

SIMULATION OF BIOMASS GASIFICATION IN FLUIDIZED BEDS USING COMPUTATIONAL FLUID DYNAMICS APPROACH

by

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A model was developed for the simulation of physical and chemical processes occurring during biomass gasification inside a fluidized bed. The commercial CFD software "FLUENT" was employed for the description of turbulent fluid flow, heat transfer, species transport, devolatilization and particle combustion and gas phase chemical reaction. The emulsion phase of the fluidized region was modeled as a porous region, while stationary "free" areas were prescribed to account for the rising gas pockets (bubbles) inside the bed. Available experimental measurements were used for model setup and validation of the calculations, in terms of species mass fractions and temperature at the gasifier outlet.

Introduction

Biomass is attracting increasing attention for power generation and it is estimated that in the next decades its share in energy production will significantly increase worldwide. It is considered a renewable energy source, extracted from a natural sustainable process, *e. g.* crops, and also has a neutral effect on the total CO₂ balance. In the European Union as a whole, during 1997 the energy production from biomass reached a total of 52309 Ktoe¹, contributing to the 63.7% of the total renewable energy sources. The target of the European Union for year 2010 is to double the contribution of the renewable energy sources from the present 6% to 12% of the total energy consumption. Hence, due to the increasing interest in biomass as a major fuel source, analogously appreciable research is under way.

The present work concerns biomass gasification in fluidized beds, in order to produce a mixture of "clean", combustible gases (*e. g.* CH₄, H₂), which may be driven to a post-combustor for energy/heat production. The whole process is confined into a fluidized-bed type vessel of upright cylindrical shape, where air is supplied from its bottom and biomass particles are fed into the emulsion phase by a worm-screw conveyor system. First the biomass undergoes a drying process, where its water content is removed, then devolatilization and finally surface combustion.

Certain assumptions were adopted during the modeling of the gasifier, mainly based on empirical aspects of fluidized bed theory ². Measurements conducted by the Farm Structures Lab. of the Agricultural University of Athens ³ were used for defining a number of operating conditions and simulation parameters, as well as for results validation. The calculations applied the gasification model of ⁴ for the description of the Firing Pyrolysis (FP) and the Char Reduction (CR) zones. All assumptions and models were fed into the commercial Computational Fluid Dynamics (CFD) code FLUENT5 ⁵, with which the simulation was performed.

Model setup

Geometry configuration

Figure 1a shows the exact (as in the experiments) and modeled geometry of the gasifier, while Fig. 1b is the corresponding close view of the air inlet region. The gasifier is a cylindrical vessel composed of three parts: the main reactor (height = 0.8 m, diameter = 0.3 m) where the fluidization and the majority of chemical reaction take place, an intermediate conical part (height = 0.1 m, diameter = 0.3/0.6 m) and the freeboard region (height = 1.2 m, diameter = 0.6 m).

Air is blown through a network of horizontal pipes that cross the gasifier near its bottom. The pipes are of 0.0254 m diameter and employ 84 holes of 0.003 m diameter in a cross-formation around the pipes' perimeter. For meshing economy reasons the pipes were modeled as plane circular holes at the gasifier bottom of 0.006 m diameter, each one

