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CFD APPROACH FOR MODELING HIGH AND LOW COMBUSTION IN A NATURAL DRAFT RESIDENTIAL WOOD LOG STOVE

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ABSTRACT

In this work, a comprehensive CFD model was developed for pyrolysis to provide significant emission reductions. In wood stoves with natural draft, the airflow is driven by buoyancy to overcome the resistance to flow within the stove. This combustion model is tested to reproduce at best the physical and chemical phenomena taking place in a natural draft wood log stove for low power (18 kW) residential heating. The RANS approach was used to solve the aerothermodynamic equations. A body fitted hexahedron mesh was adopted and the k-ε turbulence model was used to ensure closure of the Navier-Stokes equations. The chemical reaction for combustion was modeled using species transport and rate of species production formulated as the EDDY DISSIPATION CONCEPT. The key parameters for validation are based on temperature inside the combustion chamber at the center plane and the [CO]/[CO2] ratio for emissions at the exit plane. Therefore, the developed modelling approach can be used for engineering analysis and optimization of existing stoves and for relatively-quick evaluations of new stove designs.

Keywords: CFD; RANS; Turbulent flows; Biomass; Combustion; Eddy Dissipation Concept; emissions.

1. INTRODUCTION

In order to study the characteristics of a log wood stove to improve low particulate emissions, 3D numerical simulations and analysis were conducted with the commercial code ANSYS-FLUENT™. In order to meet the low particulate emissions required in the new EPA/CSA standards, manufacturers of wood burning appliances must invest heavily in R&D. The wood combustion process is especially critical at the beginning with the ignition phase and at the end of combustion when temperatures are at the lowest levels when the pyrolysing products of less volatile or toxic compounds such as CO and particulate matters are largely produced. A comprehensive CFD model for the whole stove was developed to provide significant emission reductions. The chemical reaction for pyrolysis is modeled using species transport and rate of species production with the EDDY DISSIPATION CONCEPT developed as a combustion model in FLUENT™. The RANS approach was used in this work solving the aerothermodynamic equations in the wood stove. A body fitted hexahedron mesh was adopted and the *k-ε* turbulence model was used to ensure closure of the Navier-Stokes equations. The reaction for combustion could be modeled using either the species transport or the non-premixed combustion model. In this work, only the non-premixed combustion model will be presented for the chemical reaction required for combustion. This CFD model reproduces the physical and chemical phenomena taking place within a low power (18 kW) wood stove operated in a high or low combustion regime. A high rate of combustion is considered when the vents are fully open at 100% and 40% for the low rate. A simplifying factor is to look specifically at the gas phase combustion of volatiles during the thermal decomposition of wood. The key parameters for validation are based on velocity, temperature and species concentrations inside the combustion chamber, concentrations of carbon monoxide (CO) and the [CO]/[CO_2] ratio at the exit plane for emissions. A good balance between primary and secondary air is needed to control the combustion so that there is enough secondary air to completely burn the volatile gases. Also, good mixing between air and the pyrolysis gases is needed to promote clean burning. In this work, comparison between simulation results and experimental values obtained in our combustion laboratory has shown good agreement. All measurements were completed with combined O_2, FID and FTIR analyzers. This study can reasonably confirm that most features for better wood stove performance under different operating conditions can be identified accurately by this CFD model. Future work will focus on using this model to investigate possible improvements for the design of a better air delivery system to reduce emissions. In this paper, the model is described first. The results are then presented and commented. Finally, conclusions on the stove design are made.

2. MODEL DESCRIPTION

The 3D model is divided into three parts: fluid flow, chemical mechanism and heat transfer. Model equations are

listed in a paragraph presenting the governing equations. Fig. 1 shows half of the 3D geometry with a symmetry plane to reduce the computational domain and the corresponding boundary conditions. Special attention is given to the gas phase. The heterogeneous reactions are considered negligible in the oxidation zone as oxygen reacts much faster with the generated gas from pyrolysis.

