Multiphase CFD Modelling at CSIRO

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Hybrid TFM-DEM

Coal Beneficiation Fluidised Bed
Coal Beneficiation Fluidized Bed

- Process for separating lighter coal from denser gangue particles
- Magnetite bed material $\rho = 4200 \text{ kg/m}^3$ $\phi = 200\mu\text{m}$
- Fluidized with air @ 25°C
- Coal $\rho = 1400-2700 \text{ kg/m}^3$ $\phi = 1.3-6.7\text{m}$

Numerical Approaches for Gas-Particle Systems

EE methods

1. Coarse-grid
   - Filter size

2. TFM
   - Continuous solid field
   - KTGF

3. Continuous fluid field
   - Volume/ensemble averaging

4. DEM/PPM
   - Discrete entities

5. CFD DEM
   - MDS LB PPM

6. DNS DEM
   - MP-PIC

EL methods

1. CFD

2. CPFD

3. TFM-DEM

4. TFM-DEM Hybrid Model

5. Inter-exchange

Traditional

Alternative

Computational cost (in exponential increase)

Length Scale

- 10m
- 1m
- 0.1m
- 0.01m
Segregation behaviour with coal diameter

Coal particle φ3 mm  Coal particle φ4.3 mm  Coal particle φ6.7 mm

Air velocity 0.1 m/s = 1.5 \( U_{mf} \) | Bed of 200µm magnetite particles: \( \rho = 4200 \text{ kg/m}^3 \)

Predicted and Measured

<table>
<thead>
<tr>
<th>Experiment</th>
<th>Coal particles</th>
<th>Gangue particles</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>In experiment:</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td>Coal particles</td>
<td>$d_{ds}=1-2\text{mm}$</td>
<td>$d_{ds}=3-5.5\text{mm}$</td>
</tr>
<tr>
<td>$\bar{\rho}_{ds}=1.40 \text{ g/cm}^3$</td>
<td>$\bar{\rho}_{ds}=1.38 \text{ g/cm}^3$</td>
<td></td>
</tr>
</tbody>
</table>

Effect of fluidizing velocity

Fluidised Bed Coker

Coarse Grain Modelling
1/19th Scale Syncrude Coker Geometry & BCs

From Song et al. (2004) Powder Tech. 147, 126-136
Nozzle treatment - Resolved

- Six levels of feed nozzles
- Total of 92 feed nozzles
- 5.5mm square section
- 20 attrition nozzle
- 3mm square section
- Mesh not good resolution of nozzle exit
Nozzle treatment – Sources

- Nozzles not resolved
- Mass and momentum added using source terms
- Merry jet penetration used to calculate source location

\[
\frac{L}{d_o} = 5.25 \left[ \frac{\rho_o u_o^2}{(1 - \alpha_g) \rho_s g d_p} \right]^{0.4} \left( \frac{\rho_g}{\rho_s} \right)^{0.2} \left( \frac{d_p}{d_o} \right)^{0.2} - 4.5
\]

- Jet length taken as 58% of Merry length
- Based on Li (2009) GLAB report
- Distributed along length of jet mass : 15%, 15%, 70% mom : 40%, 50%, 10%
Stage 2 – Coarse Grain Model - Drag

- Coarse grain model of Igci-Sundaresan.
- Corrections to drag, solids viscosity and solid pressure to account for sub-grid clustering effects

\[ \beta = \beta_{\text{micro}} \left[ 1 - \frac{Fr_{\text{filter}}^{-1.6}}{Fr_{\text{filter}}^{-1.6} + 0.4} h(\alpha_s) \right] \]

Where \( \beta_{\text{micro}} \) is the micro-scale drag term, Gidaspow model used here.

\[ \frac{\beta}{\beta_{\text{micro}}} = (1 - ch(\alpha_s)) \]

(\( h() \) is a complex function of volume fraction
\( Fr_{\text{filter}} \) is Froude number based on filter length)

Igci, Pannala, Benyahia & Sundaresan (2012)
Results – Drag Models

- Voidage – Good agreement mostly.
- Upper section over predicted
- Velocity over predicted in top and centre
- Up and down flow boundary reasonable

8 [s] – Coarse Grain CG4
6 [s] – Coarse Grain CG3
14 [s] – Gidaspow
- Song et al. (2003)
Solid Tracers

Solid Tracer at standpipe

Gives average solid velocity of 1.6 [m/s] c.f. measured velocity of 0.9 [m/s]
Tracer Residence Times

Tracer Break Through Times

<table>
<thead>
<tr>
<th></th>
<th>Tracer 1</th>
<th>Tracer 2</th>
<th>Tracer 3</th>
<th>Tracer 4</th>
<th>Tracer 5</th>
<th>Average</th>
</tr>
</thead>
<tbody>
<tr>
<td>Solid Break through Time [s]</td>
<td>0.61</td>
<td>0.55</td>
<td>0.49</td>
<td>0.6</td>
<td>0.66</td>
<td>0.582</td>
</tr>
<tr>
<td>Gas Break through Time [s]</td>
<td>0.2</td>
<td>0.28</td>
<td>0.21</td>
<td>0.25</td>
<td>0.23</td>
<td>0.234</td>
</tr>
</tbody>
</table>

