Supplementary materials

Multi-fluid Modeling Biomass Fast Pyrolysis in the Fluidized Bed Reactor Including Particle Shrinkage Effects

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Kinetic model

Despite the previous reports used the complex biomass pyrolysis mechanism consisting three competition reaction routes for the pyrolysis reaction and tar secondary reaction[1-3], the complex biomass pyrolysis mechanism is hard to be described by chemical equations with certain chemical formulas and stoichiometric coefficient. Therefore, the present work used a simplified reaction mechanism for biomass pyrolysis analogous to the coal pyrolysis reaction[4, 5]. After biomass pyrolysis through one-step reaction, char, tar, and light gas were obtained as shown in R1.

(R1) $$\text{biomass} \rightarrow x_c\,\text{char} + x_t\,\text{tar} + x_g\,\text{light gas}$$

where x is the mass fraction of pyrolysis products with x_c = 27.0 wt%, x_t = 28.0 wt%, and x_g = 45.0 wt%[6]. From the composition of light gas[6, 7], and on the assumption that char and tar contain pure C and C_8H_{18}, respectively, the pyrolysis reaction with certain chemical formulas and stoichiometric coefficients was determined as shown in R2:

(R2) $$C_{52.04}H_{77.75}O_{18.63} \rightarrow 22.5C + 2.46C_8H_{18} + 4.338CO + 3.947CO_2 + 1.575CH_4 + 7.2H_2 + 6.399H_2O$$

The first-order Arrhenius kinetics with rate constant (A), activation energy (E), and temperature (T) was used to model the biomass pyrolysis reaction:

$$k = Ae^{-E/RT} \tag{1}$$

where $A = 1.30\times10^{10}$ 1/s, $E = 1.505\times10^{8}$ J/kmol[8].

Variable particle density and diameter model

For the biomass pyrolysis reaction (R1), the bio-mixture solid phase includes two solid species (biomass and char). In the variable particle density and diameter model, the density of bio-mixture phase is obtained by Eq.(2) as in the previous reports.

$$\rho_{sm} = \frac{1}{\frac{Y_b}{\rho_b} + \frac{Y_c}{\rho_c}} \tag{2}$$

where ρ_{sm} is the density of bio-mixture phase. Y_b and Y_c are the mass fraction of biomass and char, respectively. ρ_b and ρ_c are the apparent density of pure biomass and char species, respectively.

However, unlike the constant diameter treatment in the previous reports, the particle diameter in the variable particle density and diameter model is determined based on the mass conservation at the particle scale during the pyrolysis process. Since the current study focused on the variation of particle density and diameter caused by the heterogeneous reaction, the particle breakage and attrition were neglected. Therefore, for an individual fresh biomass particle, because the mass fraction of the biomass species Y_b is 1, the initial apparent density equals to the density of pure biomass ρ_b according to Eq.(1). Therefore, based on the assumption that the initial particle mass is m_{b0}, the initial particle volume V_0 can be calculated through the following equation.

$$V_0 = \frac{m_{b0}}{\rho_{sm0}} = \frac{m_{b0}}{\rho_b} \tag{3}$$

Assuming m_b biomass is consumed, and m_c char is formed during the biomass pyrolysis, according to R2 the relationship between m_b and m_c can be obtained:

$$m_c = x_c m_b \tag{4}$$

The mass fraction of biomass and char can be calculated as following:

$$Y_b = \frac{m_{b0} - m_b}{m_{b0} - m_b + m_c} \tag{5}$$

$$Y_c = 1 - Y_b = \frac{m_c}{m_{b0} - m_b + m_c} \tag{6}$$

In order to obey the law of mass conservation, the particle volume should be determined according to particle mass and density. Therefore, the following equation can be obtained from Eqs. (2-6):

$$V = \frac{m_{b0} - m_b + m_c}{\rho_{sm}} = \left(m_{b0} - m_b + m_c\right)\left(\frac{Y_b}{\rho_b} + \frac{Y_c}{\rho_c}\right) = \frac{m_{b0} - m_b}{\rho_b} + \frac{m_c}{\rho_c} = V_0 - \frac{\rho_c - \rho_b x_c}{\rho_b \rho_c} m_b \tag{7}$$

