Advanced Multi-Fluid Simulations of Flow in Centrifugal Contactors

Kent E. Wardle (kwardle@anl.gov)
Chemical Sciences and Engineering Division
Argonne National Laboratory

ANS Winter Meeting
1 November 2011
Annular Centrifugal Contactor

**Solvent Extraction Equipment**
- Packed Columns
- Pulsed Columns
- Mixer Settlers
- **Centrifugal Contactors**
  - Small size
    - Physical footprint
    - Nuclear criticality
  - Short residence time
    - Low process hold-up
    - Less solvent degradation
  - High extraction efficiency
  - High throughput
  - Quick start-up/shut-down
    - Maintain conc. profile
Role of CFD Modeling in Process Simulation and Equipment Design
Context: An illustrative example

1. User wants to run a SX process simulation using a “Next Gen” package
2. Given:
   1. User inputs
      - Flow rates, O/A ratios, equipment type, chemistry
   2. Settings (defaults?) for equipment type (should be $f(\text{size})$)
      - rotor/mixer speed (mixer-settler, centrifugal contactor)
      - pulse frequency/amplitude (pulsed column)
3. SX module requires parameters for EACH STAGE
   1. stage efficiency
   2. other phase carry-over (OPCO)
   3. (stage volume)
4. Where do these values come from?
   - Current ‘state of the art’
     - Estimation based on general experience for equipment type (i.e. educated guess)
     - Estimate may be ‘function’ of equipment size, but same values for all stages
   - We know better...
     - Stage performance parameters are strong function of local stage conditions which (varies between sections of process)
     - Stage phase volumes*, total mixing zone volume, interfacial area, residence time → CFD
Design/Operational Impacts of Contactor CFD Modeling

- Quantitative investigation of the effect of various design/operational parameters on stage performance (efficiency, OPCO)
  - annular gap size, vane configuration (number, shape)
  - rotor RPM, total flow rate, O/A

- Optimize stage design/operation for given process conditions
  - Per section customized design (e.g. CSSX Plant(s))
- Exploration of contactor operation with particles, third phase(s)
CFD of Centrifugal Contactors
Three-phase Water-Oil-Air Annular Mixing Simulation Using VOF-type Solver

- Only ‘large’ droplets are resolved (~1mm)
  - Actual droplet size, ~25 µm
  - ~5 µm mesh (Δx, ~50x smaller)
    - N ~ 1×10^{11} cells
    - Δt ~ 1×10^{-7} s
    - Cr limit, as Δx ↓, Δt ↓

\[
Cr = \frac{u \Delta t}{\Delta x} \approx 0.25
\]
Three-phase VOF Simulations of Coupled Mixing/Separation Zone

Time evolution of total liquid volume for each phase in the two regions: mixing —— separation ————
Development of Advanced Multi-fluid Solver
**Coupled Multi-fluid–VOF Model Equations**

**Momentum equations for each phase** $k$:

$$ \frac{\partial \left( \rho_k \alpha_k \vec{u}_k \right)}{\partial t} + (\rho_k \alpha_k \vec{u}_k \cdot \nabla) \vec{u}_k = -\alpha_k \nabla p + \nabla \cdot \left( \mu_k \alpha_k \nabla \vec{u}_k \right) + \rho_k \alpha_k \vec{g} + \vec{F}_{D,k} + \vec{F}_{s,k} $$

**Volume fraction transport**:

$$ \frac{\partial \alpha_k}{\partial t} + \vec{u}_k \cdot \nabla \alpha_k + \nabla \cdot \left( \vec{u}_c \alpha_k (1 - \alpha_k) \right) = 0 $$

**Interface compression velocity** [1]:

$$ \vec{u}_c = C_\alpha |\vec{u}| \frac{\nabla \alpha}{|\nabla \alpha|} $$

$$ C_\alpha = \begin{cases} 
0, & \text{no interface sharpening} \\
1, & \text{interface sharpening active} 
\end{cases} $$

Multifluid-VOF Coupling Example: Collapsing Liquid-Liquid Column

cAlpha parameter controls interface compression for multifluid solver
Interface capturing ON (left, cAlpha=1) vs. OFF (right, cAlpha=0)

With interface compression on (left), ‘droplets’ form immediately (t=0.25 s →) at resolvable scale based on mesh spacing
Ex: Collapsing Water Column, w/ cAlpha Switching [2]

\[ \gamma = \frac{|\nabla \alpha|}{\text{max}(|\nabla \alpha|)} \]

for \( \gamma \geq \gamma^* \), \( C_\alpha = 1 \)

Three-phase (Water-Oil-Air) Examples

• No cAlpha switching -- interface compression applied for air/water & air/oil interfaces only
• Water/oil interface treated with multi-fluid model w/ interphase drag model of Schiller-Naumann (‘blended’ scheme)
• Fixed droplet sizes \[^3\]
  - \(d_{\text{water}} = d_{\text{oil}} = 0.150 \text{ mm}\)
  - \(d_{\text{air}} = 1 \text{ mm}\)