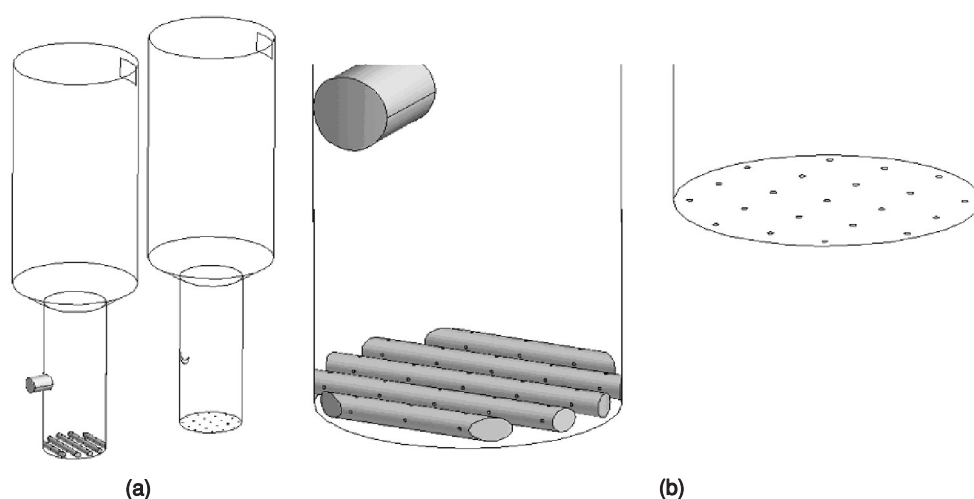


Figure 1. Geometry configuration of the biomass gasifier
(a) Total view; (b) Air inlet close-up

accounting for the joint effect of the group of four holes located around the feeding pipes, having the same area. The worm-screw conveyor system, with diameter 0.08 m, with its axis located 0.39 m above the bottom of the gasifier, was replaced by an inlet moon-shaped face, since the biomass particles before they are pushed into the emulsion adjust to that shape under the influence of gravity. The quadrilateral face observed at the top of the gasifier's side wall (0.1 × 0.2 m) is the gases outlet, through the sampling section, to the atmosphere.

Biomass & air fluxes

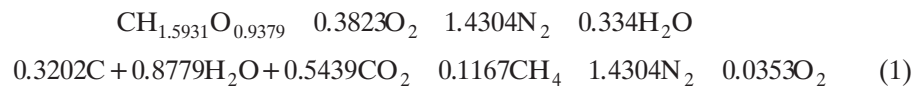
The experiments were conducted with two types of biomass; eucalyptus and miscanthus, their proximate and ultimate analysis, as well as their HHV and other properties are given in 3 . The simulations were performed for eucalyptus (water content = 15% mass, density 700 kg/m³), which was fed at a rate of 50 kg/h, while air was blown at 65 kg/h, preheated at 350 °C 5 . The exhaust gases measurements are shown in Table 1.

Table 1. Mass fluxes of exhaust gases in kg/h

Gas	H ₂	O ₂	CO	CO ₂	CH ₄	N ₂	H ₂ O	(Ash/tar)
Mass flux	0.2093	1.4080	14.4965	22.6796	3.0418	49.9500	16.2526	(6.6248)

Gasification model

Biomass gasification is described by the model of 4 . First the biomass enters the FP zone, where it is converted in char and volatiles very fast. The latter react with O₂ and char, CO₂ and H₂O is produced and part of the volatiles is cracked into CH₄. FP zone is dominated by exothermic reactions. The model assumes that no CO and H₂ are produced. The overall reaction for eucalyptus (regarding its composition, water content and the input streams of biomass and air) is written in molar form as:



Then, in CR zone, endothermic reaction dominate and the thermal energy produced by the pyrolysis-combustion process in the FP zone is transformed into chemical energy of combustible gas species, such as H₂ and CO, according to the following major reactions:





Fluidized region

Although the commercial CFD code employs a specialized model for solid-gas flows (granular multiphase model), the available computer resources for this three-dimensional (3D) turbulent flow that also includes chemical reactions forced the adoption of a more "engineering" approach to model the existence of the fluidized region. The latter was taken as an isotropic porous medium (emulsion phase), while also "free" spherical volumes were prescribed, accounting for the presence of the rising bubbles.

