Strategies to improve 3D simulation accuracy using 1D simulation for CFB boilers

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CFBC research activities at FEP CRC

Process simulation
- Experimental data, Plant efficiency

Numerical simulation
- Experimental data, Hydrodynamics/Reactions, Design evaluation

Dynamic simulation
- Operating datad, Steam-water side dynamics

0.1 MWth test-rig

Oxy-CFBC Preliminary test/Operating methods

2 MWe SC-Oxy-KIER CFBC

Material research of USC power plants
- USC material properties
- Reliability analysis data, Selection of USC material, Provide material lifetime

USC steam characteristics, Design and operation data

USC circuit test-rig

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USC circuit test-rig
Numerical simulation of 0.1 MW_{th} CFB combustor

0.1 MW_{th} Test-rig (FEP CRC)
Numerical simulation of 2 MW_e CFB boiler

2MW_e Demonstration plant

2 MW_e CFB Boiler (FEP CRC)

- 3D simulation results of 2 MW_e CFB boiler -

Solids volume fraction (-)

Gas composition (O_2, mass fraction)

Gas composition (CO_2, mass fraction)

1D 해석결과 3D 해석결과 exp

Height (m)

Concentration (ppm)

0 20 40 60 80 100 120

O2 CO2 N2 H2O CO
Numerical simulation of 2 MW$_e$ Oxy-CFB Boiler

Particle Volume Fraction

Solids volume fraction

Gas composition

Oxy combustion of 2 MW$_e$ CFB Boiler (FEP CRC)
Correct problem definitions of CFB boiler simulations

Topology of 966MW$_{th}$ supercritical CFB boiler

Ref. : 3D simulation of a commercial CFB boiler (KITECH, Seentec)
### Best practices for effective modeling with Barracuda

<table>
<thead>
<tr>
<th>#</th>
<th>Tips</th>
<th>Details</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Know expected fluidization</td>
<td>Check the Geldart particle classification and Flow regime</td>
</tr>
</tbody>
</table>
| 2  | Use available data to improve particle characterization | Verify that the particle specifications are consistent with experimental data  
- PSD and $d_{32}$  
- Sphericity, $\phi$  
- Close-pack particle volume fraction, $\varepsilon_{mf}$  |
| 3  | Verify the bed mass       |  
- history.log contains a more complete inventory of solids than the estimate from pressure drop  
- Understand the bed mass estimate  
- Place transient data points for pressure in the model to compare simulated pressure drop with Operation  |
| 4  | Use a Mass and Energy balance | Mass and energy balances are important when system contains any of the following:  
- Complex reaction scheme / Inexact components (i.e. biomass, coal, etc)  
- Strongly exothermic / endothermic reactions  
- Verify that reactant feeds and reaction scheme can produce expected gas composition under any conditions  
- Inform assumptions about material thermal properties such as heat of formation and heat capacity  
- Determine whether any significant reactions, heat losses, inputs are missing  |
| 5  | Use cyclone inlet pressure to control vessel Pressure |  
- Place a transient data point for pressure at the location where vessel pressure is measured.  
- Use SFF file for pressure BC. Initially set BC pressure to vessel pressure.  
- Periodically update SFF file to minimize difference btw simulated vessel pressure & target vessel pressure  
- Reread BC's through Interact  |
| 6  |                          | .....                                                                                                                                 |

Ref. : Advanced Best Practices: Effective Modeling with Barracuda VR 2015 CPFD user’s conference

- Total amount of solid in the boiler  
- Types and properties of particles in the boiler  
- Size distribution of each particle  
- What is the axial solid volume fraction in the boiler?  
- How much solid is circulating in the boiler?  
- What is the change in solid retention in the boiler due to load changes?  
- How much solid is coming down in the annulus region in the boiler?  
- Can you predict the change in the properties of solids due to the change in boiler operation time?  
- Can you predict the boiler's performance for fuel changes?
Characteristic flow pattern in a CFB boiler

Ref.: A. Blaszczuk et al. / Powder Technology 246 (2013) 317–326

Estimations of axial solid volume fraction in a riser

Kunii and Levenspiel model  Johnsson and Leckner model

\[ \varepsilon_s = \varepsilon_s,0 \cdot e^{-K(h - H_0)} \]
\[ \varepsilon_s,db = \varepsilon_s,0 \cdot e^{-K(h - H_0)} \]
\[ \varepsilon_s,d = \varepsilon_s,db + \varepsilon_s,db \]

Ref: C Yang, J Jeong, Y Kim, B Bang, U Lee, Powder Technology 393, (2021) 786-795
12MW\textsubscript{th} CFB boiler of Chalmers Univ. of Tech.
Operating conditions of the CUT 12MW_{th} CFB boiler

<table>
<thead>
<tr>
<th>Coal feeding rate (kg/s)</th>
<th>0.27</th>
</tr>
</thead>
<tbody>
<tr>
<td>Primary air (Nm³/h)</td>
<td>2.26</td>
</tr>
<tr>
<td>Secondary air (Nm³/h)</td>
<td>none</td>
</tr>
<tr>
<td>Superficial velocity (m/s)</td>
<td>4.7</td>
</tr>
<tr>
<td>Pressure drop (Pa)</td>
<td>9,500</td>
</tr>
<tr>
<td>The average diameter of coal particle (mm)</td>
<td>0.79</td>
</tr>
<tr>
<td>The average diameter of sand particle (mm)</td>
<td>0.22</td>
</tr>
</tbody>
</table>

Schematic of the CUT 12MW_{th} CFB boiler

Initial particle size distribution of coal and sand
The 1D simulation was conducted with varying decay constant ‘K’.

