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Development of Euler-Lagrangian Simulation of a Circulating Fluidized Bed Reactor for Coal Gasification

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Abstract

A Computational Particle Fluid Dynamics (CPFD) model based on the Multiphase Particle in Cell (MP-PIC) approach is used for Shubarkol coal gasification simulation in an atmospheric circulating fluidized bed reactor. The simulation is developed on a basis of experimental data available from a biomass gasification process. The cross-section diameter of the reactor riser is 200 mm and the height is 6500 mm. The Euler-Lagrangian simulation is validated using experimental data available in the literature and also compared with an Euler-Euler simulation. The gasification reactions kinetics model is improved, and homogenous and heterogeneous chemistry are described by reduced-chemistry, with the reaction rates solved numerically using volume-averaged chemistry. The simulations reveal gas composition, temperature, and pressure interdependencies along the height of the reactor. The product gas composition compares well with the experiment and the temperature profile demonstrate good consistency with the experiment. The developed model is used for a case study of Shubarkol coal gasification in the circulating fluidized bed reactor.

1. Introduction

Gasification is a conversion process when solid carbonaceous fuel is combusted under oxygen deficiency conditions and process is limited to intermediate gaseous products, consisting of carbon monoxide (CO), hydrogen (H_2), methane (CH_4), carbon dioxide (CO_2) and minor fractions of methane homologues, and tars. Gasification is considered a clean and efficient process that allows conversion of solid fuels to a synthesis gas which can be used in a wide variety of applications, such as in furnaces, boilers, turbines, internal-combustion engines. It also can be converted to liquid fuels, or converted to substitute natural gas. Fluidized bed gasifiers exhibit higher efficiencies and better feedstock flexibility due to the better heat and mass transfer ability [1].

The objective of this study is to develop a comprehensive three-dimensional numerical Eulerian-Lagrangian simulation of circulating fluidized bed (CFB) riser where first biomass is gasified and then Shubarkol coal gasification case study is conducted. The model describes the gas-solid flow on a basis of Eulerian-Lagrangian multiphase particle-in-cell (MP-PIC) approach, which allows the simulation of two-phase flows at affordable computational cost. Eulerian-Lagrangian models track each individual particle or particle clusters, making it possible to simulate particle size distribution and changes in physico-chemical properties [2]. Devolatilization kinetics and reaction rates are described through the Arrhenius expression. Homogeneous and heterogeneous reactions are solved with volume-average chemistry on an Eulerian grid. The data for validation of the model is taken from gasification of leached olive oil waste [3].

2. Description of mathematical model

2.1. Governing equations for gas phase

In this article a comprehensive 3D computational fluid dynamics (CFD) model using the Eulerian-Lagrangian approach is developed to simulate Shubarkol coal gasification in CFB reactor.

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Olive oil mill waste (orujillo) gasification experiment is chosen as a reference case for validation of the simulation. The method uses Eulerian equations to describe the compressible continuous gas phase and the stochastic particle method for the particle phase [4]. The computational particle fluid dynamics (CPFD) solution method solves the fluid and particle equations in three dimensions. The discrete particle phase with the particle size distribution is modelled by the Liouville equation. [4]. Gas phase continuity, gas phase momentum, momentum exchange between particles and gas phase, particle acceleration, solid phase momentum, particle volume fraction, interparticle stress equations can be found elsewhere [4, 5]. Previous studies demonstrated that the Wen-Yu and Ergun models combine adequately to predict multiphase fluid dynamics in CFB reactor [6–8].

2.2 Chemical reactions model

When fuel particles are introduced into the reactor, they undergo fast heating pyrolysis. The physico-chemical properties differ greatly among coals and other types of fuels. The rate of devolatilization is described by the Arrhenius expression. The model assumes that all volatile content fully converts to gases. Orujillo devolatilization kinetics pre-exponential factor A is 99.0 s^{-1} and activation energy E is 11.14 kj/mol. The reaction temperature exponent is set to -1.2, ms to 1510, and C_1 to 1 [9]. In case of Shubarkol coal pre-exponential factor A is set to 0.15 s^{-1} and activation energy E is set to 17.53 kj/mol, reaction temperature exponent is set to -3.9465.