Three-phase 2D Horizontal Settler *(Water-Oil-Air)*

- Inlet flow O/A = 1, initial gravity = 2g, @ t=20s gravity = 3g

---

- **No diverter disk** - Inlet flow O/A = 1, initial gravity = 2g, @ t=10s gravity = 3g

---

Time: 20.0 s

Time: 10.0 s
3D Annular Mixer

- Geometry similar to CINC-V2 mixing zone
  - \( r_{in} = 2.54 \text{ cm}, \ r_{out} = 3.17 \text{ cm} \)
  - height: 7 cm
  - initial liquid height: 2 cm water/oil
  - Rotor speed: 3600 RPM

- High shear at rotor surface requires interface sharpening to maintain liquid (multi-fluid only, two-phase✔️)

K. Wardle – Multi-Fluid Flow in Centrifugal Contactors – ANS Winter Meeting, November 1, 2011
Tee-fed Rotating Centrifuge with Baffles (Water-Oil-Air)

Partial Baffles (2), t=0 solution from VOF-only case

Full Baffles (4)

Time: 0.000 s

Time: 1.000 s

Time: 2.00 s
Annular Centrifugal Contactor (underway)

One-quarter section of contactor rotor
Initialize from two-phase, VOF-only solution
(t=1.75s shown)

Coupled mixing-, separation-zone
Initialize from VOF-only solution (t=0 shown)
Companion Experimental Effort: Multiphase Measurements in Solvent Extraction Equipment for CFD Validation
Contactor CFD Validation Using Electrical Resistance Tomography (ERT)

Contactor ERT (CERT) Facility
- Engineering-scale contactor (CINC V-5)
- Multiphase measurements using ERT
- HS-camera (Redlake X5plus, 500fps @ 4MP)

K. Wardle – Multi-Fluid Flow in Centrifugal Contactors – ANS Winter Meeting, November 1, 2011
Contactor CFD Validation Using Electrical Resistance Tomography (ERT)

Contactor ERT (CERT) Facility
- Engineering-scale contactor (CINC V-5)
- Multiphase measurements using ERT
- HS-camera (Redlake X5plus, 500fps @ 4MP)
Qualitative ERT Validation

ERT (array at TOP of vanes):
- tap water (\( \rho = 1 \)),
- 10 L/min,
- 1800RPM

Video (through vane plate):
- aqueous phase (\( \rho = 1.17 \)),
- 10 L/min,
- 1800RPM

(shows inlet orientation)

(has been mirrored match rotation of ERT measurement)
Comparison of Bottom/Top of Vanes Flow from CFD

- 3-phase simulation (600 ml/min, O/A = 1), VOF-only solver
- CINC V2 geometry
  - vane orientation shifted 45° relative to inlets, vanes go to outer wall
  - slightly larger vane-to-rotor gap
  - low mixing zone volume (lower relative flow rate)
Summary and Path Forward
Summary and Path Forward

Very Near Term (ongoing)

- Multifluid – VOF Solver
  - Testing and improvement of LES turbulence
    - Currently only implemented on mixture basis
    - Per-phase w/ interphase coupling may be needed
  - Application to full contactor model (coupled mixer/rotor geometry)
  - Resolution of residual numerical issues with multi-fluid coupling

FY12 Main Goals

- Implementation of droplet size distribution capturing
- Development of physics-based switching methodology for interface sharpening

Interface w/ Experimental Effort

- Identify specific validation test case
- Scaling required for direct comparison with ERT results (5-inch vs. 2-inch rotor)
Acknowledgements

- Chemical Sciences and Engineering Division
  - Candido Pereira and Ralph Leonard
- Industrial Tomography Systems
  - Jonathon Ritson and Edmund Talideh
- CINC Industries
  - Bret Sheldon and Chuck Harrison
- OpenCFD, Ltd.
  - Henry Weller and Mattijs Janssens

This work was supported by the U.S. Department of Energy, Office of Nuclear Energy, under Contract DE-AC02-06CH11357.

Government License Notice
The submitted manuscript has been created by UChicago Argonne, LLC, Operator of Argonne National Laboratory (“Argonne”). Argonne, a U.S. Department of Energy Office of Science laboratory, is operated under Contract No. DE-AC02-06CH11357. The U.S. Government retains for itself, and others acting on its behalf, a paid-up nonexclusive, irrevocable worldwide license in said article to reproduce, prepare derivative works, distribute copies to the public, and perform publicly and display publicly, by or on behalf of the Government.
Advanced Multi-Fluid Simulations of Flow in Centrifugal Contactors

Kent E. Wardle  (kwardle@anl.gov)
Chemical Sciences and Engineering Division
Argonne National Laboratory

ANS Winter Meeting
1 November 2011