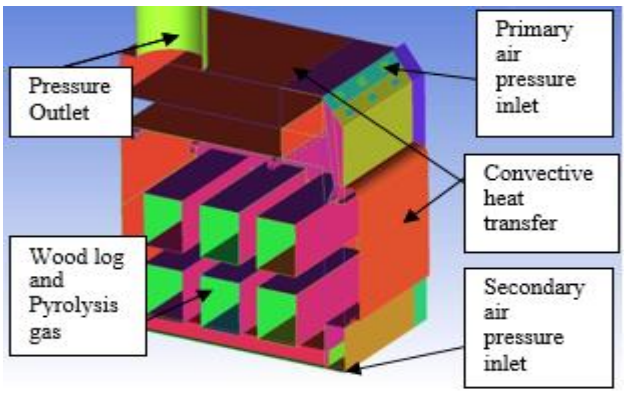

Figure 1. Geometry and boundary conditions

2.1 Governing equations

The time averaged gas phase equations for steady turbulent flow can be expressed as:

$$\frac{\partial}{\partial x_j}(\rho u_j \Phi) = \frac{\partial}{\partial x_j}\left(\Gamma_\Phi \frac{\partial \Phi}{\partial x_j}\right) + S_\Phi \qquad (1)$$

where Φ, Γ_Φ and S_Φ are respectively the representative dependent variables, the effective diffusion coefficient and the source term for the gas phase respectively as shown in equation (1). Replacement of Φ with a value of 1 yields the continuity equation, while a substitution with u, v and w represents the momentum equation in the x, y and z directions, and substitution of Φ with T, k, ω and y yields respectively the equations of energy, turbulent kinetic energy, dissipation rate of the turbulent kinetic energy and species transport. In this work, the following models were selected: Eddy Dissipation Concept (EDC) Model for turbulent combustion reaction, discrete ordinates model for radiation heat transfer, and k-ε equations for the turbulence model.

Eddy dissipation concept model. For a solid fuel such as wood, it is not possible to provide a mixture equivalent to that obtainable with a gas or a volatile liquid. It requires that each carbon atom or hydrogen waits its turn in the queue before being oxidized. When the first flies off the solid surface as volatilized product from when heated by combustion, then the neighbor becomes available to fly off next, and so on. This process delays the oxidation of the log mass and therefore decreases the efficiency of heat production. It has been confirmed by a number of researchers [3], [4], [5], [6] and [7] that, in the residential stove, the combustion reaction can be regarded as approaching equilibrium. Furthermore, it is reasonable that, in the wood pyrolysis process, each substance to form a particle is uniformly released. Concerning homogeneous reactions, a combined model is used. The finite rate Eddy dissipation concept model computes both the Arrhenius rate and the Eddy dissipation rate and uses the lower of the two. The combustion mechanism of Westbrook and Dryer [10] is used here; it consists of the partial oxidation of tar and light hydrocarbons (Reactions (R1), (R5), and (R6)), the complete oxidation of carbon monoxide (Reaction (R2)) and hydrogen (Reaction (R4)) and the dissociation of carbon dioxide (Reaction (R3)) which is significant at high temperatures.

Chemical kinetics used here is based on a global reduced mechanism, with the following reactions:

$$CH_4 + 1{,}5\ O_2 \rightarrow CO + 2\ H_2O \qquad (R1)$$
$$CO + 0{,}5\ O_2 \rightarrow CO_2 \qquad (R2)$$
$$CO_2 \rightarrow CO + 0{,}5\ O_2 \qquad (R3)$$
$$H_2 + 0{,}5\ O_2 \rightarrow H_2O \qquad (R4)$$
$$C_2H_2 + 2{,}5\ O_2 \rightarrow 2\ CO_2 + H_2O \qquad (R5)$$
$$C_2H_4 + 3\ O_2 \rightarrow 2\ CO_2 + 2H_2O \qquad (R6)$$

The kinetic rates for the mechanism are listed in Table 1.

