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Modelling of bio-oil steam gasification in a fluidized bed reactor

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ABSTRACT

This paper reports a three-dimensional CFD model for bio-oil gasification in a fluidized bed reactor. The model considered three-phase hydrodynamics, heat and mass transfer, bio-oil atomization, spray droplet vaporization and thermal decomposition in gas–solid flow. It employed a Euler-Lagrange method, in which gas and solid flow were solved using the Eulerian method and the bio-oil droplets were tracked using the Lagrangian approach. Droplet trajectory was calculated via equation of motion using discrete phase model in the Lagrangian frame, considering the interactions with flow field. Experimental data were obtained for bio-oil injection characteristics and simulations were conducted for generating the Rosin-Rammler distribution function under different injection conditions. As the droplets were injected into a fluidised-bed reactor, the depletion in bio-oil droplet size as a result of evaporation could not be described by the D^2-law due to the complex composition of bio-oil. Spray penetration into the reactor increased substantially with increasing droplet size. The predictions from the CFD model for bio-oil steam gasification were in good agreement with the experimental data available in the literature, in terms of cold gas efficiency (CGE) and syngas compositions at various bed temperatures, steam-carbon molar ratios and methane equivalent gas hourly space velocity (G_{C1}HSV) of feed. Sensitivity analyses on these key process parameters were also carried out.

1. Introduction

Biomass is considered as a renewable energy source for future sustainable development [1]. However, it has a high moisture content, a low energy density, being bulk and widely distributed so that direct utilisation of biomass is fundamentally limited to small scale [2]. These undesired fuel properties associated with biomass may be addressed via distributed biomass pyrolysis at 450–550 °C to convert biomass into high-energy-density bio-oil and biochar suitable for transport [2,3]. While biochar can be applied locally for soil amendment and carbon sequestration [4], bio-oil can be transported to centralised plants for centralised processing. One application is to use bio-oil as a feedstock for hydrogen production [5] via fluidized-bed steam gasification processes [6–9]. Previous studies were carried out on experimental investigations and thermodynamic equilibrium modelling on bio-oil steam gasification [10–12]. For those models, the predictions were for bio-oil conversion under thermodynamic equilibrium conditions hence may not agree well with the experimental results [13–18]. Therefore, the objective of this study is to develop a bio-oil gasification model based on computational fluid dynamics (CFD), considering atomization, hydrodynamics, heat and mass transfer and chemical kinetics in a fluidised-bed reactor. A series of simulations were carried out to evaluate the effect of key parameters on bio-oil gasification.

2. Methodology

Bio-oil gasification in a fluidised bed includes three phases of solid, liquid and gas and involves injecting bio-oil in the gas-solid fluidized bed. The CFD code was developed based on Eulerian-Eulerian multiphase flow approach which is of relatively low computational cost and suitable for fluidized-bed reactor [19,20]. The continuity and momentum equations apply for both phases with the equation of particles granular temperature. The Syamlal–O'Brien drag model was employed for predicting the hydrodynamic behaviour of gas-solid fluidized bed reactor [21]. The droplet flow field was examined by Eulerian-Lagrangian approach in which the fluids phase (the gas–solid flow) is treated as continuous and fuel droplets as discrete phase. The discrete phase model (DPM) was used for predicting droplet trajectory, considering interactions with the continuous phase in terms of momentum, heat and mass transfer. The droplet size distribution from atomisation was based on experimental data [22] and presented in terms of the cumulative frequency of mass distribution curve in the Rosin-Rammler format.

2.1. Conservation equations of flow field (continuous phase)

Continuous flow field can be modelled by Eulerian approach in a

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Nomenclature

A_d	Droplet surface (m^2)
B_M	Spalding mass transfer number
B_T	Spalding heat transfer number
c_p, c_v	heat capacity at constant pressure and volume ($J\,kg^{-1}\,K^{-1}$)
D_{ij}	mass diffusion coefficient of components i and j (m^2/s)
H	total enthalpy (energy/mass)
J	diffusion flux ($kg/(m^2s)$)
h	convective heat transfer coefficient ($W/(m^2K)$)
k	thermal conductivity ($W/(mK)$)
Le	Lewis number (ratio of thermal diffusivity to mass diffusivity)
m	Droplet mass (kg)
$\dot{m}$	evaporation rate ($kg\,s^{-1}$)
M	molecular weight ($kg\,kmol^{-1}$)
Nu	Nusselt number
P	pressure (Pa)
P_{vpr}	reduced vapour pressure
q	heat flux (W/m^2)
r	reaction rate (units vary)
Sh	Sherwood number
T	temperature (K)
$T_{r,i}$	reduced temperature of component i at actual temperature
$T_{br,i}$	reduced temperature of component i at boiling point
Y	mass fraction
$y_{i,s}$	mass fraction of species i at droplet surface
$y_{i,\infty}$	mass fraction of species i at free stream
$\sum_v$	diffusion volume
$\Delta H_{vb,i}$	latent heat at the normal boiling point
α	volume fraction
ρ	density (kg/m^3)
ε_i	fraction of vaporization rate for component i

