

### **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  $ρ = 4200 kg/m<sup>3</sup> φ = 200μm$
- Fluidized with air @ 25°C
- Coal  $p = 1400 2700$  kg/m<sup>3</sup>  $\phi = 1.3 6.7$ m





**Qinggong Wang et al. (2015) Chem. Eng J. 260, 240-257**

### **Numerical Approaches for Gas-Particle Systems**



![](_page_3_Picture_2.jpeg)

### **Segregation behaviour with coal diameter**

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

![](_page_4_Figure_4.jpeg)

Air velocity 0.1 m/s = 1.5 U<sub>mf</sub> | Bed of 200µm magnetite particles:  $\rho = 4200 \text{ kg/m}^3$ 

**Qinggong Wang et al. (2015) Chem. Eng J. 260, 240-257**

5 | Peter Witt | NETL Workshop, 9-10 August 2016

![](_page_4_Picture_8.jpeg)

### **Predicted and Measured**

![](_page_5_Figure_1.jpeg)

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**Qinggong Wang et al. (2015) Chem. Eng J. 260, 240-257**

## **Effect of fluidizing velocity**

![](_page_6_Figure_1.jpeg)

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# **Fluidised Bed Coker**

# **Coase Grain Modelling**

![](_page_7_Picture_2.jpeg)

![](_page_7_Picture_3.jpeg)

![](_page_7_Picture_4.jpeg)

### **1/19th Scale Syncrude Coker Geometry & BCs**

![](_page_8_Figure_1.jpeg)

![](_page_8_Picture_2.jpeg)

### **Nozzle treatment - Resolved**

![](_page_9_Picture_1.jpeg)

![](_page_9_Picture_2.jpeg)

![](_page_9_Picture_3.jpeg)

- 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

![](_page_9_Picture_10.jpeg)

### **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%

![](_page_10_Figure_8.jpeg)

![](_page_10_Picture_9.jpeg)

### **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

$$
\beta = \beta_{micro} \left[ 1 - \frac{Fr_{filter}^{-1.6}}{Fr_{filter}^{-1.6} + 0.4} h(\alpha_s) \right]
$$
  $h()$  is a complex function of volume fraction  
where  $\beta_{micro}$  is the micro-scale drag term, Gidaspow model used here.

![](_page_11_Figure_4.jpeg)

![](_page_11_Figure_5.jpeg)

![](_page_11_Picture_6.jpeg)

### **Results – Drag Models**

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

![](_page_12_Figure_5.jpeg)

![](_page_12_Figure_6.jpeg)

**Time averaged** 

![](_page_12_Picture_7.jpeg)

•

14 [s] – *Gidaspow* 

Song *et al.* (2003)

### **Solid Tracers**

#### **Solid Tracer at standpipe**

![](_page_13_Figure_2.jpeg)

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

![](_page_13_Figure_4.jpeg)

![](_page_13_Picture_5.jpeg)

![](_page_14_Figure_0.jpeg)

#### **Tracer Break Through Times**

![](_page_14_Picture_283.jpeg)

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

![](_page_14_Picture_4.jpeg)

### **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 *etal.*

![](_page_15_Figure_6.jpeg)

![](_page_15_Picture_7.jpeg)

### **Feed Nozzle Model**

### **Discharging into air**

#### **Gas Volume Fraction**

![](_page_16_Figure_3.jpeg)

![](_page_16_Figure_4.jpeg)

#### **Bubble Diameter [m]**

![](_page_16_Figure_6.jpeg)

#### **Drop Diameter [m]**

![](_page_16_Figure_8.jpeg)

![](_page_16_Picture_9.jpeg)

### **Comparison to Measurements**

![](_page_17_Figure_1.jpeg)

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## **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

![](_page_18_Picture_5.jpeg)

# **Thickener Modelling**

# **Two phase slurry flow with Population Balance**

![](_page_19_Picture_2.jpeg)

### **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

![](_page_20_Figure_13.jpeg)

**OTAL** 

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## **Solid-liquid separation in thickener/clarifier**

![](_page_21_Figure_1.jpeg)

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

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### **Flocculation Process**

![](_page_22_Figure_1.jpeg)

 $\rightarrow$ 

**Turbulent flocculant/particle mixing**

**Flocculant adsorption (turbulent collision)**

**Aggregation (turbulent collision)**

**Breakage (turbulent shear)**

![](_page_22_Picture_6.jpeg)

![](_page_22_Picture_7.jpeg)

![](_page_22_Picture_8.jpeg)

![](_page_22_Picture_9.jpeg)