Chemical reactions are formulated as stochiometric equations with rate coefficients based on the Arrhenius law [3]. Reaction rate coefficients for homogeneous and heterougeneous reactions are given in Table 1. T is the reaction zone temperature between solid phase and gas phase, which is assumed as the average temperature between solid and gas phases. Solid particle concentration is expressed as solids mass per volume, $m_s = \rho_s \theta_s$ [4].

3. Model setup

3.1. Reactor description

The experimental data for this study reference case are taken from gasification of leached orujillo (olive oil waste) [3]. The CFB gasification reactor is an atmospheric air-blown installation. The reactor consists of riser, cyclone, standpipe, and a loop seal. In order to reduce computation time, the model is simplified to a three-dimensional riser section. The total height of the reactor is 6500 mm, with fluidized bed reactor diameter 200 mm. The fuel is injected into the reactor from a port with 100 mm diameter and 370 mm above the bottom of the riser.

Table 1
Homogeneous and heterogeneous reaction rates [4, 10]

Stoichiometric equation	Kinetic reaction rate expression, mol $m^{-3}s^{-1}$
$C(s) + H_2O \rightarrow CO + H_2$	$R_0 = 1.272\ m_s\ Texp\ (-22.645/T)\ [H_2O]$
$CO + H_2 \rightarrow C(S) + H_2$	$R_1 = 1.044 \times 10^{-4}\ m_s T^2 exp\ (-6319/T-17.29)\ [CO]\ [H_2]$
$C(s) + CO_2 \rightarrow 2CO$	$R_2 = 1.272\ m_s Texp\ (-22.645/T)\ [CO_2]$
$2CO \rightarrow C(S) + CO_2$	$R_3 = 1.044 \times 10^{-4}\ m_s T^2 exp\ (-2363/T-20.92)\ [CO]_2$
$0.5C(s) + H_2 \rightarrow 0.5CH_4$	$R_4 = 1.368 \times 10^{-3}\ m_s Texp\ (-8078/T-7.087)\ [H_2]$
$0.5CH_4 \rightarrow 0.5C\ (s) + H_2$	$R_5 = 0.151\ m_s T^{0.5} exp\ (-13578/T-0.372)\ [O_2]$
$2C(s) + O_2 \rightarrow CO_2$	$R_6 = 4.34 \times 10^7\ \alpha_p T^{0.5} exp\ (-13590/T-0.372)\ [O_2]$
$CO + H_2O \rightarrow CO_2 + H_2$	$R_7 = 7.68 \times 10^{10}\ Texp\ (-36640/T)\ [CO]^{0.5}\ [H_2O]$
$CO_2 + H_2 \rightarrow CO + H_2O$	$R_8 = 6.4 \times 10^9\ Texp\ (-39260/T)\ [H_2]^{05}\ [CO_2]$
$CO + 0.5O_2 \rightarrow CO_2$	$R_9 = 5.62 \times 10^{12}\ Texp\ (-16000/T)\ [CO]\ [O_2]$
$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2$	$R_{10} = 3.552 \times 10^{11}\ T^{-1}\ exp\ (-15700/T)\ [CH_4]\ [O_2]$
$H_2 + 0.5O_2 \rightarrow H_2O$	$R_{11} = 1.63 \times 10^{11}\ T^{-1.5}\ exp\ (-3430/T)\ [H_2]^{1.5}\ [O_2]$
$C_2H_4 + O_2 \rightarrow 2CO + 2H_2$	$R_{12} = 1 \times 10^{12}\ T^{-1.5}\ exp\ (-20818.3/T)\ [H_2]^{1.5}\ [C_2H_4]\ [O_2]$
$CH_4 + H_2O \rightarrow CO + 3H_2$	$R_{13} = 3.0 \times 10^5\ exp\ (-15042/T)\ [CH_4]\ [H_2O]$

Table 2
Proximate and ultimate analysis of fuel [3, 9]

	Leached orujillo	Shubarkol Coal		Leached orujillo	Shubarkol coal
Proximate analysis (wt%, dry basis)			Ultimate analysis (wt%, dry ash free)		
Volatile matter	74.4	40.3	C H	52.7 7.2	70.93 5.05
Fixed carbon	17.1	51.3	N S	1.6 0.07	1.81 <0.01
Ash	7.7	2.44	Cl	0.37	
Lower heating value (LHV)	18.5 Mj/kg	26.97 Mj/kg	O	38.1	22.19

