Development of a Dense discrete phase model for 3D numerical simulation of coal combustion in an industrial scale circulating fluidized bed boiler

Department of Mechanical Engineering
Yonsei University

Massoud Massoudi Farid, Hyo Jae Jeong, Jungho Hwang

2015.11.5
Circulating Fluidized Beds in Korea

- Korea South-East Power Co.
  - Co-firing (coal + biomass or waste), 10%
  - CFB boiler at Yeosu Power Plant

- Korea Southern Power Co.
  - Co-firing (coal + biomass), 5%
  - Super Critical CFB boiler at Samcheok Power Plant (under construction until 2015)

- Korea East-West Power Co.
  - 100% Biomass, 30MW
  - CFB boiler at Donghae Power plant
Numerical methods for particle laden flows

**Eulerian-Lagrangian**

Discrete Phase Method (DPM)

- In Eulerian frame
- In Lagrangian frame

It is suitable for low volume fraction of solids since:
1) Solid Volume fraction was neglected.
2) Particles interaction was neglected.

**Eulerian-Eulerian**

Multiphase Eulerian-Granular Method (MEGM)

- In Eulerian frame
- In Eulerian frame

Disadvantages:
1) It just shows general flow behavior.
2) It is not possible to model particle surface reactions.
3) We have to define lots of phases to handle particle size distributions.
**Dense Discrete Phase Method (DDPM)**

Assumptions

1) Trajectory of a discrete phase particle is predicted by integrating the force balance equation of the particle on lagrangian reference of frame.
2) N.S equations are solved for fluid phases on Eulerian reference of frame.
3) For calculation of the particles interactions, first the position of the particles are mapped on the Eulerian grid and the interactions are calculated on the Eulerian grid, then calculated interaction terms are mapped back on the particles positions.

Advantages:

1) It predicts more exact details of flow
2) Size distribution is modeled in a natural way in the Lagrangian formulation
Zhang et al. analyzed cold flow at a 150MWe circulating fluidized bed (CFB) employing a 3D unsteady Eulerian granular multiphase model. They presented the whole loop pressure profile, solids volume fraction profiles and solids vertical velocity.

Adamczyk et al. analyzed combustion at an industrial circulating fluidized bed (CFB) employing a 3D unsteady DDPM. They presented pressure drop, solids volume fraction profiles and temperature profile. However, no information about combustion products were presented.

Boiler Geometry

Real CFB

Due to computational barriers

340 MWe CFB boiler located in Yeosu, Korea.

Symmetry B.C

Simulated zone and mesh
### Boundary condition and PSD

#### Boundary and operating Conditions

<table>
<thead>
<tr>
<th>Hydrodynamic Boundary conditions</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary air inlet</td>
<td>101 (kg/s)</td>
</tr>
<tr>
<td>Return leg inlet</td>
<td>0.361 (kg/s)</td>
</tr>
<tr>
<td>Secondary air inlet</td>
<td>54.2 (kg/s)</td>
</tr>
<tr>
<td>Outlet pressure</td>
<td>-91.5 Pa</td>
</tr>
<tr>
<td>Wall B.C</td>
<td></td>
</tr>
<tr>
<td>Gas</td>
<td>No Slip</td>
</tr>
<tr>
<td>Solid</td>
<td>Reflect</td>
</tr>
</tbody>
</table>

#### Heat transfer Boundary Conditions

| Primary air Temperature                                | 482.15 K    |
| Secondary air Temperature                             | 498.15 K    |
| Return Leg air Temperature                            | 1073.15 K   |
| Wall Temperature                                       | 632.15 K    |
| Division wall Temperature                              | 632.15 K    |
| Wing wall tubes Temperature                            |             |
| 1st Super heater                                       | 686.65 K    |
| 2nd Super heater                                       | 766.65 K    |

#### Size distribution (Rosin Rammler)

<table>
<thead>
<tr>
<th>Coal</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min Diameter</td>
<td>1 mm</td>
</tr>
<tr>
<td>Max Diameter</td>
<td>16 mm</td>
</tr>
<tr>
<td>Mean Diameter</td>
<td>6.5 mm</td>
</tr>
<tr>
<td>Spread parameter</td>
<td>1.120114</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Sand</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Min Diameter</td>
<td>50 µm</td>
</tr>
<tr>
<td>Max Diameter</td>
<td>2000 µm</td>
</tr>
<tr>
<td>Mean Diameter</td>
<td>1000 µm</td>
</tr>
<tr>
<td>Spread parameter</td>
<td>1.98931</td>
</tr>
</tbody>
</table>