The m_b can be substituted from Eqs. (3-5):

$$Y_b m_{b0} - Y_b m_b + Y_b x_c m_b = m_{b0} - m_b \tag{8}$$

$$m_b\left(1 - Y_b + Y_b x_c\right) = m_{b0}\left(1 - Y_b\right) \tag{9}$$

$$m_b = \frac{m_{b0}\left(1 - Y_b\right)}{1 - Y_b\left(1 - x_c\right)} = \frac{\rho_b V_0\left(1 - Y_b\right)}{1 - Y_b\left(1 - x_c\right)} \tag{10}$$

Therefore, the equation for particle volume V can be developed from Eqs. (7 and 10):

$$V = V_0\left(1 - \frac{\rho_c - \rho_b x_c}{\rho_c}\frac{1 - Y_b}{1 - Y_b\left(1 - x_c\right)}\right) \tag{11}$$

For spherical biomass particle, the particle diameter d_p can be determined from the initial particle diameter d_{p0}, mass fraction (Y_b and Y_c), apparent density (ρ_b and ρ_c), and mass yield of char in the pyrolysis reaction x_c:

$$d_p = d_{p0}\left(1 - \frac{\rho_c - \rho_b x_c}{\rho_c}\frac{1 - Y_b}{1 - Y_b\left(1 - x_c\right)}\right)^{1/3} = d_{p0}\left(1 - \frac{\rho_c - \rho_b x_c}{\rho_c}\frac{Y_c}{1 - \left(1 - Y_c\right)\left(1 - x_c\right)}\right)^{1/3} \tag{12}$$

Specially, for the pyrolysis reaction with constant diameter, the particle diameter keeps constant during the pyrolysis reaction:

$$d_p = d_{p0} \tag{13}$$

The apparent density for bio-mixture can be calculated from Eqs. (3-7 and 13)：

$$
\begin{aligned}
\rho_{sm} &= \frac{m_{b0} - m_b + m_c}{V} \\
&= \frac{m_{b0} - m_b + m_c}{V_0} \\
&= \frac{m_{b0} - m_b + m_c}{\dfrac{m_{b0}}{\rho_b}} \\
&= \frac{1}{\dfrac{m_{b0} - m_b + m_b}{\rho_b}\dfrac{1}{m_{b0} - m_b + m_c}} \\
&= \frac{1}{\dfrac{m_{b0} - m_b}{m_{b0} - m_b + m_c}\dfrac{1}{\rho_b} + \dfrac{m_c / x_c}{m_{b0} - m_b + m_c}\dfrac{1}{\rho_b}} \\
&= \frac{1}{\dfrac{Y_b}{\rho_b} + \dfrac{Y_c}{x_c \rho_b}}
\end{aligned} \tag{14}
$$

In order to obtain the same formulation as Eq. (2), the apparent density of char should be defined as:

$$\rho_c = x_c \rho_b \tag{15}$$

Hence, if the particle diameter is assumed to be unchanged during the pyrolysis reaction, the apparent density of biomass and char should be related by Eq. (15), which was ignored in the previous MFM with variable particle density while constant diameter.

CFD model

The multi-fluid model based on Eulerian-Eulerian method is used to simulate the biomass pyrolysis process in the fluidized bed reactor. The primary phase is the gas mixture phase, whereas the secondary phases are the solid phases. In order to close the governing equations for each solid phase, the kinetic granular theory assuming that the random motion of particles is analogous to the motion of molecules in gas is used[9]. A set of conservation equations for mass, momentum, energy, and species are formulated for all the phases. The Gidaspow drag model with a monotonic function was used to determine the gas-solid drag coefficient to avoid the discontinuous behavior[10]. The solid-solid drag coefficient was described by the Syamlal drag model[11]. The gas-solid heat transfer coefficient was obtained from the Nusselt number which was calculated through the experience correlation developed by Gunn[12]. Since the previous report indicates that the ratio between particle-particle heat transfer and gas-solid heat transfer is rather low[13], the present work neglected the heat transfer between the sand and biomass-mixture phase. The Governing equations and constitutive equations are summarized in Table S1. It should be mentioned that the particle diameter of bio-mixture phase varies during the heterogeneous reactions with the variable particle density and diameter model, which indicates that polydisperse biomass particles will be formed in the fluidized bed reactor. However, the number of solid phases is still restricted to two in each grid cell, i.e. the bio-mixture phase and the sand phase, which is consistent with the simulation using the previous MFM. Although for the polydisperse particles the polydisperse kinetic theory should be more suitable[14], the monodisperse kinetic theory was used in many published reports, and reasonable results were obtained[1, 3, 15]. Therefore, the monodisperse kinetic theory used in the present work is acceptable.