Gives average solid velocity of 1.6 [m/s] c.f. measured velocity of 0.9 [m/s]
Feed Nozzle Model

- 2D axi-symmetric
- 2 / 3 Phase
  steam / bitumen
  steam / bitumen / coke
- Phase inversion bubble to drops
- Number density model for bubble/drop diameter
- Based on work from UBC Pougatch et al.
Feed Nozzle Model

Discharging into air

Gas Volume Fraction

Liquid Volume Fraction

Bubble Diameter [m]

Drop Diameter [m]
Comparison to Measurements
Feed Nozzle into a Fluidized Bed

- 2D model not really adequate
- 3D transient model needed
- Sources for momentum, gas and liquid deposition could be determined
- Sources used in full coker model to improve results
Thickener Modelling

Two phase slurry flow with Population Balance
AMIRA P266 Improved Thickener Technology

- Multi sponsor project over 20 yrs
- 21 Industrial Customers
- Over $750mil NPV savings
- Multiphase slurry flow
  - CFD & UVP measurements
- Flocculation Expt. & Population balance, CFD
- Slurry unified rheology:
  - Hindered settling
  - Sedimentation
  - Yield stress
- Raking
- Control
Solid-liquid separation in thickener/clarifier

- Continuous gravity settling tank
- High solid underflow, clear overflow
- Feedwell dissipates feed momentum + mixing chamber to flocculate particles to increase settling rate.
Flocculation Process

1. Turbulent flocculant/particle mixing
2. Flocculant adsorption (turbulent collision)
3. Aggregation (turbulent collision)
4. Breakage (turbulent shear)
Combined population balance & CFD model

Mean aggregate size

- Full PB size distribution in each cell
- ~100,000-500,000 nodes
- Coded as Fortran subroutine in CFX-4, CFX-5 & OpenFOAM
- Fully coupled to flow solution (viscosity, settling velocity, shear)
- Allows feedwell optimisation (geometry, flocculant addition point, dilution)

Pilot-scale validation

Feedwell sub-model validation

CFD simulation:
- very similar flow structures
- velocity profiles agree well

LDV time-averaged velocity measurements in a model feedwell

Aggregate size measured by Lasentec probe at feedwell outlet and compared to CFD prediction.
Feedwell Design Improvements

Closed feedwell – current design

Main features:

- New concept: separate zones for momentum dissipation and flocculation
- Ability to cope with wide range of feed variations
- Simple design and easy to manufacture and retrofit

CSIRO Novel feedwell
Potential for Control …

Carry out a matrix of CFD simulations

Develop surrogate models to cover the window of operating conditions

- CFD is not being used for control.
- Interrogation of surrogates is simple/rapid.

Interrogate surrogates as part of thickener control on the basis of monitored feed properties
**Example 1-to-1 CFD (Sunrise Dam)**

**Problem:**
- Paste thickener treating gold tailings that are then pumped to a central tailings discharge area.
- Low underflow density 55 wt%, low yield stress (7-12 Pa).
- Severely shear thinning; zero beach angle limits storage capacity.

**Approach:**
- CFD model used to determine factors limiting flocculation efficiency within the full-scale feedwell.

**Recommendation:**
- Install half-shelf and remove existing baffles.
- Add flocculant through two specific sparges locations.

**After:**
- Underflow density increased to 60-66 wt%, gave beach angle 2°.
- Eliminated need to duplicate Tailings Storage Facility (saved $20 m).
- Increased water recovery, reduced flocculant dosage, reduced cyanide to tailings (saved >$0.15 m pa).

*Images and outcomes courtesy of AngloGold Ashanti*
Aluminium Electrolysis Process

Multi-phase & Multi-physics Modelling
Reduction of Alumina to Al Metal
Aluminium Electrolysis Process

• 15g Coke can requires 0.9kWh elec.
40W globe 23hrs or 11 laptop batteries @ 0.08kWh
• Aluminium metal refined from alumina.
• Operates at ≈960°C.
• Very high electric currents and magnetic fields.
• Lorentz, Marangoni & electro-chemical effects

The schematic diagram of one cell

Al$_2$O$_3$ powder
CO$_2$ (g)

Current 150 – 600 kA

Carbon anode
Cryolite melt (bath) (960°C)
Al (l)

Cathode

Cell 1

Cell 2

Al$_2$O$_3$
Multi-physics in Al Reduction Cells

Aim to:
- Save energy;
- Increase current efficiency;
- Optimize cell’s operation and design;
- Develop new cells