Table 1. Parameters for Arrhenius rates

Reaction	A*	E_a	a	b
R1	$5.012 \cdot 10^{11}$	$2.000\ 10^8$	0.7	0.8
R2	$2.239 \cdot 10^{12}$	$1.700\ 10^8$	1.0	0.25
R3	$5.000 \cdot 10^8$	$1.700\ 10^8$	1.0	
R4	$9.870\ 10^8$	$3.100\ 10^7$	1.0	1.00
R5	$1.125\ 10^{10}$	$1.256\ 10^8$	0.1	1.65
R6	$3.655\ 10^{10}$	$1.256\ 10^8$	0.5	1.25

The advantage is that it requires less computation time, but it is limited to six (6) stages. In this EDC model, the total space is divided into smaller spaces to account for reaction, called fine structures. The reactions are assumed to take place in these fine structures. These models are described in more detail in the theory section of the user's guide for the commercial code FLUENT ™.

The volatile stream composition is defined by selecting appropriate species and setting their mole fractions. The equilibrium system for homogenous combustion consists of 8 species (CH4, CO, CO2, C2H2, H2, H2O, C2H4 and O2).

2.2 Numerical scheme

The computational model uses a 3D steady-state solver and a second-order discretization scheme where gradients and derivatives are evaluated through the Green-Gauss method. Table 2 summarizes the characteristics of the solver. For the discretization of all conservative equations (momentum, continuity, energy, mixture fraction, turbulent kinetic energy, turbulent kinetic energy dissipation rate and mass fraction of chemical species), a second-order upwind scheme was used [9], [10] and [11]. In this discretization scheme, quantities at the cell faces are determined by assuming that the cell-center values represent an average value and hold throughout the entire cell; the face quantities are identical to the cell quantities.

Table 2. Solver parameters

Characteristic	**Value**
Formulation	Implicit
Velocity Formulation	Absolute
Gradient Option	Green-Gauss
Pressure-Velocity Coupling	Phase Coupled SIMPLE
Discretization	Second Order Upwind
Under-Relaxation	Variables

3. EXPERIMENTAL FACILITIES

3.1 Facilities

The appliance is a residential wood stove with an 18 kW thermal capacity and the air required for combustion is fed by natural draft. Fig. 2 shows the experimental setup as used to obtain all the data at the four different burning categories as given in Table 2.

3.2 Method of investigation

The flue gas composition is determined by gas analysis with a probe sampling inside the flue gas at the area shown in Fig.3. The gas analyzer probe is equipped with multi-stage filters that prevent solid particles to reach the analyzers. The gas analyzers include 3 modules: an Oxygen (O_2) analyzer, a Fourier transform infrared spectrometer (FTIR) and a Flame ionization detector (FID). The position of all K-type thermocouples used in the experimental set-up is marked with small rectangles in Fig. 3. The main purpose of the installed thermocouples is to obtain temperature data from the firebox and from the chimney. Temperatures at the inlet and exit of the stack allow calculation of the wood stove efficiency. The inlet temperature to the stack gives also a good approximation of the overall combustion gas temperature. The internal thermocouple positions are described into Fig.4. Experiments were performed with Douglas fir wood logs. Wood moisture was maintained at 20.5% of the total mass. The wood equivalent formula is $C_{4.6}\,H_{6.87}\,O_{2.775}$. Since all tests were completed with standardized wood, the atomic composition of the fuel is well known allowing calculation of the equivalence ratio Φ from a global reaction. In addition a detailed evaluation of Φ is performed on the basis of a MATLAB routine from FTIR data. Φ is defined as the ratio between the actual fuel/air ratio and the stoichiometric fuel/air ratio required for a complete combustion of the fuel. Two preload must be burned to heat the stove before introducing the test load and take experimental measurements.