The solid material used in the experiments was rounded quartz sand of sphericity, $\phi_s = 0.86$, and mean diameter, $d_p = 250 \mu\text{m}$ and density $= 1600 \text{ kg/m}^3$, which falls into the Group B of Geldart classification [2]. For minimum fluidization conditions the porosity is $\varepsilon_m = 0.43$. The pressure losses in the emulsion phase are described by [6] for porous media of such type, according to:

$$\frac{\Delta P}{\Delta x_i} = \frac{\mu}{\alpha} U_i + \frac{1}{2} C_2 \rho U_i^2$$

where

$$\alpha = \frac{d_p^2 \phi_s^2}{150} \frac{\varepsilon_m^3}{(1 - \varepsilon_m)^2}, \quad C_2 = \frac{3.50}{d_p \phi_s} \frac{(1 - \varepsilon_m)}{\varepsilon_m^3} \quad (3)$$

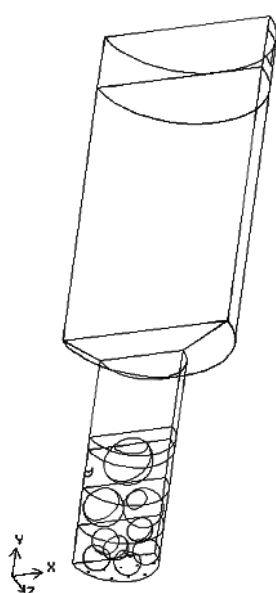


Figure 2. Bubble modeling

where μ = gas viscosity kg/m/s , ρ = gas density kg/m^3 , U_i = gas velocity component in the i -direction m/s , and x_i = coordinates ($i = 1, 2, 3$ for a 3D problem) m . eq. (3) return $\alpha = 7.5412 \cdot 10^{-11} \text{ m}^2$ and $C_2 = 1.1671 \cdot 10^6 \text{ m}^{-1}$, which were fed into FLUENT's porous model.

The analysis above concerns the emulsion phase, *i. e.* the fluidized region except the rising bubbles. The latter were modeled as open spheres, according to an empirical model of [7]. As the present case falls within the bubbling fluidized beds, a model, based on available empirical relations [2], was devised by [7] in order to calculate inside the fluidization region the bubble diameter and rising velocity as a function of the height from the air injection location. For this purpose the whole fluidized region was divided in 4 horizontal slices, where different diameter, rising velocity and turbulence levels were prescribed for the bubbles. The arrangement of the bubbles is shown in Fig. 2, where it is obvious that the bottom slice employs small bubbles, while the top one (as

the rising bubbles coalesce) only a big one. It must be noted that the bubble formation is a transient phenomenon, which however was modeled as a time-averaged equivalent. The empirical method does not violate the overall mass balance of the initial sand load and returns the correct local value of the emulsion voidage, as given by the empirical relations of 2 . Note that although the bubble volumes are fixed in space, they possess a rising velocity, which appears as a momentum source term in the mixture momentum equations. The total height at steady operation was found 0.4975 m, compared to the initial 0.32 m for normally packed bed conditions.

Gas phase governing equations

Fluid (gas) turbulent flow is described by the steady, 3D, Reynolds-averaged form of the Navier-Stokes equations (continuity and momentum), combined with the standard $k-\varepsilon$ model of turbulence 8 . In the momentum equations source terms were prescribed in order to incorporate the flow resistance described by eq. (3) and the interaction between the biomass particles and the gases. The energy equation is also solved for the gas phase, taking into account source/sinks terms due to chemical reactions in the gas, as well as in gas-solid phase .

Finally, transport equations are solved for all gas species of Table 1, accounting for mass sources/sinks due to gas-phase reactions, as well as for mass addition released from the biomass particles. Also, the gas-phase reaction (2d) was set into the code with its coefficients taken from FLUENT's database.

Dispersed phase equations

While all previously mentioned equations are solved in an Eulerian reference frame, the history of the biomass particles is calculated according to a Lagrangian one. Their motion is described by:

$$\frac{dU_{p,i}}{dt} = F_D(U_i - U_{p,i}) - g_i \frac{\rho_p - \rho}{\rho} - F_i, \quad \frac{dx_i}{dt} = U_{p,i} \quad (4)$$

where U_i and $U_{p,i}$ = particle and gas velocity respectively, t = time, g_i = gravitational acceleration, ρ_p = particle density, and F_i = other forces (subscript i denotes the i -direction, hence eq. (4) can be written separately for the three co-ordinates). The first equation is a momentum balance, while the second calculates the position of the particle as it moves inside the main (gas) phase. F_D accounts for the drag force exerted on the particle moving at a relative velocity $(U_i - U_{p,i})$ in the gas phase and is calculated by appropriate empirical relations for spherical bodies 8 , depending on the Reynolds number. F_i stands for the virtual mass and pressure gradient force 8 . All forces appearing in eq. (4) enter the gas phase momentum equations as source terms with opposite sign, enabling the coupled calculation of the dispersed-main phase interaction.