Table S1. Governing equations and constitutive equations.

Governing equations

1. Continuity equations of gas and solid phases

$$\frac{\partial}{\partial t}\left(\alpha_g\rho_g\right)+\nabla\cdot\left(\alpha_g\rho_g\overrightarrow{v_g}\right)=S_g,\ \frac{\partial}{\partial t}\left(\alpha_{sn}\rho_{sn}\right)+\nabla\cdot\left(\alpha_{sn}\rho_{sn}\overrightarrow{v_{sn}}\right)=S_{sn},\ \alpha_g+\sum_{n=1}^{2}\alpha_{sn}=1 \tag{16}$$

2. Momentum equations of gas and solid phases

$$\frac{\partial}{\partial t}(\alpha_g\rho_g\overrightarrow{v_g})+\nabla\cdot\left(\alpha_g\rho_g\overrightarrow{v_g}\overrightarrow{v_g}\right)=-\alpha_g\nabla p+\nabla\cdot\overline{\overline{\tau}}_g+\alpha_g\rho_g\vec{g}+\sum_{n=1}^{2}\beta_n(\overrightarrow{v_{sn}}-\overrightarrow{v_g})+S_g^v \tag{17}$$

$$\begin{aligned}&\frac{\partial}{\partial t}(\alpha_{sn}\rho_{sn}\overrightarrow{v_{sn}})+\nabla\cdot\left(\alpha_{sn}\rho_{sn}\overrightarrow{v_{sn}}\overrightarrow{v_{sn}}\right)=-\alpha_{sn}\nabla p+\nabla\cdot\overline{\overline{\tau}}_{sn}+\alpha_{sn}\rho_{sn}\vec{g}+\beta_n(\overrightarrow{v_g}-\overrightarrow{v_{sn}})\\&+\zeta_{nm}(\overrightarrow{v_{sm}}-\overrightarrow{v_{sn}})+S_{sn}^v\end{aligned} \tag{18}$$

3. Energy equations of gas and solid phases

$$\frac{\partial}{\partial t}(\alpha_g\rho_g H_g)+\nabla\cdot(\alpha_g\rho_g\overrightarrow{v_g}H_g)=\nabla\cdot\left(K_g\nabla T_g\right)+\sum_n\left[h_{gsn}\left(T_{sn}-T_g\right)\right]+S_g^H \tag{19}$$

$$\frac{\partial}{\partial t}(\alpha_{sn}\rho_{sn}H_{sn}) + \nabla\cdot(\alpha_{sn}\rho_{sn}\overrightarrow{v_{sn}}H_{sn}) = \nabla\cdot\left(K_{sn}\nabla T_{sn}\right) + h_{gsn}\left(T_g - T_{sn}\right) + S_{sn}^{H} \tag{20}$$

4. Species transport equations of gas and solid phases

$$\frac{\partial}{\partial t}(\alpha_g\rho_g Y_{g,k}) + \nabla\cdot(\alpha_g\rho_g\overrightarrow{v_g}Y_{g,k}) = \nabla\cdot(\alpha_g\rho_g D_{k,mix}\nabla Y_k] + S_g^k \tag{21}$$

$$\frac{\partial}{\partial t}(\alpha_{sn}\rho_{sn}Y_{sn,k}) + \nabla\cdot(\alpha_{sn}\rho_{sn}\overrightarrow{v_{sn}}Y_{sn,k}) = \nabla\cdot(\alpha_{sn}\rho_{sn}D_{k,mix}\nabla Y_{sn,k}] + S_{sn}^k \tag{22}$$