<table>
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<th>Operating conditions</th>
<th>Run 1*</th>
</tr>
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<tr>
<td>Coal feeding rate (kg/s)</td>
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</tr>
<tr>
<td>Primary air (Nm³/h)</td>
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<td>-</td>
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<td>4.7</td>
</tr>
<tr>
<td>Pressure drop, Pa</td>
<td>9,500</td>
</tr>
<tr>
<td>Particle mean diameter, mm</td>
<td>0.32</td>
</tr>
</tbody>
</table>

*Johnsson and Leckner, 1995

Operating conditions of the Chalmers CFB boiler
<Chalmers CFB boiler(12 MW_th)> Comparison of 1-D simulation with experimental value

1) Different gas velocity (mean particle size: 0.32 mm)

2) Different particle size (gas velocity: 2.7 m/s)

Calculation condition

<table>
<thead>
<tr>
<th>Gas velocity(m/s)</th>
<th>4.7</th>
<th>3.5</th>
<th>2.7</th>
<th>1.8</th>
</tr>
</thead>
<tbody>
<tr>
<td>Riser pressure drop(Pa)</td>
<td>9500</td>
<td>8200</td>
<td>8500</td>
<td>7700</td>
</tr>
<tr>
<td>a</td>
<td>4</td>
<td>4</td>
<td>8</td>
<td>12</td>
</tr>
<tr>
<td>K</td>
<td>0.7</td>
<td>0.15</td>
<td>0.23</td>
<td>0.023</td>
</tr>
<tr>
<td>Feed inert(kg/s)</td>
<td>0.05</td>
<td>0.06</td>
<td>0.09</td>
<td>0.09</td>
</tr>
</tbody>
</table>

Mean particle size(mm) | 0.2 | 0.32 | 0.44 |
Riser pressure drop(Pa) | 10500 | 8500 | 8000 |
| a | 4.5 | 8 | 12 |
| K | 0.23 | 0.23 | 0.023 |
| Feed inert(kg/s) | 0.05 | 0.09 | 0.05 |
The whole PSD (char + sand) profiles in CTH have an almost same peak and the peaks are shifted toward fine particle sizes with increasing furnace height.

In the 1D results, these peaks also are shifted to fine particle sizes and the mean particle diameter has changed along the height.
Comparison of axial pressure profile between experiments and 1D simulation results

Effects of sand attrition coefficients

Effects of fuel fragmentation coefficients
Distribution of axial pressure drop (a) and solids concentration (b) along the height.

**Diagram (a):**
- **Experiment**
- **Simulation**
- \( K = \frac{0.8}{(u-u_t)}, a = 6u_t/u \)
- Attrition coefficient: 3.5E-6
- Fragmentation coefficient: 1.0

**Diagram (b):**
- **Experiment**
- **Simulation**
- \( K = \frac{0.8}{(u-u_t)}, a = 6u_t/u \)
- Attrition coefficient: 3.5E-6
- Fragmentation coefficient: 1.0
PSD of inert (silica sand only) and whole bed materials

Sold mass fraction (Sand)

CTH_H=0.56m
IEA2.3.4

Sold mass fraction (Sand + Char/Ash)

CTH_H=0.56m
IEA2.3.4
Change of PSD along with the height of the riser

- CTH_H=0.56m
- CTH_H=3.7m
- CTH_H=5.35m
- CTH_H=7.9m
Axial pressure drop of Chalmers boiler
(Experiments, 3D CFD results with different inputs)
0.1 MW_{th} test-rig simulation results

− Result – Hydrodynamic characteristics

[Diagrams showing fluid velocity, solid volume fraction, particle size, and fluid pressure contours]
0.1 \text{ MW}_{th} \text{ test-rig simulation results}

\section*{Result – Temperature & combustion gas compositions}

\begin{itemize}
  \item \textit{Fluid temperature contour (K)}
  \item \textit{Temperature profile (oxy-40\%)}
  \item \textit{Temperature profile (oxy-50\%)}
  \item \textit{Temperature profile (oxy-60\%)}
  \item \textit{Flue gas compositions through flow time}
  \item \textit{Flue gas compositions (oxy-40\%)}
  \item \textit{Flue gas compositions (oxy-50\%)}
  \item \textit{Flue gas compositions (oxy-60\%)}
\end{itemize}
Welcome to FBRBuddy

Fluidized Bed Reactor Simulator

- CFBuddy: Numerical simulation of CFB reactors
- BFBuddy/DFBuddy: Numerical simulation of BFB and DFB reactors
- DesignBuddy: Conceptual design of a fluidized bed

Operating conditions and pre-calculation

Fuel Data Base Management

Derivation of reactor design data
Welcome to FBRBuddy

Fluidized Bed Reactor Simulator

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Problem definition for a 3D simulation (Barracuda/OpenFoam)

Numerical simulation of a BFB reactor

Big data generation and management
Important features of CFBuddy

Major functions (Project management, Analysis):
- Project setting,
- Model selection,
- Operating conditions (Thermal input, operating conditions, pre-calculation)
- Simulation results
- Reports
- Various additional functions for analysis

Important features of CFBuddy:
- General condition
- Input condition (Geometry, Particle, Fluid property, Particle property, PSD)
- Analysis condition
- Boundary conditions
- Reaction parameter
1. Interactive online CFB boiler manual based on CFD
   • Interactive guide for design and operation
   • Boiler performance check & improvement
   • Training of operator-linking with existing simulator
   • Smart boiler management system

2. CFB boiler design S/W based on simulation
   • Conceptual/Basic design verification
   • Preliminary design for bidding

3. Operation support based on multidimensional simulation
   • 1D CFB simulator with GUI
   • 1D-3D CFD co-simulation for fluidized bed systems

4. Machine learning-based CFB boiler optimization
   • Big data generation
   • Correlation of big data from operation and CFD
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