#### Diagram

- Symmetric Boundary condition
- 9t/h
- 10t/h
- 20t/h
- 20t/h
- 10t/h
- 9t/h
- 14t/h
- 20t/h
- 20t/h
- 14t/h
Results

Pressure drop and circulation rate:

<table>
<thead>
<tr>
<th>Gs (kg/s)</th>
<th>Cyclone A</th>
<th>Cyclone B</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>384</td>
<td>305</td>
</tr>
</tbody>
</table>

![Graph showing pressure drop and circulation rate](image)

![Diagram showing pressure distribution](image)
Results

Solid VOF:

H=1

H=3

H=6

H=10

H=15

H=20

H=35

Walls

X=0
Results

Gas Velocity:

<table>
<thead>
<tr>
<th>H</th>
<th>Averaged velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>6.18</td>
</tr>
<tr>
<td>3</td>
<td>5.4</td>
</tr>
<tr>
<td>6</td>
<td>5.21</td>
</tr>
<tr>
<td>10</td>
<td>5.11</td>
</tr>
<tr>
<td>20</td>
<td>5.1</td>
</tr>
<tr>
<td>35</td>
<td>4.71</td>
</tr>
</tbody>
</table>
Results

Temperature:

<table>
<thead>
<tr>
<th>H</th>
<th>Averaged Temperature</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>1212.445</td>
</tr>
<tr>
<td>3</td>
<td>1178.197</td>
</tr>
<tr>
<td>6</td>
<td>1156.205</td>
</tr>
<tr>
<td>10</td>
<td>1149.343</td>
</tr>
<tr>
<td>20</td>
<td>1135.411</td>
</tr>
<tr>
<td>35</td>
<td>1042.409</td>
</tr>
</tbody>
</table>
Results

O₂ mole fraction:

<table>
<thead>
<tr>
<th>H</th>
<th>Averaged O₂ mole fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.4</td>
<td>0.116889</td>
</tr>
<tr>
<td>3</td>
<td>0.079107</td>
</tr>
<tr>
<td>6</td>
<td>0.077509</td>
</tr>
<tr>
<td>10</td>
<td>0.071479</td>
</tr>
<tr>
<td>20</td>
<td>0.044502</td>
</tr>
<tr>
<td>35</td>
<td>0.041857</td>
</tr>
</tbody>
</table>
Results

**CO₂ mole fraction:**

<table>
<thead>
<tr>
<th>H</th>
<th>Averaged CO₂ mole fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>z₁=0.4</td>
<td>0.088602</td>
</tr>
<tr>
<td>z₂=3</td>
<td>0.110953</td>
</tr>
<tr>
<td>z₃=6</td>
<td>0.104716</td>
</tr>
<tr>
<td>z₄=10</td>
<td>0.110959</td>
</tr>
<tr>
<td>z₅=20</td>
<td>0.128557</td>
</tr>
<tr>
<td>z₆=35</td>
<td>0.130368</td>
</tr>
</tbody>
</table>
### Results

#### Heat Fluxes:

<table>
<thead>
<tr>
<th>Component</th>
<th>Heat Flux (Mega Watts)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SH1</td>
<td>10.7</td>
</tr>
<tr>
<td>SH2</td>
<td>8.2</td>
</tr>
<tr>
<td>SH3</td>
<td>12</td>
</tr>
<tr>
<td>SH4</td>
<td>9.3</td>
</tr>
<tr>
<td>SH5</td>
<td>9.7</td>
</tr>
<tr>
<td>SH6</td>
<td>9.9</td>
</tr>
<tr>
<td>SH7</td>
<td>8.2</td>
</tr>
<tr>
<td>SH8</td>
<td>17.8</td>
</tr>
<tr>
<td>SH9</td>
<td>11</td>
</tr>
<tr>
<td>SH10</td>
<td>5.3</td>
</tr>
<tr>
<td>SH11</td>
<td>5.7</td>
</tr>
<tr>
<td>SH12</td>
<td>3.6</td>
</tr>
<tr>
<td>SH13</td>
<td>6.3</td>
</tr>
<tr>
<td>SH14</td>
<td>12.5</td>
</tr>
<tr>
<td>SH15</td>
<td>2</td>
</tr>
<tr>
<td><strong>Total Heat Fluxes</strong>:</td>
<td><strong>246 Mega Watts</strong></td>
</tr>
</tbody>
</table>

The calculated total heat flux is 246 Mega Watts, which is close to the measured value.
Conclusion

Numerical simulation of an industrial scale fluidized bed furnace was done using DDPM.