As for the thermal and chemical processes occurring on the dispersed phase (biomass), a number of particle laws is offered by FLUENT, which are sequential as the particle moves in the gas phase. In the present work the droplet and combustible particle types were selected, to simulate the water content evaporation and devolatilization/surface combustion, respectively. First, both types undergo the inert heating law, where they are heated up (heat exchange with the hot gas phase) to a prescribed temperature (300 K for droplets, 400 K for combustible) before the next law begins. For the droplet type the next law is the droplet vaporization which is followed by droplet boiling, when the boiling point is reached (373.15 K). Boiling stops when all liquid water has changed phase. For the combustible type, the second law is the devolatilization, where the volatile matter of the biomass enters the gas phase according to the constant rate kinetic model. When all volatile mass is consumed, surface combustion is initiated according to an Arrhenius expression for the reaction kinetics. If all combustible matter is consumed, the particles (ash) return to inert heating law. The kinetics of the reactions (2a) to (2c) were taken from FLUENT's database.

Devolatilization was used to model the gas release described by eq. (1) during the biomass gasification inside the FP zone, *i. e.* appropriate volatile matter was prescribed to be released in the form of CO_2 and CH_4 . During all laws, both for droplet and combustible type, energy is also consumed/created. Mass and thermal energy terms enter the gas phase species and energy equations, respectively, as sources with opposite sign, enabling the coupling between the main and the dispersed phase. The various properties, variable values and empirical constants required for the implementation of the dispersed phase calculation are described in 7.

Numerical mesh, boundary conditions and material properties

The simulations were performed for steady state operations, and due to geometrical and flow symmetry only one half of the domain was calculated. Figure 3 displays the surface mesh of the gasifier, as well as a close view of the volume mesh inside the fluidized region. In total, the computational cells were 22085 (6302 hexahedral, 15461 tetrahedral and 142 pyramids).

At biomass and air inlets the mass flow rate was prescribed, while at gases' exit atmospheric pressure level was assigned. At the walls their materials (steel and insulation) and corresponding thicknesses and heat conduction coefficients were prescribed, as well as the ambient temperature conditions (25°C).

All materials (gas species, solid biomass particles) were assigned appropriate properties from standard thermodynamic tables. The properties of the gas species (density, ρ , viscosity, μ , thermal conductivity, k , specific heat capacity, C_p) were allowed to vary with local main phase temperature and the mixture's effective value was calculated from its local composition and available FLUENT laws (ideal gas law for ρ and mass-weighted mixing law for μ , k and C_p).