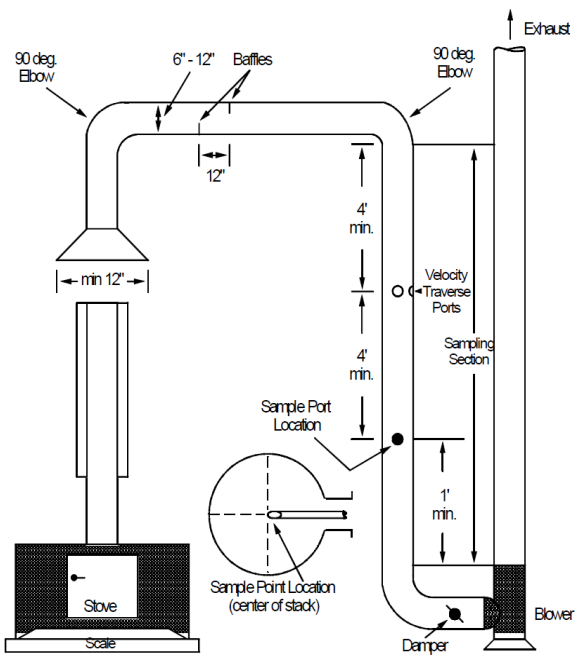

Figure 2. Experimental setup

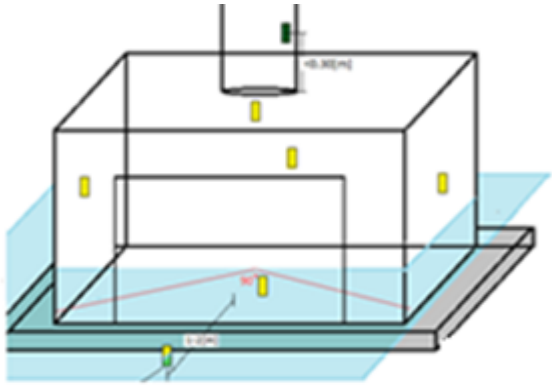

Figure 3. Small yellow boxes represent the external thermocouples

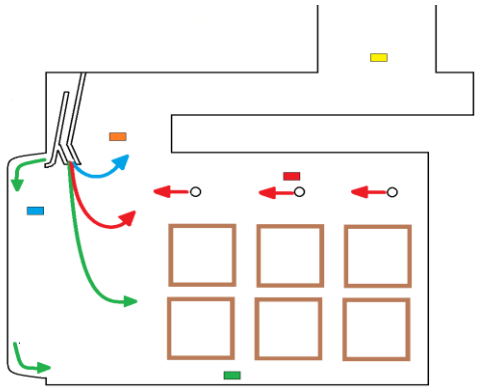

Figure 4. Small colored boxes represent the internal thermocouples

4. SIMULATION CONDITIONS

4.1 Geometry and grid

The computational domain of the 3D geometry used in this study includes unstructured grid of tetrahedral mesh elements as seen at Fig.5. A grid independent study was performed with coarse, medium and fine grids. The results for the velocity field at the symmetry plane of the combustion chamber show a small difference between the medium and fine grids. The medium grid with 934 705 nodes was selected for this CFD analysis. The initial boundary conditions for the flow are shown in Fig.1.

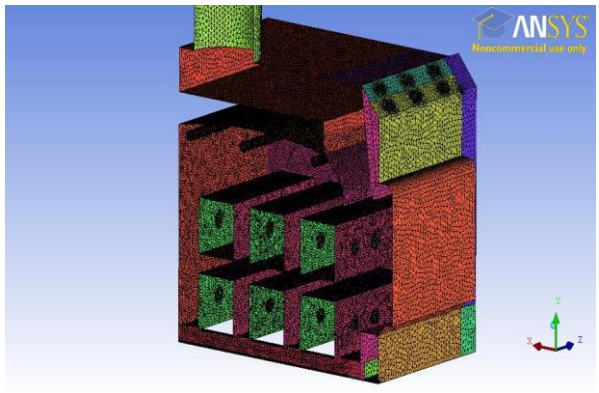

Figure 5. Tetrahedral grid

4.2 Validation cases

The validation study is to simulate two types of stove operating conditions defined by the Environmental Protection Agency (EPA) as follows: category 1: Low combustion (low burn) and category 4: high combustion (high burn) as seen at Table 3. In this paper, only the high and low combustion are presented but temperature and species contours are shown only for category 4 (high combustion).

Indeed, prior to complex simulations, it is necessary to know the behavior of the computer code for this type of physics and thus to evaluate the accuracy of results that can be achieved. In our validation, the CFD results were compared with experimental values that were obtained specifically for this validation study.

These comparisons have thus helped to refine the methodology as it was possible to identify the strengths and weaknesses of the code, and make adjustments as necessary.

Table 3. Different burning categories

	Categ. 1	**Categ. 4**
Rate of combustion in kg / h	< 0.80	> 3.5 Maxi- rate
Case	4 , 5	1 , 2 , 3

Tables 4, 5 and 6 summarize all the operating conditions presented in this study. The air flow distribution as input to the model is estimated as follows at the high burn category:

- 88% for the primary air,
- 12% for the secondary air.