Pressure drop, Solid volume fraction contour, Temperature and species profiles and contours were displayed.

Details of heat fluxes were presented.

Pressure drop, temperature, $O_2$ mole fraction, and heat fluxes were matched with measurements.
Thank you for your attention
Appendix
Discrete Phase Method (DPM)

Assumptions

1) Solid particles have low Volume fraction and they cannot affect fluid motion. Hence Volume fraction is not considered in N.S equations.
2) There is no particles interaction.
3) Trajectory of a discrete phase particle is predicted by integrating the force balance equation of the particle.
4) Coal particles interact directly only by gas phase via drag force.
5) Coal particles do not interact directly by sand phase.
6) Coal particles transfer heat directly only to gas phase.

\[
\frac{\partial u_p}{\partial t} = F_D(u - u_p) + \frac{g(\rho_p - \rho)}{\rho_p} + \vec{F}_x
\]

Particle force balance for Solid Phase
Assumptions
1) It is a multiphase flow method and N.S equations are solved for both phases.
2) Solid and fluid phases are treated in the same way as interpenetrating continua.
3) Granular properties are added to solid phase by solving an additional equation for solids fluctuating energy or granular temperature.
4) There is no limitation for volume fraction. Hence effects of volume fraction should be considered in N.S equations.
Multiphase Eulerian-Granular Method (MEGM)

\[
\frac{1}{\rho_g} \left( \frac{\partial}{\partial t} (\alpha_g \rho_g) + \nabla \cdot (\alpha_g \rho_g \vec{v}_g) \right) = 0
\]
The kinetic energy due to the random motion of particles is represented by the granular temperature of the solid phase ($\Theta_s$). Utilizing the kinetic theory, the transport equation of the granular temperature takes the form:

$$\frac{3}{2} \left[ \frac{\partial}{\partial t} (\alpha_s \rho_s \Theta_s) + \nabla \cdot (\alpha_s \rho_s \vec{v}_s \Theta_s) \right] = (-p_s \bar{I} + \bar{\tau}_s) : \nabla \vec{v}_s + \nabla \cdot (k_s \nabla \Theta_s) - \gamma_s + \varphi_{gs}$$

**Granular Temperature**

- Generation of energy by the solid stress tensor
- Diffusion of energy or diffusive flux of granular energy
- Unit tensor
- Diffusion coefficient
- Collisional dissipation of energy
- Energy exchange between the two phases
Important features:

- Coal and sand particles interact directly by gas phase via drag force.

- Coal particles interact directly by sand phase via solid stress tensors of sand and coal, \( \tau_{sand} \) and \( \tau_{coal} \), respectively.

- Coal and sand particles transfer heat directly by each other and gas phase.

- In DDPM there is no restriction for the volume fraction of the discrete phase. So, volume fraction of the discrete phase should be considered in the gas momentum equations. Hence, relation between volume fractions becomes \( \phi_{coal} + \phi_{sand} = 1 \).
\[
\frac{1}{\rho_{rg}} \left( \frac{\partial}{\partial t} \left( \alpha_g \rho_g \right) + \nabla \cdot \left( \alpha_g \rho_g \vec{v}_g \right) \right) = 0
\]
Granular Temperature

Generation of energy by the solid stress tensor

\[ \frac{3}{2} \left[ \frac{\partial}{\partial t} \left( \alpha_s \rho_s \Theta_s \right) + \nabla \cdot \left( \alpha_s \rho_s \vec{v}_s \Theta_s \right) \right] = \left( -p_s \bar{I} + \tau_s \right) : \nabla \vec{v}_s + \nabla \cdot \left( k_{\Theta_s} \nabla \Theta_s \right) - \gamma_{\Theta_s} \]

For calculation of particles interactions we need to calculate solid Stress-strain tensor on Eulerian Grid. This tensor is a function of the kinetic energy due to the random motion of particles which is represented by the granular temperature of the solid phase. Utilizing the kinetic theory, the transport equation of the granular temperature takes the form.

