An Euler-Euler CFD Model for Biomass Gasification in Fluidized Bed

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Objectives

- Provide MFIx-based Euler-Euler CFD models for polydisperse, reacting, variable density solid particles

- Facilitate the numerical simulation and scale up of energy systems such as gasifier
Background: Multiphysics & Multiscales

![Graphs showing y-component of velocity and axial height in bed](image)

- y-component of velocity (cm/s)
- Axial height in bed (cm)
- Averaged apparent density (g/cm³)

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**Physical**
- Density
- Size
- Drying

**Chemical**
- Volatile reaction
- Tar cracking
- Char oxidation and gasification
- Devolatilization

**Fuel**
- Biomass
- Volatiles (CO, CO₂, H₂, C₃H₆)
- Bio/Char

**Produced Gas**

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Polydisperse Biomass Gasification

May 22-24
Physical Models

- Spherical particle assumption
- Porosity and moisture modeled
- Uniform conversion model for micro-particles
  - Constant particle diameter ($d_p$)
  - Variable particle density ($\rho_p$) with increasing pores
  - Intra-particle transport ignored for micro-particle
- Couple continuity and species equation to update $\rho_p$

\[
\frac{1}{\rho_{\text{apparent}}} = \sum_{n=1}^{N} \frac{X_{s,n}}{(\rho_n)_{\text{true}}}
\]
Chemical Models

- **Devolatilization:** Biomass $\rightarrow$ light gas (CO, CO$_2$, H$_2$, CH$_4$) + tar + char + H$_2$O
- **Tar reaction:** Tar (g) $\rightarrow$ light gas (CO+ CO$_2$ + H$_2$ + CH$_4$ + H$_2$O) + inert Tar
- **Volatile reaction:**
  - Carbon monoxide oxidation: CO + 1/2 O$_2$ $\rightarrow$ CO$_2$
  - Hydrogen oxidation: H$_2$ + 1/2 O$_2$ $\rightarrow$ H$_2$O
  - Methane oxidation: CH$_4$ + 2 O$_2$ $\rightarrow$ CO$_2$ + 2 H$_2$O
  - Water-gas shift: CO + H$_2$O $\leftrightarrow$ CO$_2$ + H$_2$

**Char combustion**
- Partial combustion: C + 1/2 O$_2$ $\rightarrow$ CO

**Char gasification:**
- Boudouard reaction: C + CO$_2$ $\rightarrow$ 2 CO
- Steam gasification: C + H$_2$O $\rightarrow$ CO + H$_2$
- Hydrogen gasification: C + 2 H$_2$ $\rightarrow$ CH$_4$

Reaction rate based on $\text{min}[k = \exp[-E/RT], C(2\bar{S}_{ij}\bar{S}_{ij})^{1/2}]$
Implementation in MFIX-Continuum

- Time-splitting approach coupling hydrodynamics and kinetics
  \[ \phi(t) \xrightarrow{\text{transport}} \phi^*(t + \Delta t) \xrightarrow{\text{chemical reaction}} \phi(t + \Delta t) \]

- Synchronized time-step for transport and reaction

![Diagram](image-url)
A Lab-scale Fluidized-bed Reactor

- syngas
- biomass
- air (N$_2$+O$_2$) / steam

Dimensions:
- 3.81 cm
- 10.62 cm
- 34.29 cm
## Simulation Conditions

<table>
<thead>
<tr>
<th>Phase</th>
<th>Species (n)</th>
<th>$X_n$</th>
<th>$T$ (K)</th>
<th>$\epsilon_g, \epsilon_{sm}$</th>
<th>$\rho_{true}$ (g/cm$^3$)</th>
<th>$d$ (cm)</th>
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<td></td>
<td>void</td>
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<td>same as gas</td>
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</table>

$^a$ equation of state for an ideal gas
$^b$ includes CO, CO$_2$, H$_2$O, H$_2$, CH$_4$
$^c$ includes active tar and inert tar
$^d$ air fuel ratio ($\dot{m}_{air}/\dot{m}_{biomass}$) is 1.5
## Simulation Cases

<table>
<thead>
<tr>
<th>Cases</th>
<th>air/biomass ratio</th>
<th>biomass moisture (wt%)</th>
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<td>base</td>
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<td>1.5</td>
<td>25</td>
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</table>
Convergency History

- Gas Temperature and mass inside reactor

![Graph showing temperature and mass over time]

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Biomass Apparent Density

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Time- and Spatial-Averaged Density and Temperature (160-200 s)

- y-component of velocity (cm/s)
  - Axial height in bed (cm)
  - Averaged apparent density (g/cm³)
  - y-velocity
  - Apparent density

- Averaged temperature (K)
  - Axial height in bed (cm)
  - Averaged temperature (K)
  - Gas phase
  - Sand phase
  - Biomass phase
Gas Molar Fraction @180 s

- O2
- N2
- CO
- H2
- CO2
- CH4
- Tar
Biomass Mass Fraction @180 s

Bio

Char

Pore

Ash

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Polydisperse Biomass Gasification
May 22-24
Mass Flow Ratio (Air/Biomass)

Gas composition vs. mass flow ratio

Product yield vs. mass flow ratio

CO, CO₂, H₂, CH₄, Tar, N₂
Bed Temperature

Gas composition vs. temperature

Product yield vs. temperature
Moisture Content

Gas composition vs. moisture content

Product yield vs. moisture content
Variable particle density implemented for modeling bio-particle transport

Biomass (wood) gasification kinetics implemented

The model captures the key features of gasification

Different conditions tested
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