Table 3
Particle size distribution of fuel particles [10]

size (mm)	0.10	0.25	0.35	0.50	1.00	1.41	2.83	5.00
cumulative (%)	0.00	1.90	2.40	3.10	6.20	12.00	94.60	100.00

Table 4
Composition of gases evolved from volatile matter

Gas species	CO_2	CO	CH_4	C_2H_4	H_2	Benzene
Leached orujillo [12]	29.0	46.2	16.2	5.3	1.3	2
Shubarkol coal [11]	31.1	46.8	17.9	4.2	0	0

3.2. Grid characteristics

The reactor domain has been discretized using a uniform Cartesian grid. The reactor grid is built and simulated in CPFD Barracuda. The grid is built uniformly, to investigate grid independence, three grids were created with 10692 cells for coarse grid, 21060 cells for medium grid, and 42120 cells for fine grid. Each grid consists of hexahedral and tetrahedral cells, and grid independence tests conducted.

3.3. Materials

One of the distinctive features of Eulerian Lagrangian MP-PIC method is the capability to describe in detail fuel particle characteristics. Details that need to be defined are proximate analysis, ultimate analysis, released volatile composition, pyrolysis rate, and particle size distribution. Proximate and ultimate analysis of leached orujillo and Shubarkol coal are given in the Table 2. Particle size distribution is assumed to be the same as it was described by Gómez-Barea et al. [10], described in Table 3. Gas composition evolved from volatiles is given in Table 4.

3.4. Initial and boundary conditions

Initial conditions of the reference case simulation are initialized into the model to repeat exactly the operating conditions of the experiment [3]. Figure 1a illustrates initial conditions and boundary conditions of the model. It is assumed that the reactor is preheated to 500 °C and completely filled with air. The model has two flow boundary conditions that describe the air inlet and the fuel feed port. Air is introduced through a perforated plate located at the bottom of the reactor. In the first case fuel is biomass and in the second case Shubarkol coal. The simulation contains two types of particles, which includes sand and fuel. Sand particles are initialized to the bottom of the reactor, with close pack volume equal to 0.55.

4. Results and discussion

4.1. Flow patterns

Figure 1b displays the granular flow formation and its development. Fluidized bed flow patterns are displayed with colored particle volume fraction. Flow steady state conditions set after 0.7 s.

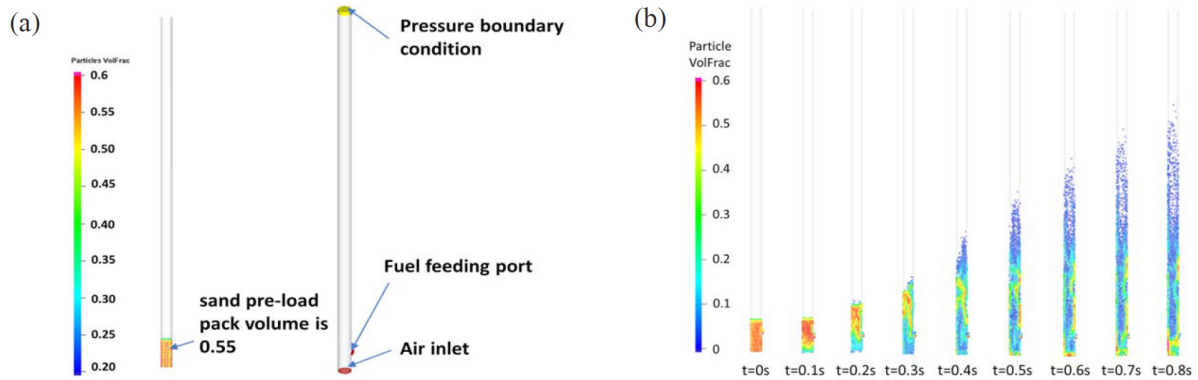

Fig. 1. (a) – Initial conditions and boundary conditions; (b) – onset of granular flow particle volume fraction.

Devolatilization of the fuel, combustion of volatiles, and combustion of pyrolysis products cause formation of bubbles above the fuel inlet.

4.2. Model validation

One of the most important characteristics of the fluidized bed combustion and gasification process is the reactor temperature. Reactor temperature influences chemical reactions kinetics and gasification products composition. Figure 2a demonstrates comparison of model simulations with three grid resolutions and their comparison with experimental measurements. Simulation with the fine grid having 42120 cells demonstrate satisfactory conformity with experimental measurements. Simulation results also demonstrate good conformity with experimental results.

