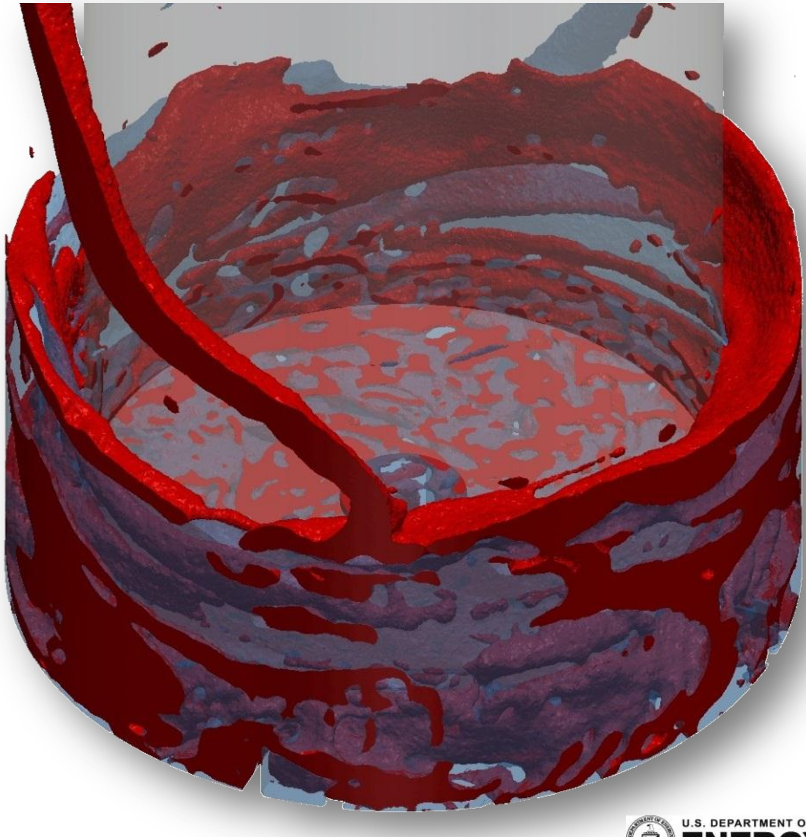
Advanced Multi-Fluid Simulations of Flow in Centrifugal Contactors



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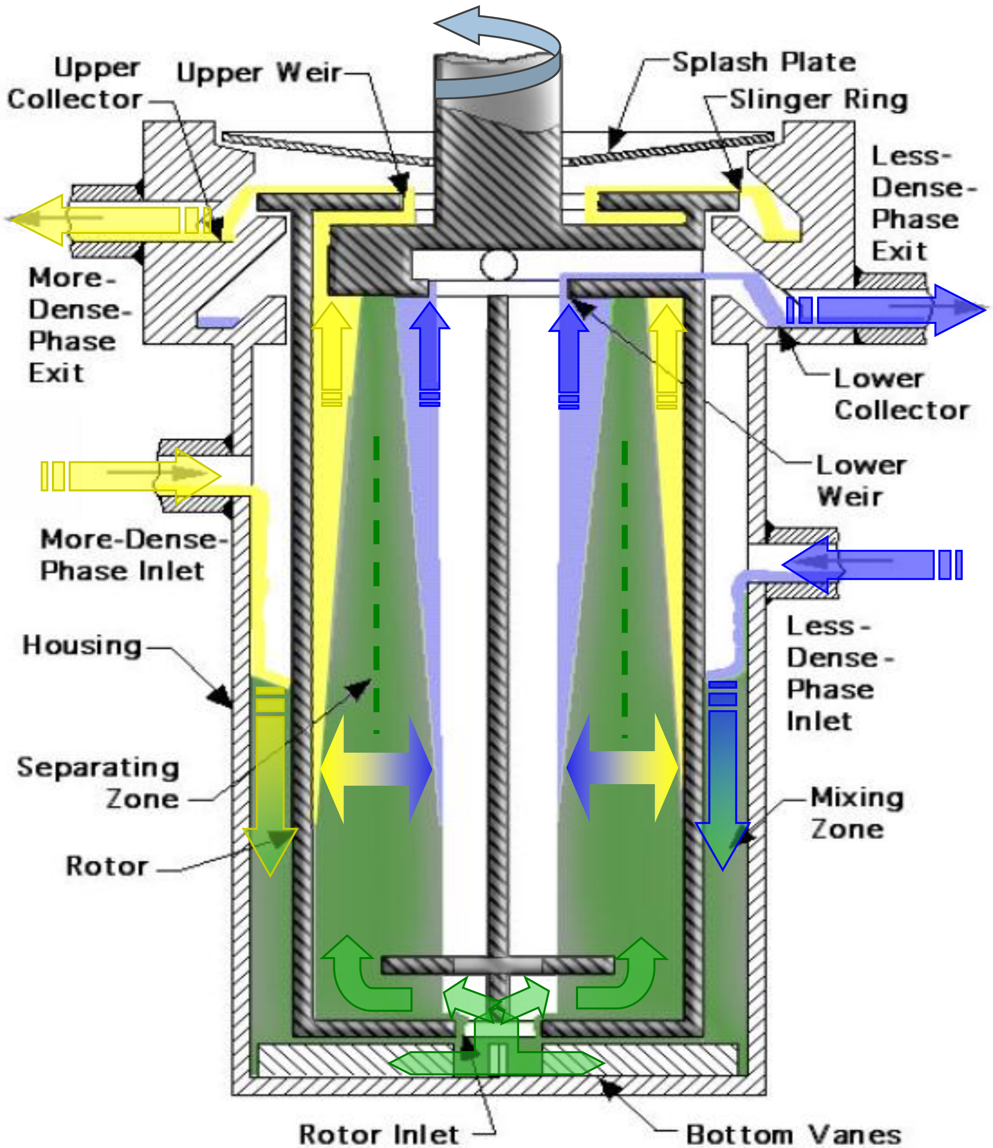
ANS Winter Meeting
1 November 2011