Table 4. Calculation assumptions

parameters	**Assumptions**
State	steady-state
Fuel	Volatile composition
Flow of volatiles	evaluated experimentally (mass change of the wood logs)
Airflow	evaluated experimentally (from a molar balance using data from FTIR analyzer and chemical equations)

Table 5. Overall operating conditions

Inlet static pressure	0 Pa
Outlet static pressure	Variable natural draft
Turbulence intensity at the inlet	10%
Hydraulic diameter at the inlet	0.05 m
Turbulence intensity at the exit	10%
Hydraulic diameter at the exit	0.05 m
External Wall treatment (convective heat transfer type boundary condition) External emissivity External temperature	8 W/m² K 0.1 300 K

For each simulated case, a flow calculation must be done to adjust the natural draft in the chimney to meet the value of the overall equivalence ratio Φ. Therefore the Φ is set by changing the draft at the exit of the chimney to adjust the air feed rate and the fuel rate. The calculations are based on the detailed measurements done for the composition of combustion products and temperature distribution inside the combustion chamber. The results are compared with the experimental data to better understand the effects of temperature and Φ on the CO/CO_2 ratio.

Chimney draft (outlet pressure) varies within a range of 1.5 Pa (0.006 in H_2O) to 31.1 Pa (0.125 in H_2O). The fuel rate is evaluated experimentally (mass change of consumed wood logs), although only the gas phase is considered. The fuel volatile composition at the wood log boundary is listed in Table 6.

Table 6. Composition of Volatiles at wood log boundary

Gas	CO	H_2	H_2O	CH_4	CO_2	C_2H_4	C_2H_2
Vol %	36.3	23.6	16.0	15.4	6.1	1.7	0.9

5. RESULTS AND DISCUSSIONS

Table 7 shows the different operating conditions simulated throughout this work. Five (5) cases were selected for the validation of the numerical model. For all cases, calculation times are approximately two days in a parallel computer using 32 cores.

Table 7. Operating conditions

Operating conditions	**1** HB 100 % open	**2** HB 100% open	**3** HB 100 % open	**4** LB 20% open	**5** LB 20% open
Fuel(kg/s)	0.0025	0.001	0.0004	0.0115	0.0074
Air(kg/s)	0.022	0.011	0.009	0.0012	0.0007
Φ	0.7	0.5	0.26	0.64	0.58
CO (%)	36.3	36.3	36.3	36.3	36.3
H_2 (%)	23.6	23.6	23.6	23.6	23.6
H_2O (%)	16.0	16.0	16.0	16.0	16.0
CH_4 (%)	15.4	15.4	15.4	15.4	15.4
CO_2 (%)	6.1	6.1	6.1	6.1	6.1
C_2H_2 (%)	1.7	1.7	1.7	1.7	1.7
C_2H_4 (%)	0.9	0.9	0.9	0.9	0.9

(HB: 100% open air inlet and LB: 20% open air inlet)

Table 8. Predicted and experimental results

Case	Predicted T (℃) at symmetric plane	Experimental T (℃) at symmetric plane	Predicted Ratio CO/CO_2 at exit plane	Experi-mental Ratio CO/CO_2 at exit plane
1	652	742	1.5	0.125
2	786	730	0.059	0.08
3	442	491	0.292	0.03
4	616	591	1.44	0.2
5	574	594	0.3	0.07

In order to verify the accuracy of this model, simulation results are compared with experimental values tested in Combustion laboratory at Université Laval under the corresponding conditions. The temperature distributions in the combustion chamber are in accordance with the experimental measurements. Calculated temperatures are of

the same order of magnitude as the measured values and taking into account the overall mechanism for the simplified combustion model, the differences are acceptable as seen in Table 8. The simulated flame shape for most cases was found conform to experimental observations as seen on Figs. 7 to 9. Numerical modeling reproduces reasonably well the physical phenomena occurring in the combustion chamber for temperature as shown in Fig. 7 to 9, for aerodynamics in Fig. 12, and for chemical species in Figs. 10 and 11. Aerodynamics shown in Fig 12 were validated from experimental observations. Velocity measurements are planned in future work. Numerical results are in acceptable agreement with the experimental data and Fig. 6 shows the comparisons between predicted and experimental temperatures versus the Φ at the central plane of the combustion chamber.