Diffusion coefficient

Collisional dissipation of energy

Dense Discrete Phase Method (DDPM)
There is a limit for maximum VOF in a cell equal to 0.63% of cell volume.

If VOF is over limit, redistribution of VOF to neighbor cells occurs.

If all neighbor cells are full and the number of iteration per time step is low, mass loss is calculated.

3. Calculation of pressure drop along furnace based on mass of particles in each section.
5. Calculation of PSD at furnace outlet.
6. Non-uniform boundary condition at inlet. The air mass flow rate at the bottom of at different sections has different values.
## Reactions

### Gas Phase Reactions

<table>
<thead>
<tr>
<th>Reactions</th>
<th>$A_r$</th>
<th>$E_r$ (J/kmol)</th>
<th>m</th>
<th>a</th>
<th>b</th>
<th>c</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{CH}_2\text{.84O}_0\text{.761} \rightarrow 0.239\text{CH}_4 + 0.761\text{CO} + 0.942\text{H}_2$</td>
<td>$4.26 \times 10^8$ [1/s]</td>
<td>$1.08 \times 10^8$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$\text{CH}_2\text{.84O}_0\text{.761} + 1.33\text{O}_2 \rightarrow \text{CO}_2 + 1.42\text{H}_2\text{O}$</td>
<td>$2.12 \times 10^{12}$ [1/K/s]</td>
<td>$2.03 \times 10^7$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$\text{CO} + 0.5\text{O}_2 \rightarrow \text{CO}_2$</td>
<td>$2.239 \times 10^{12}$ [(m$^3$/kmol)$^{0.75}$/s]</td>
<td>$1.674 \times 10^8$</td>
<td>0</td>
<td>1</td>
<td>0.25</td>
<td>0.5 [H$_2$O]</td>
</tr>
<tr>
<td>$\text{H}_2 + 0.5\text{O}_2 \rightarrow \text{H}_2\text{O}$</td>
<td>$6.8 \times 10^{15}$ [(m$^3$/kmol)$^{0.75}$/K$^{1}$/s]</td>
<td>$1.67 \times 10^8$</td>
<td>-1</td>
<td>0.25</td>
<td>1.5</td>
<td>0</td>
</tr>
<tr>
<td>$\text{CO} + \text{H}_2\text{O} \rightarrow \text{CO}_2 + \text{H}_2$</td>
<td>$275$ [(m$^3$/kmol)$^{0.5}$/s]</td>
<td>$8.374 \times 10^7$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$\text{H}_2 + \text{CO}_2 \rightarrow \text{CO} + \text{H}_2\text{O}$</td>
<td>$0.0265$ [(m$^3$/kmol)$^{0.5}$/s]</td>
<td>$3960$</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>$\text{CH}_4 + 0.5\text{O}_2 \rightarrow \text{CO} + 2\text{H}_2$</td>
<td>$4.4 \times 10^{11}$ [(m$^3$/kmol)$^{0.75}$/s]</td>
<td>$1.25 \times 10^8$</td>
<td>0</td>
<td>0.5</td>
<td>1.25</td>
<td>0</td>
</tr>
<tr>
<td>$\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$</td>
<td>$8.7 \times 10^7$ [(m$^3$/kmol)$^{0.5}$/s]</td>
<td>$2.51 \times 10^8$</td>
<td>0</td>
<td>0.5</td>
<td>1</td>
<td>0</td>
</tr>
</tbody>
</table>

### Solid Phase reactions

<table>
<thead>
<tr>
<th>Reactions</th>
<th>$A_r$ [kg/m$^2$/sec/Pa$^{0.5}$]</th>
<th>$E_r$(J/kmol)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{C(s)} + 0.5\text{O}_2 \rightarrow \text{CO}$</td>
<td>0.052</td>
<td>$6.1 \times 10^7$</td>
</tr>
<tr>
<td>$\text{C(s)} + \text{CO}_2 \rightarrow 2\text{CO}$</td>
<td>0.0732</td>
<td>$1.125 \times 10^8$</td>
</tr>
<tr>
<td>$\text{C(s)} + \text{H}_2\text{O}\rightarrow \text{CO} + \text{H}_2$</td>
<td>0.0782</td>
<td>$1.15 \times 10^8$</td>
</tr>
</tbody>
</table>
Governing Equations:

\[
\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla \cdot (\alpha_q \rho_q \vec{v}_q) = \sum_{p=1}^{n} (\dot{m}_{pq} - \dot{m}_{qp})
\]