Annular Centrifugal Contactor

<u>Solvent Extraction Equipment</u>

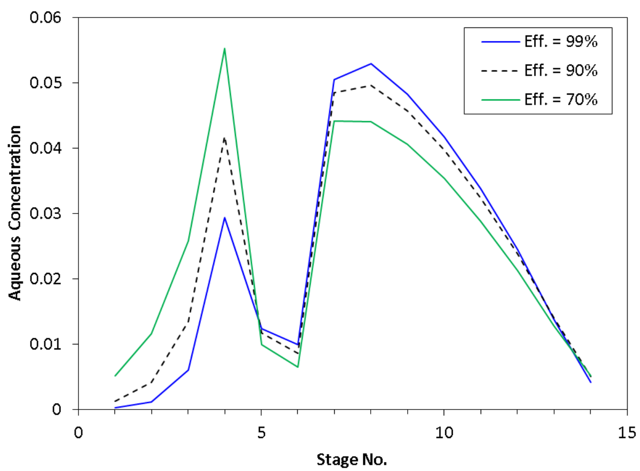
- Packed Columns
- Pulsed Columns
- Mixer Settlers
- **Centrifugal Contactors**
  - Small size
    - Physical footprint
    - Nuclear criticality
  - Short residence time
    - Low process hold-up
    - Less solvent degradation
  - High extraction efficiency
  - High throughput
  - Quick start-up/shut-down
    - Maintain conc. profile



Role of CFD Modeling in Process Simulation and Equipment Design

Context: An illustrative example

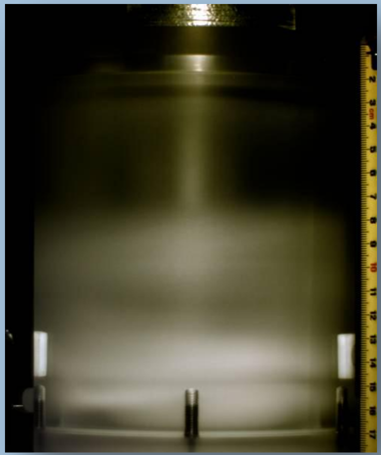
1. User wants to run a SX process simulation using a "Next Gen" package
2. Given:
   1. User inputs
      - Flow rates, O/A ratios, equipment type, chemistry
   2. Settings (defaults?) for equipment type (should be *f*(size))
      - rotor/mixer speed (mixer-settler, centrifugal contactor)
      - pulse frequency/amplitude (pulsed column)
3. SX module requires parameters for EACH STAGE
   1. stage efficiency →
   2. other phase carry-over (OPCO)
   3. (stage volume)

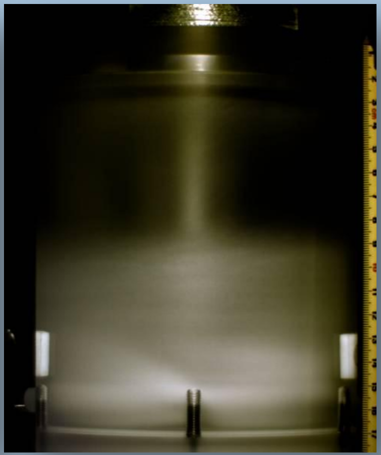


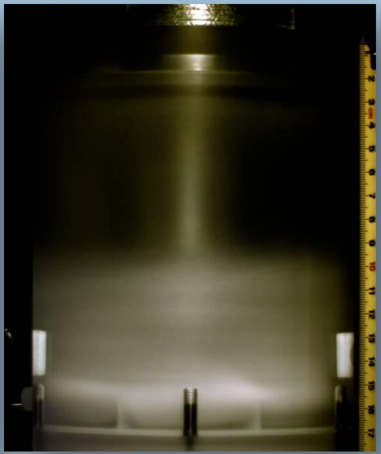
4. Where do these values come from?
   – Current 'state of the art'
      - Estimation based on general experience for equipment type (i.e. educated guess)
        – Estimate may be `function' of equipment size, <u>but same values for all stages</u>
   – We know better…
      - Stage performance parameters 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***