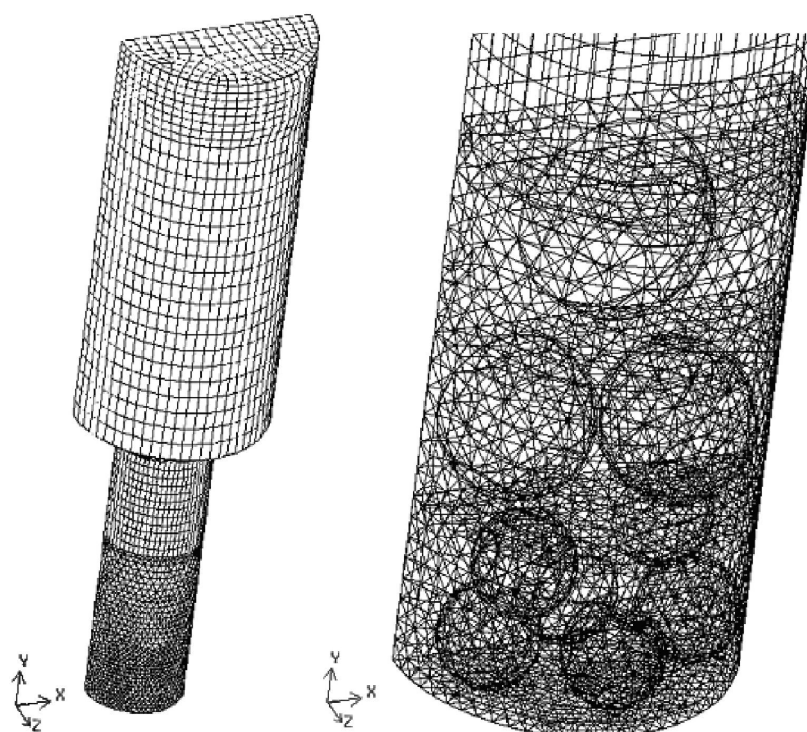


Figure 3. Surface and volume computational mesh

Results and discussion

Table 2 shows the measured and computed exhaust gases' composition. Their exit temperature was found 1068 K, in reasonable agreement with experiment 3 ($\cong 700\text{--}750^\circ\text{C}$). The major disagreement is found in the fractions of CO and CO₂. The numerical model overestimates the produced amount of CO and consequently underestimates the CO₂ one.

Table 2. Measured and computed mass fractions of exhaust gases

Gas	H ₂	O ₂	CO	CO ₂	CH ₄	N ₂	H ₂ O
Measured	0.001931	0.012992	0.133765	0.209273	0.028068	0.460890	0.149967
Computed	0.002078	0.012981	0.209930	0.131203	0.024324	0.460521	0.155853

Figure 4(a) shows the main phase path lines, initiated from the air inlets at the gasifier bottom, while Fig. 4(b) the flow field in the form of velocity vectors (at two planes at 30° and 150° with respect to the symmetry plane). The flow pattern exhibits a degree of distortion due to the interchange between emulsion (porous medium; high flow resistance) and the bubbles (zero flow resistance; free volumes). In Fig. 4(c) the particle

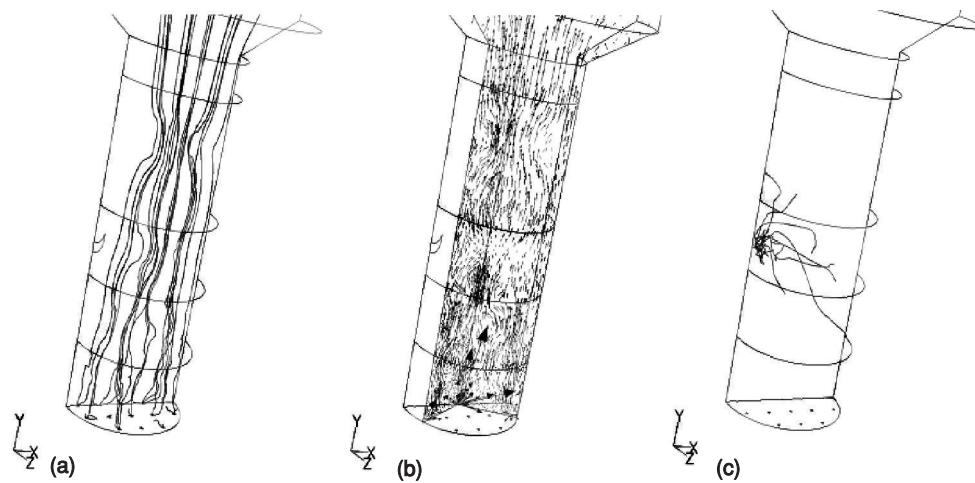


Figure 4. (a) Gas phase path lines; (b) Gas phase velocity vectors; (c) Dispersed phase droplet paths