4.3. Case study

Temperature profile of Shubarkol coal gasification simulation exhibits relatively stable temperature profile, reaching maximum at 850 °C (Fig. 3a). Overall air-to-fuel equivalence ratio during the case study is 0.35. At this equivalence ratio Shubarkol coal gasification produced gas with composition is given on Fig. 3b.

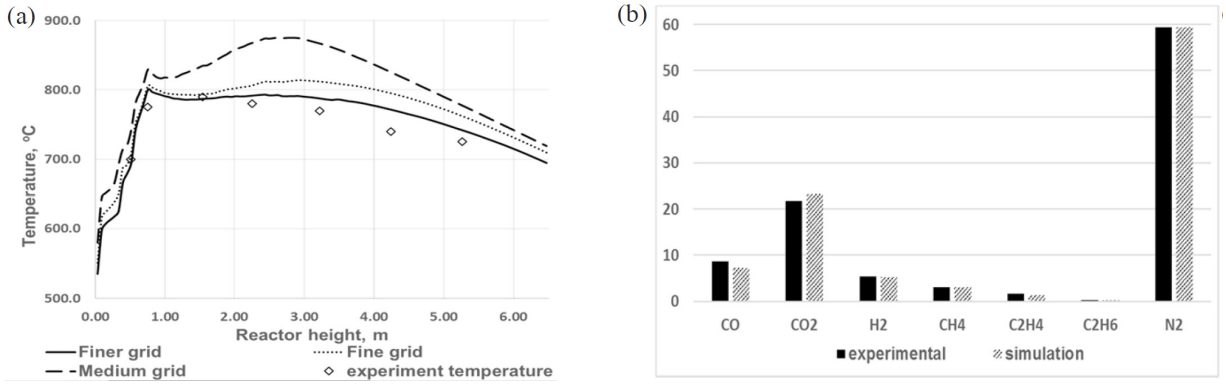

Fig. 2. (a) – Temperature profile of three simulations with coarse, medium and fine grid for grid independence test; (b) – experiment and simulation outlet gas composition.

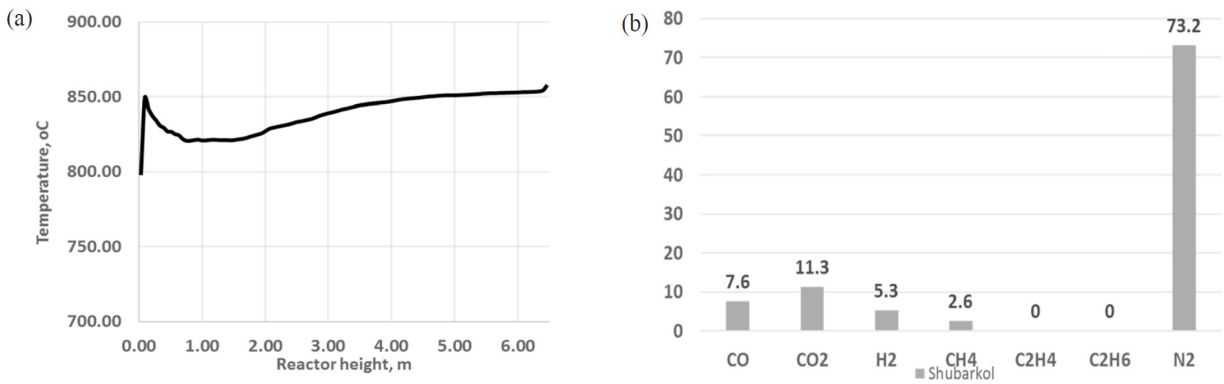

Fig. 3. (a) – Shubarkol coal gasification temperature profile along the length of the fluidized bed reactor; (b) – gas composition at the outlet from the reactor riser.

5. Conclusions

The CFB reactor simulation comprised complex multiphase flow, heat and mass transfer, and heterogeneous chemical reactions. The reaction model included devolatilization, combustion of released volatile gases and char particles. The uniformities of the temperature in the furnace and composition of evolved gases were analyzed and compared with the experiment in order to validate the model. Based on the validated biomass gasification simulation the Shubarkol coal gasification model was developed [11].

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