Volume Fraction Equation

Continuity
Governing Equations:

\[
\begin{align*}
\frac{\partial}{\partial t}&\left(\alpha_s \rho_s \Theta_s\right) + \nabla \cdot \left(\alpha_s \rho_s \vec{v}_s \Theta_s\right) = \left(-p_s \bar{I} + \tau_s\right) : -\nabla \vec{v}_s + \\
\n\n\n\end{align*}
\]
Volume Fraction

Density

Velocity

Mass transfer between Phases

Pressure

Phase Stress-Strain Tensor

Gravitational accelerate

Interphase momentum exchange coefficient
Lift Force:

\[ \vec{F}_{\text{lift}} = -0.5 \rho_p \alpha_p (\vec{v}_q - \vec{v}_p) \times (\nabla \times \vec{v}_q) \]

• Due to velocity gradients

• Important for large particles
Virtual Mass Force:

\[
\frac{d}{dt} \Phi_p = \frac{\partial \phi}{\partial t} + (\mathbf{v}_q \cdot \nabla) \phi
\]

- Important when secondary phase density is much smaller than primary phase
  - Due to Relative acceleration of Phase \( p \) to the primary Phase \( q \)
Fluid-Solid exchange coefficient

\[ K_{sl} = \frac{3}{4} C_d \frac{\alpha_s \alpha_l \rho_l |\bar{v}_s - \bar{v}_l|}{d_s} \alpha_l^{-2.65} \]

For

Gidaspow model
Solid Pressure

\[ p_s = \alpha_s \rho_s \Theta_s + 2 \rho_s (1 + e_{ss}^s) \alpha_s^2 g_{0,ss} \Theta_s \]

- Due to using Maxwellian velocity distribution, granular temperature appears

 radially distribution function

Coefficient of restitution for particle collision (around 0.9)
Radial distribution function

\[ g_0 = \left[ 1 - \left( \frac{\alpha_s}{\alpha_{s,\text{max}}} \right)^{\frac{1}{3}} \right]^{-1} \]

- Governs the transition from compressible condition to incompressible condition
- Is a correction factor to modify the probability of collisions in dense beds

Max Packing Volume fraction
Solid Shear Stresses:

\[
\tau_s = \alpha_s \mu_s (\nabla \vec{v}_s + \nabla \vec{v}_s^T) + \alpha_s (\lambda_s - \frac{2}{3} \mu_s) \nabla \cdot \vec{v}_s I
\]

Stress-strain tensor for solid phase:

Shear viscosity

Gidaspow model
Granular Temperature

\[
\frac{\partial}{\partial t} (\alpha_s \rho_s \Theta_s) + \nabla \cdot (\alpha_s \rho_s \vec{v}_s \Theta_s) = (-p_s \bar{I} + \tau_s) : -\nabla \vec{v}_s + \\
\nabla \cdot (k_{\Theta_s} \nabla \Theta_s) - \gamma_{\Theta_s} + \phi_{ls}
\]

The generation of energy by the solid stress tensor

The collisional dissipation of energy

The diffusion of energy
\[ k_{\Theta_s} = \frac{1}{150} \sqrt{\Theta} \quad \text{(Diffusion Coefficient)} \]  

(Gidaspow model)
Boundary Conditions

Wall: No slip
Inlet: Velocity inlet
Outlet: Atmosphere Pressure

Solid Phase:
Wall: Partial slip:
Outlet: Atmosphere Pressure

Liquid Phase:

\[ \bar{t}_s = -\frac{\pi}{6} \sqrt{3\phi} \frac{\alpha_s}{\alpha_{s,\text{max}}} \rho_s g_0 \sqrt{\Theta_s} \bar{U}_s,|| \]

Granular Boundary condition:
\[
\frac{\partial}{\partial x} \left[ u_i (\rho e + p) \right] = \frac{\partial}{\partial x_i} \left( k \frac{\partial T}{\partial x_i} - \sum_j h \cdot J_j + u \cdot \tau_{ij} \right) + S_h
\]

Conservation of Fluid Mass

Conservation of momentum
Governing Equations-Gas phase

Turbulence model (Realizable $k$-$\varepsilon$) for SCGP

\[ \frac{\partial}{\partial x_i} \left( \rho k u_i \right) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \varepsilon - Y_M + S_k \]

Turbulence model (Standard $k$-$\varepsilon$) for E-Gas

$G_k$ represents the generation of turbulence kinetic energy due to the mean velocity gradients.

