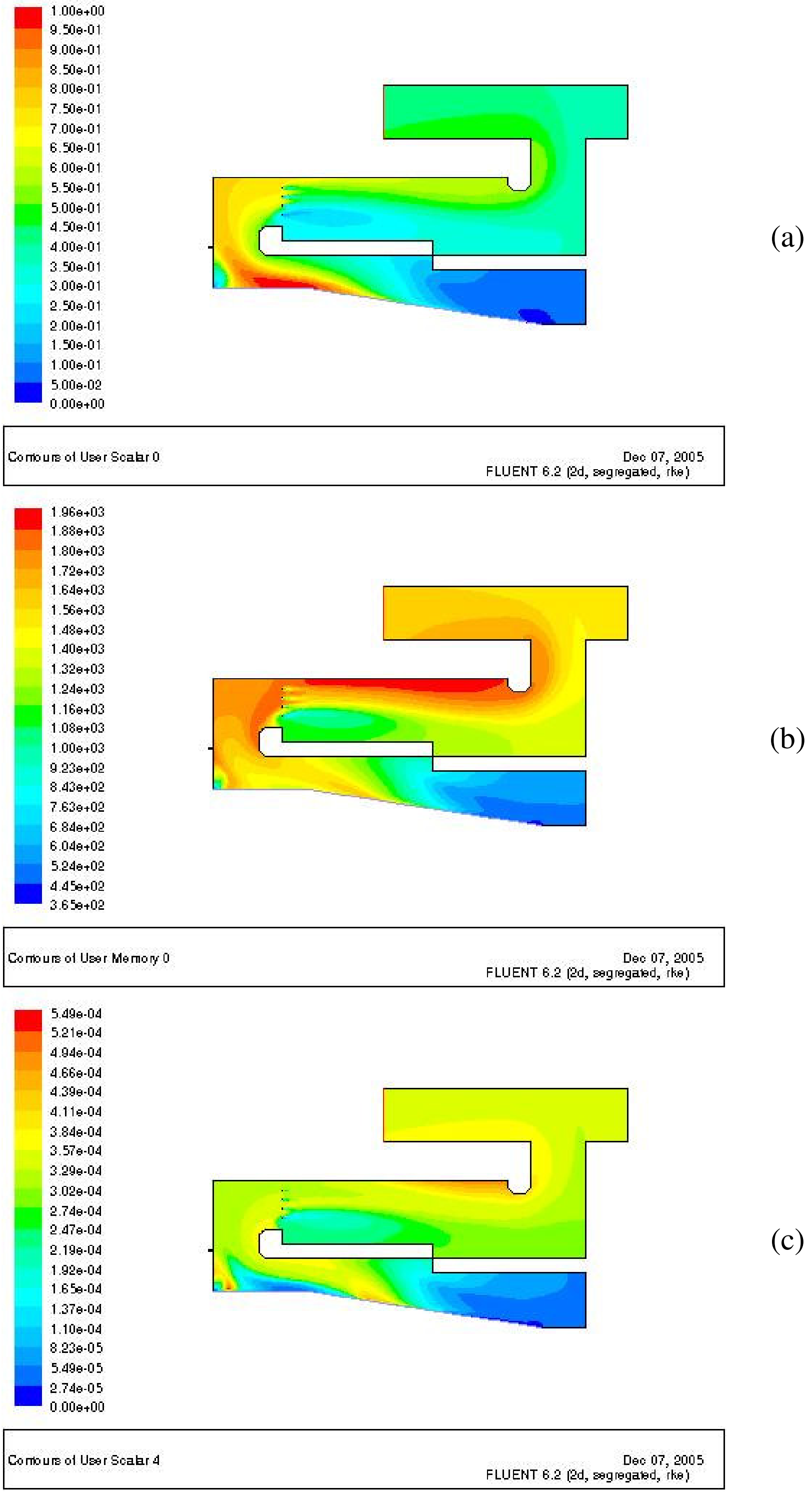


Figure 3: 2D predicted profiles of (a) mean mixture fraction, (b) mean temperature and (c) mean NO mass fraction, for the biomass grate furnace.

7 Conclusions

- The present flamelet model uses premixed flamelets to describe the combustion chemistry. The code employs the mean and the variance of the mixture fraction and a progress variable to model a turbulent combustion process. The turbulence-chemistry interaction is described by an assumed shape PDF approach.
- NO formation is predicted by solving an additional transport equation for the NO mass fraction.
- The model predictions agree well both qualitatively and quantitatively with the measurements for the Sandia Flame D.
- The flamelet model was used to simulate a biomass grate furnace in a 2D geometry. The preliminary results are encouraging. The addition of an enthalpy variable to take into account the heat loss in the furnace is expected to improve the numerical predictions.

8 Acknowledgements

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