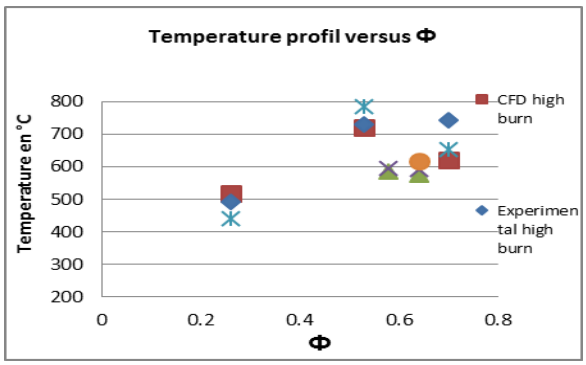

Figure 6. Comparisons between predicted and experimental temperatures versus the (Φ)

As for the CO/CO_2 ratio, it is clear that CO is produced right in the primary zone around the logs and it burns incompletely in the secondary area as you see at Figs. 10 and 11. According to experimental data, the calculation returns a high ratio results. The predicted CO/CO_2 ratio is not of the same order of magnitude as the experimental data. The high CO/CO_2 ratio seems to be caused by the fact that the distribution of volatile species was obtained from a generic correlation, not specific for the wood used in the present experiments. Also, the CO/CO_2 ratio must be better understood to explain the char combustion mechanism. During char combustion, the CO_2 and CO produced in primary zone result from heterogeneous reactions.