Abbreviations

SMD	Sauter Mean Diameter
CGE	cold gas efficiency

Subscripts

i	species
s	solid
s	droplet surface
g	gas
d	droplet

fluidized bed reactor. The continuity, volume fraction, momentum and heat transfer equations, species transport and volumetric reactions are considered. The Syamlal–O'Brien drag model [23,24] is used for calculating drag forces and then fluid–solid exchange coefficient. The turbulence flow is simulated used the standard k–ε model [25]. The internal energy balance can be written for gas and solid phases as:

$$\frac{\partial}{\partial t}(\alpha_g \rho_g H_g) + \nabla.\,(\alpha_g \rho_g \nu_g H_g) = -\nabla.\,q_g + S_{hg} + Q_{sg} \tag{1}$$

$$\frac{\partial}{\partial t}(\alpha_s \rho_s H_s) + \nabla.\,(\alpha_s \rho_s \nu_s H_s) = -\nabla.\,q_s - Q_{sg} \tag{2}$$

The term S_{hg} in Eq. (1) considers the rate of energy transfer between bio-oil droplet and gas while $Q_{sg} = -Q_{gs}$ is the heat transfer rate between gas and solid phase, related to heat transfer coefficient (correlated to the particle Nusselt number) and temperature difference between gas and solid phases. In the case of granular flows the Nusselt number is determined by Gunn correlation [26]. The individual species transport equations need to be considered when there is mass transfer happen between bio-oil droplets and gas phase due to droplet vaporization.

$$\frac{\partial}{\partial t}(\rho_g Y_i) + \nabla.\,(\rho_g \nu_g Y_i) = -\nabla.\,J_i + R_i + S_i \tag{3}$$

where S_i and J_i are the mass sources for the bio-oil species due to droplet thermal decomposition and the diffusion flux of species i (due to concentration and temperature gradient), respectively. R_i is the net rate of production of species i by chemical reactions.

2.2. Trajectory, heat and mass transfer of bio-oil droplets

Lagrangian discrete phase model was employed for tracking bio-oil droplets, considering interactions between droplets and flow field via interphase exchange of momentum, heat, and mass transfer. The drag model by Saboni and Alexandrov [27] was employed to predict the drag coefficients (C_D) of dispersed liquid phase in gas phase, as a function of Reynolds number, density ratio, and the viscosity ratio ($\kappa = \mu_d/\mu_c$) between the dispersed phase and the continuous phase.

$$C_{D,d} = \frac{\left[\kappa\left(\frac{24}{Re} + \frac{4}{Re^{1/3}}\right) + \frac{14.9}{Re^{0.78}}\right]Re^2 + 40\frac{3\kappa+2}{Re} + 15\kappa + 10}{(1+\kappa)(5+Re^2)} \tag{4}$$

The bio-oil vaporization was modelled with a discrete component approach, with the droplet assumed to be ideal liquid mixture. The pseudo-steady species equation [28] in the gas phase is solved, considering the forced convection between the drop and ambient gas.

$$\dot{m}_{tot} = \frac{\dot{m}_i}{\varepsilon_i} = 2\pi R \rho Sh_{i,o} D_{i,g} \ln(1 + B_{M,i}) \tag{5}$$

where $\dot{m}_{tot}$ and $\dot{m}_i$ are total evaporation rate and evaporation rate of component i respectively, $Sh_{i,0}$ is Sherwood number, ε_i is the fraction of vaporization rate for component i with $\varepsilon_i = \dot{m}_i/\dot{m}_{tot}$ and $\sum \varepsilon_i = 1$, $D_{i,g}$ is the binary diffusivity between fuel component i and ambient gas, and $B_{M,i}$ is Spalding mass transfer number ($B_{M,i} = y_{i,s} - y_{i,\infty}/\varepsilon_i - y_{i,s}$) where $y_{i,s}$ and $y_{i,\infty}$ are mass fraction of species i at droplet surface and free stream. At equilibrium, the mole fraction of the components of vapour phase at the interface can be estimated by the Raoult's law [29].

For a liquid droplet with two components i and j, its diffusivity is related to Spalding mass transfer number via Eq. (6). The vapour pressure is estimated using Eq. (7) [29].

$$D_{i,g}\ln(1 + B_{M,i}) = D_{j,g}\ln(1 + B_{M,j}) \tag{6}$$

$$\ln(P_{vpr}) = f^{(0)}(T_r) + \omega f^{(1)}(T_r) \tag{7}$$

The multicomponent diffusion flux was simplified to binary

Table 1
Different operating conditions of bio-oil steam gasification in fluidized bed reactor [10].

Run ID	Temperature	H_2O/C	$G_{C1}HSV$	Discrete phase flow rate	Mass source of steam and nitrogen	Mole fraction of N_2 inlet
	K	mol/mol	m^3/m^3	kg/s	kg/s	mol %
1020_B	1020	5.225	338.53	7.12E−05	4.63E−04	58.2
1063_B	1063	5.446	331.81	6.97E−05	4.63E−04	59.4
1073_B	1073	5.833	215.23	4.52E−05	3.95E−04	50.5
1081_B	1081	7.451	343.02	7.20E−05	5.64E−04	67.7
1105_B	1105	5.718	334.05	7.00E−05	4.73E−04	61.2