5. Granular temperature equation[9]

$$\frac{3}{2}\left[\frac{\partial}{\partial t}\left(\alpha_{sn}\rho_{sn}\Theta_{sn}\right) + \nabla\cdot\left(\alpha_{sn}\rho_{sn}\overrightarrow{v_{sn}}\Theta_{sn}\right)\right] = \overline{\overline{\tau_{sn}}} : \nabla\overrightarrow{v_{sn}} + \nabla\cdot\left(k_{\Theta_{sn}}\nabla\Theta_{sn}\right) - \gamma_{\Theta_{sn}} - 3(\beta_n + \zeta_{nm})\Theta_{sn} \tag{23}$$

Constitutive equations

1. Gas shear stress

$$\overline{\overline{\tau_g}} = \alpha_g\mu_g\left[\nabla\overrightarrow{v_g} + \left(\nabla\overrightarrow{v_g}\right)^{\mathrm{T}} - \frac{2}{3}\left(\nabla\cdot\overrightarrow{v_g}\right)\overline{\overline{I}}\right] \tag{24}$$

2. Solids shear stress

$$\overline{\overline{\tau_{sn}}} = \left(-p_{sn} + \alpha_{sn}\lambda_{sn}\nabla\cdot\overrightarrow{v_{sn}}\right)\overline{\overline{I}} + \alpha_{sn}\mu_{sn}\left[\nabla\overrightarrow{v_{sn}} + \left(\nabla\overrightarrow{v_{sn}}\right)^{\mathrm{T}} - \frac{2}{3}\left(\nabla\cdot\overrightarrow{v_{sn}}\right)\overline{\overline{I}}\right] \tag{25}$$

3. Solids pressure

$$p_{sn} = \left[1 + 2\sum_{n=1}^{2}\left(\frac{d_{sn}+d_{sm}}{2d_{sn}}\right)^3\left(1+e_{nm}\right)\alpha_{sm}g_{nm}\right]\alpha_{sn}\rho_{sn}\Theta_{sn} \tag{26}$$

4. Solids shear viscosity[16, 17]

$$\mu_{sn} = \frac{4}{5}\alpha_{sn}\rho_{sn}d_{sn}g_{nm}\left(1+e_{nm}\right)\sqrt{\frac{\Theta_{sn}}{\pi}} + \frac{10\rho_{sn}d_{sn}\sqrt{\Theta_{sn}\pi}}{96\alpha_{sn}\left(1+e_{nm}\right)g_{nm}}\left[1 + \frac{4}{5}g_{nm}\alpha_{sn}\left(1+e_{nm}\right)\right]^2 + \frac{p_{sn}\sin\theta_{sn}}{2\sqrt{I_{2D}}} \tag{27}$$

5. Solids bulk viscosity[18]

$$\lambda_{sn} = \frac{4}{3}\alpha_{sn}\rho_{sn}d_{sn}g_{nm}\left(1+e_{nm}\right)\sqrt{\frac{\Theta_{sn}}{\pi}} \tag{28}$$

6. Diffusion coefficient of granular energy[16]

$$k_{\Theta_{sn}} = \frac{150\rho_{sn}d_{sn}\sqrt{\Theta_{sn}\pi}}{384\left(1+e_{nm}\right)g_{nm}}\left[1 + \frac{6}{5}\alpha_{sn}g_{nm}\left(1+e_{nm}\right)\right]^2 + 2\rho_{sn}\alpha_{sn}^2d_{sn}\left(1+e_{nm}\right)g_{nm}\sqrt{\frac{\Theta_{sn}}{\pi}} \tag{29}$$

7. Collisional energy dissipation[18]

$$\gamma_{\Theta_{sn}} = \frac{12\left(1-e_{nm}^2\right)g_{nm}}{d_{sn}\sqrt{\pi}}\rho_{sn}\alpha_{sn}^2\Theta_{sn}^{3/2} \tag{30}$$