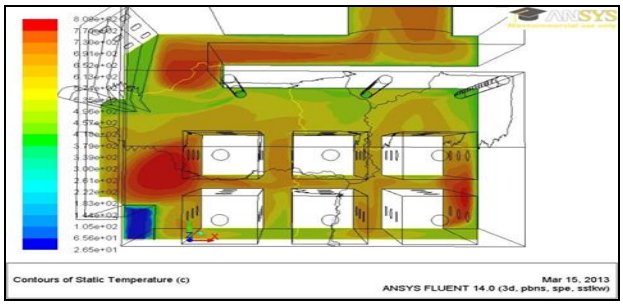

Figure 7. Validation cat. 4, temperature contour at the central plane

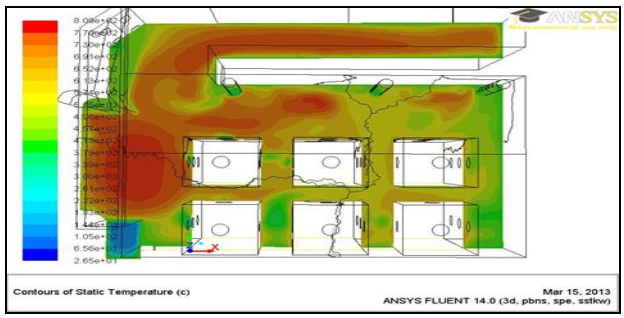

Figure 8. Validation cat. 4, temperature contour near the wall

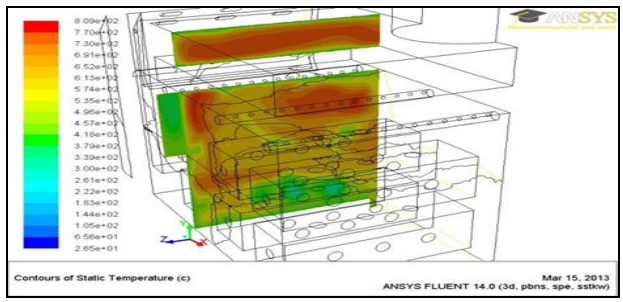

Figure 9. Validation cat. 4, temperature contour between two log

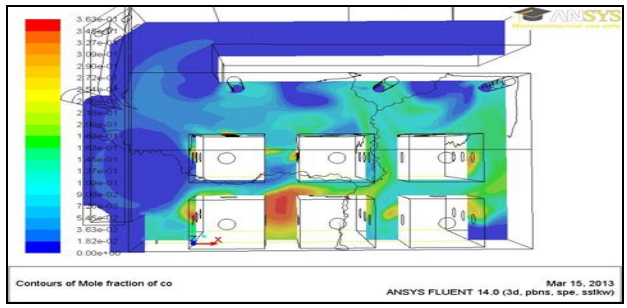

Figure 10. Validation cat. 4, CO contour at the central plane

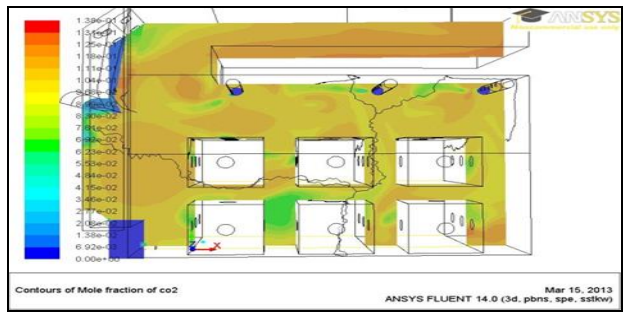

Figure 11. Validation cat. 4, CO_2 contour at the central plane

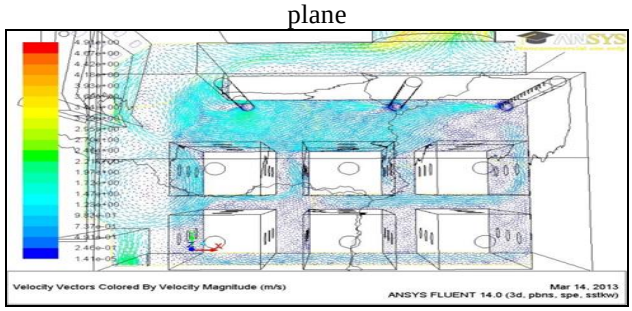

Figure 12. Validation cat. 4, velocity field at central plane

As well for the high combustion, we can reasonably conclude that the CFD results are acceptable and in good agreement with experimental measurements at a low combustion regime also. The difference could certainly be the result of the simplifying assumptions: a) considering only the gas phase and b) also considering a global reaction mechanism. The combustion of solid biomass is a multi-step process: gasification, pyrolysis, heterogeneous phase and homogeneous phase. The CO/CO_2 ratio for the heterogeneous reactions for biomass combustion will be investigated in future simulations, including the effect of homogeneous reactions. The Eddy Dissipation Concept (EDC) model deserves to be further tested in future work in order to reflect more accurately the high number (at least 40 equations) of chemical reactions involved in the combustion process [12] and [13]. The three-dimensionality of the present model would allow for design changes to include geometrical modifications and/or alterations in the operating and boundary conditions and capture their effects numerically. This allows the model to be used for analysis and optimization of existing wood stoves and to study new designs with corresponding operating conditions in reasonable turnaround times, regardless of the geometrical complexity of a combustion chamber.

6. CONCLUSIONS

The CFD model was calibrated and validated using operating conditions and experimental measurements available in the Combustion Laboratory at Université Laval. Numerical results are in acceptable agreement with the experimental data. The CFD model is capable of describing the fluid dynamics and chemical processes taking place in the overall combustion process, capturing known phenomena like air velocity, temperature distribution and chemical species concentrations. However, since the model was developed in the framework of a commercial code, it can also handle more complex geometries and operating boundary conditions. Therefore, it can be used for the analysis and optimization of existing stove and for relatively quick evaluations of new designs. In future works, the combustion of solid biomass will be taken into consideration knowing that is generally assumed to be a multi-stage process (drying, gasification/pyrolysis, homogeneous combustion of the released volatiles, and heterogeneous combustion of the char residue). The CO/CO_2 ratio of the heterogeneous reactions for biomass combustion will also be investigated in the future, including the effect of the homogeneous reactions.

The integration of this multi-step model in an accurate and stable manner with moderate computational requirements will be one of the next ambitious steps. Furthermore, a model for the generation of NOx-emissions from fuel-N using several precursor species would be introduced.

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