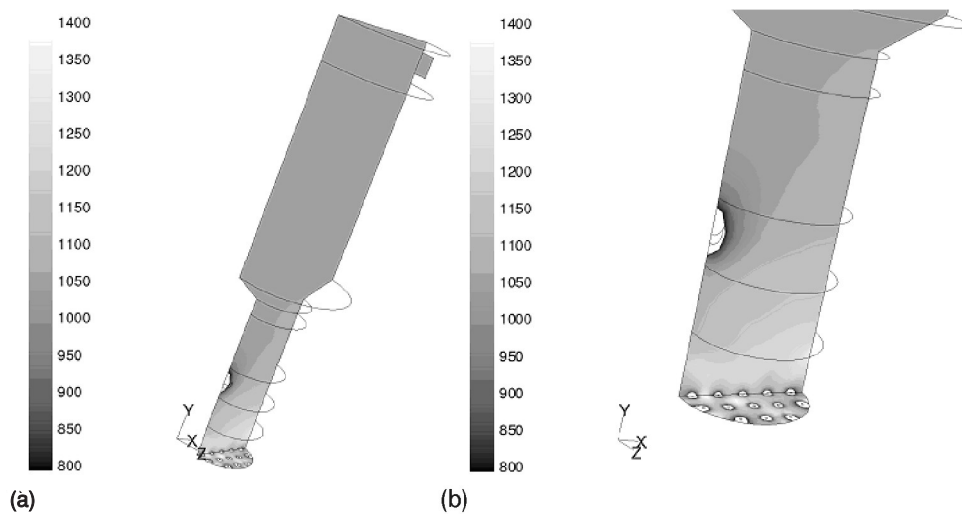


Figure 5. Temperature contours

tracks of the droplet injection (modeling the moisture content of the biomass solids) are shown. Their tracks are terminated very fast (all fluid phase is evaporated) after their entering in the gasifier, as the gas temperature is considerably high (Fig. 5) and the droplets are quickly heated up and evaporated. The "random" shape of the droplet trajectories is due to a statistical tracking model of FLUENT that was used to better describe their turbulent and stochastic nature. In essence, the particles are not expected to follow the same geometrical routes every time they are injected into the flow field, they rather follow a scattered (around a time-mean path) route which is determined by a random number generator determined by the local turbulence levels.