8. Radial distribution function

$$g_{nm} = \frac{d_{sn}g_{sm} + d_{sm}g_{sn}}{d_{sn}+d_{sm}},\ g_{sn} = \frac{d_{sn}}{2}\sum_{m=1}^{2}\frac{\alpha_{sm}}{d_{sm}} + \left[1 - \left(\frac{\alpha_s}{\alpha_{s,\max}}\right)^{\frac{1}{3}}\right]^{-1},\ \alpha_s = \sum_{n=1}^{2}\alpha_{sn} \tag{31}$$

$\alpha_{s,\max}$ is determined by the correlations proposed by Fedors and Landel[19] with

$d_{sn} > d_{sm}$, $X_n = \frac{\alpha_{sn}}{\alpha_s}$:

for $X_n \le \frac{\alpha_{sn,\max}}{\alpha_{sn,\max} + \left(1-\alpha_{sn,\max}\right)\alpha_{sm,\max}}$

$$\begin{aligned}\alpha_{s,\max} &= \left[\alpha_{sn,\max} - \alpha_{sm,\max} + \left(1-\sqrt{\frac{d_{sm}}{d_{sn}}}\right)\left(1-\alpha_{sn,\max}\right)\alpha_{sm,\max}\right] \\ &\times\left[\alpha_{sn,\max} + \left(1-\alpha_{sn,\max}\right)\alpha_{sm,\max}\right]\frac{X_n}{\alpha_{sn,\max}} + \alpha_{sm,\max}\end{aligned} \tag{32}$$

otherwise

$$\alpha_{s,\max} = \left(1-\sqrt{\frac{d_{sm}}{d_{sn}}}\right)\left[\alpha_{sn,\max} + \left(1-\alpha_{sn,\max}\right)\alpha_{sm,\max}\right]\left(1-X_n\right) + \alpha_{sn,\max} \tag{33}$$

9. Gas–solid drag coefficient[10]

$$\beta_n = \phi\beta_{n,\text{Ergun}} + \left(1-\phi\right)\beta_{n,\text{Wen-Yu}} \tag{34}$$

$$\beta_{n,\text{Ergun}} = 150\frac{\alpha_{sn}(1-\alpha_g)\mu_g}{\alpha_g {d_{sn}}^2} + 1.75\frac{\rho_g\alpha_{sn}\left|\overrightarrow{v_g} - \overrightarrow{v_{sn}}\right|}{d_{sn}} \tag{35}$$

$$\beta_{n,\text{Wen-Yu}} = \frac{3}{4}C_D\frac{\alpha_g\alpha_{sn}\rho_g\left|\overrightarrow{v_g} - \overrightarrow{v_{sn}}\right|}{d_{sn}}{\alpha_g}^{-2.65} \tag{36}$$

$$C_D = \begin{cases}\frac{24}{\text{Re}_{sn}}\left[1 + 0.15\left(\text{Re}_{sn}\right)^{0.687}\right], & \text{Re}_{sn} \le 1000 \\ 0.44, & \text{Re}_{sn} > 1000\end{cases} \tag{37}$$

$$\text{Re}_{sn} = \frac{\alpha_g\rho_g\left|\overrightarrow{v_g} - \overrightarrow{v_{sn}}\right|d_{sn}}{\mu_g} \tag{38}$$

$$\phi = \arctan\left(\frac{150\times1.75\left(0.2-\alpha_s\right)}{\pi}\right) + 0.5 \tag{39}$$

10. Solid-solid drag coefficient[11]

$$\zeta_{nm} = \frac{3\left(1+e_{nm}\right)\left(\frac{\pi}{2} + C_{fr,nm}\frac{\pi^2}{8}\right)\alpha_{sn}\rho_{sn}\alpha_{sm}\rho_{sm}\left(d_{sn}+d_{sm}\right)^2 g_{nm}}{2\pi\left(\rho_{sn}d_{sn}^3 + \rho_{sm}d_{sm}^3\right)}\left|\overrightarrow{v_{sn}} - \overrightarrow{v_{sm}}\right| \tag{40}$$