**Electric Field**
- Current Density Distribution
- Electric Field Distribution

**Electromagnetic Effect**

**Magnetic Field**
- Magnetic Field Distribution

**Flow Field**
- Electrolyte Flow
- Metal Flow/Variation
- Anode Effect

**Anodic Bubble**
- \( \text{Al}_2\text{O}_3 \) dissolution and diffusion; Al dissolution and diffusion; bath-metal interface variation; ledge profile; sludge et.al

**Thermal Field**
- Temperature Distribution
- Ledge Profile
- Energy Balance
- Phase Transition
- Thermal Stability

**Thermal Expansion**

**Thermal-stress Distribution**

**Stress Field**
- Deformation

**Joule Effect**

**Erosion**
Multi-scale, Multi-physics Simulation Environment

Prep
MHD flow + Bubble flow = Bath flow

Proc
Bath flow + Transient feeding curve = Species concentrations

Mesh adjustments:

• Dynamic tracking of Bath/Metal interface using Fluent VOF (volume fraction 0.5) and sliding mesh approach to adjust anode bottom shape to metal pad profile

• Spring smooth is used to improve volume mesh quality

J. Hua et al, Light Metals 2014, 691
Steady state metal pad profile and MHD prediction

Simulation result:

Metal surface speed
• Metal pad surface speed transferred to full cell bath flow model

J. Hua et al, Light Metals 2014, 691
CSIRO’s integrated modelling approach to electrolyte modelling

CFD model development cycle

Water model

Macro-scale model

Micro-scale model

Plant measurements

Concept of likely critical design factors

Develop CFD model framework

Validate/Calibrate CFD model fundamentals

Detailed lab-scale flow measurements

Plant measurements

Validation/Calibrate plant model

Use CFD model to optimise/design

Plant trials

Determine additional critical factors

predict

validate

predict

validate

bubble dynamics
Air-Water flow in CSIRO 3 anode model

Bubble dynamics in ACD

Case 1 CO2-cryolite, contact angle $60^\circ$, $\sigma 0.132$ N/m, $\rho 0.4 / 2100$ kg/m$^3$

Case 2 Air-water, contact angle $120^\circ$, $\sigma 0.072$ N/m, $\rho 1.2 / 998$ kg/m$^3$

Case 3 Air-water, contact angle $60^\circ$, $\sigma 0.132$ N/m, $\rho 0.4 / 2100$ kg/m$^3$

Using bubble flow and resolved bubble models to improve two fluid model closures

Zhao, Zhang, Feng et.al., (2014) Australasian Fluid Mechanics Conference, Melbourne, Australia
Steady State Full Cell Bath Flow Model

Bath Flow Model – Steady State

• Eulerian-Eulerian, two-fluid model
• Conservation equations for phase mass and phase momentum (gas and cryolite)
• MHD forces & current density included (no induced currents and fields*)
• Modified $\kappa$-$\varepsilon$ turbulence model in liquid phase only.
• Bubble drag and phase turbulence from zero equation model.
• Time averaged gas distributions, gas & liquid velocities and turbulence quantities.
• Anode shape, metal pad profile & velocity boundary condition.

*) $\sigma_{\text{bath}} = 250 \text{ S/m, } \sigma_{\text{Al}} = 3000000 \text{ s/m}$
Modelling implementation

- Anodes of different age considered
- Ledge profile of sides and ends
- Metal pad profile

Steady State Full Cell Bath Flow Model
Steady State Full Cell Bath Flow Model

Simulation results

• Velocity field stable against temperature changes
• Velocity field stable against viscosity changes
• Turbulent viscosity 1000 time higher than bath viscosity
• High cross flow speed in area with no slots
Steady State Full Cell Bath Flow Model

Simulation results

• Gas accumulation below anode and in slot visible
• Simulation indicating performance deficit of anode toward end of anode cycle
• Reduced current flow under old anodes
• Coupling between gas generation and current
Transients Bubble and Chemical Reaction Flow Model

Model application

The impact of the slots for guiding the bubble from the anode bottom
Simulation results – Full Cell

• Underfeeding and overfeeding cycles can be evaluated

Critical areas can be identified

To low concentration => anode effect
To high concentration => sludging

Modelling approach

Transient transport model

• Time averaged fluxes used to transport of reacting species

• Steady state bath flow field is fixed boundary condition.

• Chemical reaction model with 6 species developed
Conclusion

Presented multi-scale & multi-physic examples of where we have used CFD for industrial applications including:

- Hybrid TFM-DEM model for Coal Beneficiation Fluidised Bed
- Coarse grain simulation of a coker
- Population balance model for slurry flow in a thickener
- Hall-Héroult aluminium reduction cell

Further improvements needed in sub-model (drag, turbulence..)
Better ways to link resolved models to large scale “process” models
Twelfth International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries
30 May – 1 June 2017, Trondheim, Norway

Announcement:
SINTEF to organise next conference in Norway.

Industries Covered:
- Pragmatic industrial modelling
- Oil & Gas pipeflow & processing
- Chemical processing
- Multiscale modelling
- CFD in Cardiovascular medicine
- Metallurgical applications
- Others…

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