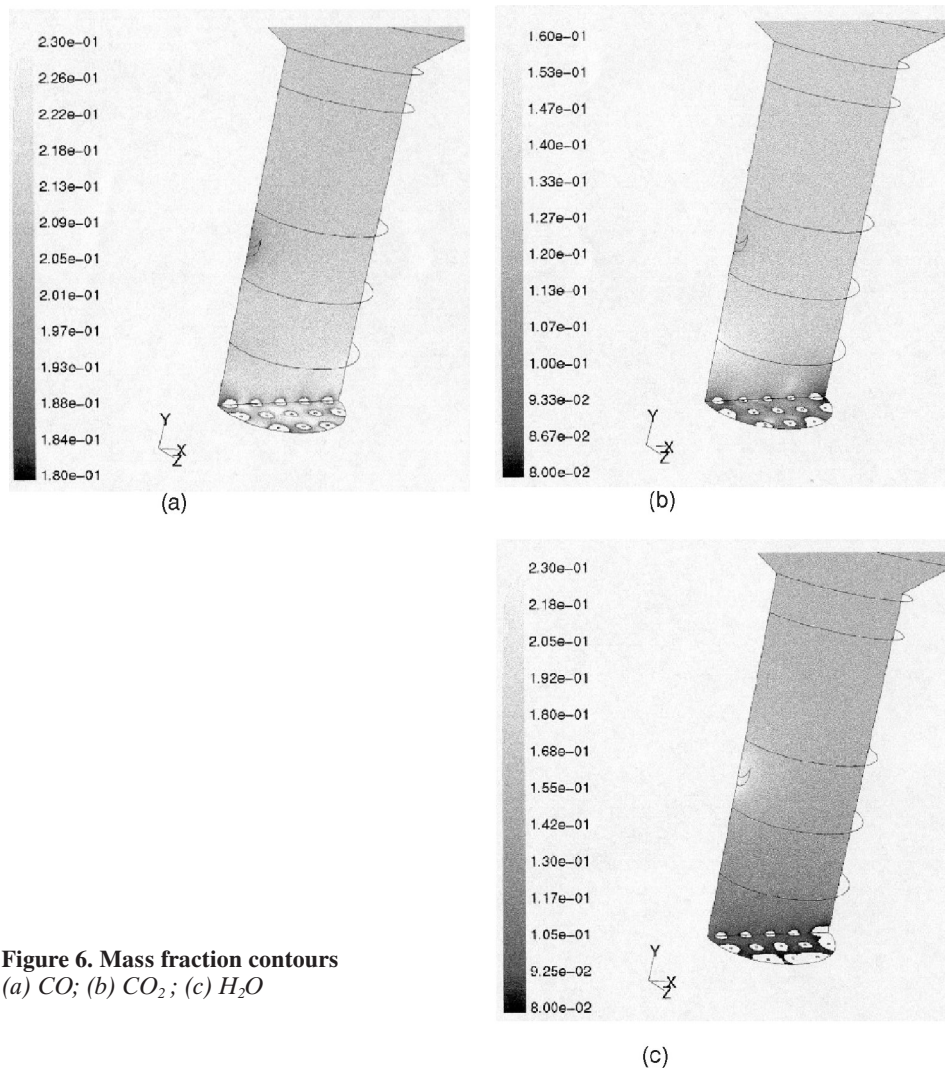


Figure 6. Mass fraction contours
(a) CO ; (b) CO_2 ; (c) H_2O

The temperature field is presented in Fig. 5(a) (whole view) and 5(b) (close view of the fluidized region). Note that the "empty areas" denote values outside the plotted range (limited for clarity reasons). Near the biomass and air inlets the temperature employs its minimum values, as the gases are cooled by the colder input fluxes. The highest temperatures are detected near the bottom of the reactor, where the reaction rates exhibit their higher values and the exothermic reactions are very intense due to high O_2 concentration. The overall field shows, except near the gasifier bottom, uniformity in the horizontal directions, while a certain temperature variation is noticed along the gasifier's height. Above the fluidized region, temperature remains up to the exit almost constant ($\approx 1100\text{ K}$), due to negligible reaction rates and efficient wall insulation.

Finally, Fig. 6 shows the contours of the CO , CO_2 and H_2O mass fractions in the gas mixture (see above note for "empty areas"). The higher values for CO are located immediately above the air inlets, while for CO_2 , at a greater height. Both gases acquire their exit values (Table 2) very quickly, below the freeboard area. H_2O values are large near the biomass inlet (see Fig. 4c), its production inside the intense reaction zone results in reduced concentrations and obtains its exit value immediately above the biomass inlet.

Conclusions

Biomass gasification process is a very complex and difficult case for numerical investigation, as it entails multiphase flow, turbulent dynamics, heat transfer, species transport and chemical reactions. Its numerical simulation with commercial CFD code FLUENT entailed several assumptions in order to arrive at practical modeling approach for this complex and demanding problem.

The numerical results show a satisfactory agreement with experimental evidence, considering the adopted engineering simplifications that were made to the problem. Yet, several issues were proven to require further elaboration and research. For instance, the biomass particle trajectories are by no means representative of the real situation, as the effect of solid-to-solid interaction (sand-to-biomass) was ignored by the modeling of emulsion phase as a porous medium. Also, due to data unavailability, certain modeling parameters were adopted by the corresponding measurements.

On the other hand the simulation produced fast and reasonably accurate results of practical use for biomass gasification design. CFD simulations are nowadays easy to perform and when sufficiently validated through experimental data become a powerful design and optimization tool. When industrial application is concern, accurate simulation tools may be safely utilized for scaling up purposes.

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