![](_page_22_Picture_10.jpeg)

![](_page_22_Picture_11.jpeg)

## **Combined population balance & CFD model**

![](_page_23_Figure_1.jpeg)

- **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)

![](_page_23_Figure_7.jpeg)

### **Feedwell sub-model validation**

![](_page_24_Figure_1.jpeg)

#### CFD simulation:

- very similar flow structures
- velocity profiles agree well

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

![](_page_24_Picture_6.jpeg)

### **Feedwell Design Improvements**

#### Closed feedwell – current design CSIRO Novel feedwell

![](_page_25_Figure_3.jpeg)

#### **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**

![](_page_25_Picture_8.jpeg)

### **Potential for Control …**

![](_page_26_Figure_1.jpeg)

Carry out a matrix of CFD simulations

![](_page_26_Figure_3.jpeg)

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

![](_page_26_Picture_8.jpeg)

### **Example 1-to-1 CFD (Sunrise Dam)**

![](_page_27_Picture_1.jpeg)

![](_page_27_Picture_2.jpeg)

![](_page_27_Picture_3.jpeg)

#### *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).

![](_page_27_Picture_17.jpeg)

# **Aluminium Electrolysis Process**

# **Multi-phase & Multi-physics Modelling**

![](_page_28_Picture_2.jpeg)

![](_page_28_Picture_3.jpeg)

### **Reduction of Alumina to Al Metal Aluminium Electrolysis Process**

![](_page_29_Picture_1.jpeg)

- 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

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![](_page_29_Figure_7.jpeg)

### **Multi-physics in Al Reduction Cells**

![](_page_30_Figure_1.jpeg)

![](_page_30_Picture_2.jpeg)

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

![](_page_31_Figure_1.jpeg)

### **Steady state metal pad profile and MHD prediction**

#### 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

![](_page_32_Figure_3.jpeg)

• Spring smooth is used to improve volume mesh quality

![](_page_32_Picture_5.jpeg)

J. Hua et al, Light Metals 2014, 691

![](_page_33_Figure_0.jpeg)

#### J. Hua et al, Light Metals 2014, 691

### **CSIRO's integrated modelling approach to electrolyte modelling**

CFD model development cycle

![](_page_34_Figure_2.jpeg)

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### **Air-Water flow in CSIRO 3 anode model**

![](_page_35_Picture_1.jpeg)

Feng et.al., (2010) J. Comp. Multiphase Flows 2(3) 179-188

![](_page_35_Picture_3.jpeg)

# **Bubble dynamics in ACD**

![](_page_36_Figure_1.jpeg)

function with time

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

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#### 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 κ-ε 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 S/m,  $\sigma_{\text{Al}}$  = 3000000 s/m

Witt et al, 10<sup>th</sup> Int. Conf. on CFD in Oil & Gas, Metallurgical &Proc. Ind. Trondheim, Norway

![](_page_37_Picture_12.jpeg)

#### **Modelling implementation**

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

![](_page_38_Figure_5.jpeg)

Witt et al, 10<sup>th</sup> Int. Conf. on CFD in Oil & Gas, Metallurgical &Proc. Ind. Trondheim, Norway

![](_page_38_Picture_7.jpeg)

#### **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

![](_page_39_Figure_6.jpeg)

Witt et al, 10<sup>th</sup> Int. Conf. on CFD in Oil & Gas, Metallurgical &Proc. Ind. Trondheim, Norway

![](_page_39_Figure_8.jpeg)

![](_page_39_Picture_10.jpeg)

#### **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

![](_page_40_Figure_5.jpeg)

![](_page_40_Picture_6.jpeg)

### **Transient Bubble and Chemical Reaction Flow Model**

#### **Model application**

The impact of the slots for guiding the bubble from the anode bottom

![](_page_41_Figure_3.jpeg)

### **Transient Alumina Reaction and Distribution Model**

#### **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

![](_page_42_Figure_6.jpeg)

![](_page_42_Figure_7.jpeg)

#### **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

![](_page_42_Picture_12.jpeg)

# **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
- Coase 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

![](_page_43_Picture_7.jpeg)

![](_page_44_Picture_0.jpeg)

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…

![](_page_44_Picture_13.jpeg)

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![](_page_44_Picture_16.jpeg)

### **Acknowledgements**

![](_page_45_Picture_1.jpeg)

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![](_page_45_Picture_3.jpeg)

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![](_page_45_Picture_5.jpeg)

**Mike Wormsbecker Kevin Reid Craig McKnight**

![](_page_45_Picture_7.jpeg)

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![](_page_45_Picture_11.jpeg)