$G_b$ generation of turbulence kinetic energy due to buoyancy.

$Y_M$ contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate.

$\sigma_k$ and $\sigma_\varepsilon$ turbulent Prandtl numbers for $k$ and $\varepsilon$, respectively.

$S_k$, $S_\varepsilon$ user-defined source terms.
Governing Equations - Particle phase

\[
\frac{du_p}{dt} = F_D(u - u_p) + \frac{g_x(p - \rho)}{\rho_p} + F_x
\]

Particle motion equation

Drag force

Turbulent (stochastic) tracking model

- Conservation of energy for particle
Governing Equations-Radiation sub model

Discrete Ordinates (DO) radiation model

\[ \nabla \cdot (IS) + (a + a_P + \sigma_P)I(\vec{r},\vec{s}) = an^2 \frac{\sigma T^4}{\pi} + E_P + \frac{\sigma_P}{4\pi} \int_0^{4\pi} I(\vec{r},\vec{s}') \Phi(\vec{s} \cdot \vec{s}')d\Omega' \]

\( a \) : path length (m)
\( a \) : absorption coefficient of gas phase
\( a_p \) : equivalent absorption coefficient due to the presence of particulates
\( n \) : refractive index
\( \sigma \) : Stefan-Boltzmann constant (5.669 \times 10^{-8} \text{ W/m}^2\text{K}^4)

\( a_p \) : equivalent particle scattering factor
\( I \) : radiation intensity (W/sr)
\( E_P \) : equivalent emission
\( T \) : local temperature (K)
\( \Phi \) : phase function
\( \Omega' \) : solid angle

Weighted Sum of Gray Gases Model (WSGGM)

Radiation heat source is included in the source term in the energy equation.
Coal Reaction sub model

Evaporation

\[
\frac{dm_p}{dt} = -A_p k c \rho_\infty \ln(1 + B_m)
\]

- \( m_p \): water droplet mass (kg)
- \( k \): mass transfer coefficient (m/s)

Devolatilization

Homogeneous reaction

- \( A_r \): droplet surface area (m²)
- \( \rho_\infty \): density of bulk gas (kg/m³)

- \( R_1 \) and \( R_2 \): competing rates that control the devolatilization over different temperature ranges.
- \( m_{v}\): volatilized mass at time \( t \) (kg)
- \( m_{a} \): ash content of coal (kg)
- \( m_{m} \): initial coal particle mass (kg)
- \( \xi_{w,0} \): mass fraction of evaporating/boiling material

- \( k_{mix} \): turbulence mixing rate
- \( k \): function of turbulence kinetic energy
- \( \varepsilon \): dissipation rate of turbulence kinetic energy
- \( x_R \) and \( x_P \): mole fractions of reactant \( x_R \) and product \( x_P \)
- \( C_1 \) and \( C_2 \): molar concentrations of the first and second reactants
- \( m \): exponent of temperature
- \( E_r \): activation energy (J/mol)
- \( A \): pre-exponential factor
- \( R \): universal gas constant (8314 J/mol·K)
- \( C_{1,2} \): concentration of a third species
- \( c \): corresponding reaction order.
Coal Reaction sub model

Heterogeneous reaction (Volume Reaction Model)

\[ \frac{dx}{dt} = \eta_r A_r P_i^n e^{-E_r / RT} (1 - x) \sqrt{1 - \psi \ln(1 - x)} \]

\( \eta_r \): effectiveness factor
\( A_r \): pre-exponential factor
\( E_r \): activation energy (J/mol)
\( P_i \): partial pressure of species \( i \) (Pa)
\( R \): universal gas constant (8314 J/mol K)
\( \psi \): pore structure parameter
\( n \): apparent reaction order

Heterogeneous reaction (Random Pore Model)

\( D_{0r} \): diffusion rate coefficient for reaction \( r \) (kg/m\(^2\)/sec/Pa\(^{0.5}\))
\( \rho_c \): bulk partial pressure of the gas phase (Pa)
\( \Delta P_{\text{kin},r} \): kinetic rate of reaction \( r \) (kg/m\(^2\)/sec/Pa\(^{0.5}\))

\( x \): carbon conversion of char particle
\( \eta_r \): effectiveness factor
\( A_r \): pre-exponential factor
\( E_r \): activation energy (J/mol)