11. Gas-solid heat transfer coefficient[12]

$$h_{gsn} = \frac{6\lambda_g\alpha_g\alpha_{sn}Nu_{sn}}{d_{sn}^2} \tag{41}$$

$$Nu_{sn} = (7-10\alpha_g + 5\alpha_g^2)(1 + 0.7\,\text{Re}_{sn}^{0.2}\,\text{Pr}_g^{1/3}) + (1.33 - 2.4\alpha_g + 1.2\alpha_g^2)\,\text{Re}_{sn}^{0.7}\,\text{Pr}_g^{1/3} \tag{42}$$

$$\Pr_g = \frac{c_{p_g}\mu_g}{\lambda_g} \tag{43}$$

12. Source terms[20]

Mass source for the i^{th} phase

$$S_i = S_{p_i} + S_{r_i},\ S_{r_i} = -R\sum_{r_i}\gamma_j^r M_j^r,\ S_{p_i} = R\sum_{p_i}\gamma_j^p M_j^p,\ R = k\prod_{j=1}^{NR}\frac{Y_j\rho_i\alpha_i}{MW_j} \tag{44}$$

Momentum source for the i^{th} phase

$$S_i^v = S_{p_i}\vec{v}_{net} - R\sum_{r_i}\gamma_j^r M_j^r\vec{v}_i,\ \vec{v}_{net} = \frac{\sum_r \gamma_j^r M_j^r \vec{v}_{r_j}}{\sum_r \gamma_j^r M_j^r} \tag{45}$$

Species source for k^{th} species in the i^{th} phase

$$S_i^k = S_{p_i}^k + S_{r_i}^k,\ S_{r_i}^k = -R\sum_{r_i^k}\gamma_j^{r^k} M_j^{r^k},\ S_{p_i}^k = R\sum_{p_i^k}\gamma_j^{p^k} M_j^{p^k} \tag{46}$$

Energy source

$$S_i^H = S_{p_i}H_{net} - R\left(\sum_{r_i}\gamma_j^r M_j^r H_j^r + \sum_{p_i}\gamma_j^p M_j^p h_j^{f\,p}\right),\ H_{net} = \frac{\sum_r \gamma_j^r M_j^r\left(H_j^r + h_j^{f\,r}\right)}{\sum_r \gamma_j^r M_j^r} \tag{47}$$

NOMENCLATURE

Symbols

A	pre-exponential factor, s^{-1}
C_D	particle drag coefficient
d	particle diameter, m
C_{fr}	friction coefficient
c_p	specific heat, J kg^{-1} K^{-1}
e	restitution coefficient
E	activation energy, J $kmol^{-1}$
g	gravitational acceleration, m s^{-2}
g_{sn}	radial distribution function
g_{nm}	constitutive function, dimensionless identity tensor
h	heat transfer coefficient, W m^{-2} K^{-1}
h^f	formation enthalpy, J $kmol^{-1}$

H	enthalpy, J kmol^{-1}
I_{2D}	second invariant of the deviatoric stress tensor
k	reaction constant
$k_{\Theta_{sn}}$	diffusion coefficient for the granular temperature, kg s^{-1} m^{-1}
K	thermal conductivity, W m^{-1} K^{-1}
M	molecular weight, kg kmol^{-1}
Nu	Nusselt number
p	pressure, Pa
Pr	Prandtl number
R	reaction rate, kmol m^{-3} s^{-1}
S	Source term
Re	particle Reynolds number
v	velocity, m s^{-1}

Greek symbols

α	volume fraction
β	drag force coefficient, kg m^{-3} s^{-1}
γ	stoichiometric coefficient
$\gamma_{\Theta_{pi}}$	collisional dissipation of fluctuating energy, kg m^{-1} s^{-3}
λ	particle bulk viscosity, kg m^{-1} s^{-1}
μ	shear viscosity, kg m^{-1} s^{-1}
θ	angle of internal friction
τ	viscous stress tensor, kg m^{-1} s^{-2}
Θ	granular temperature, m^2 s^{-2}
ρ	density, kg m^{-3}
ζ	drag force coefficient, kg m^{-3} s^{-1}

Subscripts

g	gas phase
sn	n^{th} particle phase
i	generic phase
j,k	species
p	product
r	reactant

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