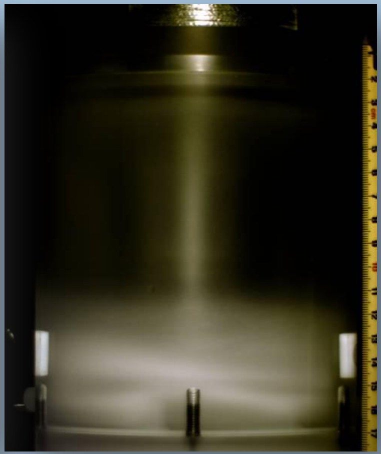
Design/Operational Impacts of Contactor CFD Modeling

- 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


4V


6V

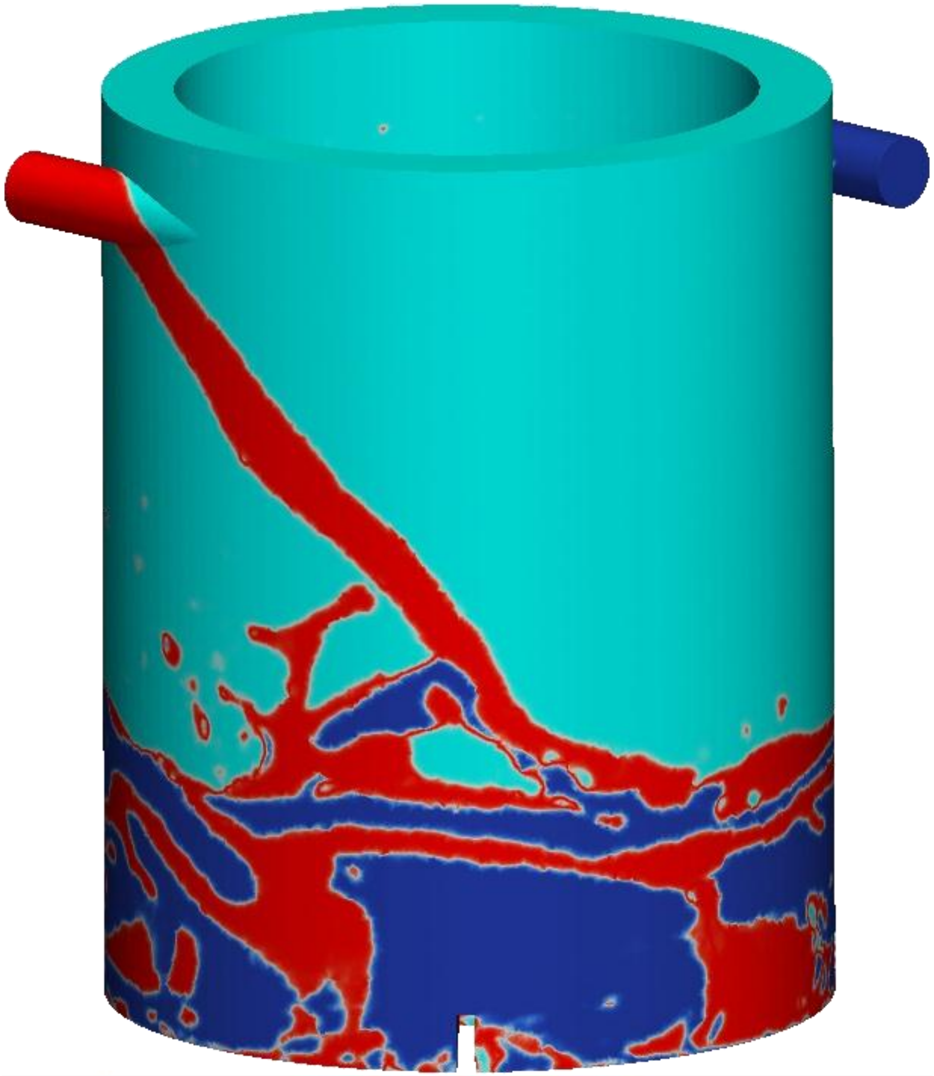

8V


CV

- 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)

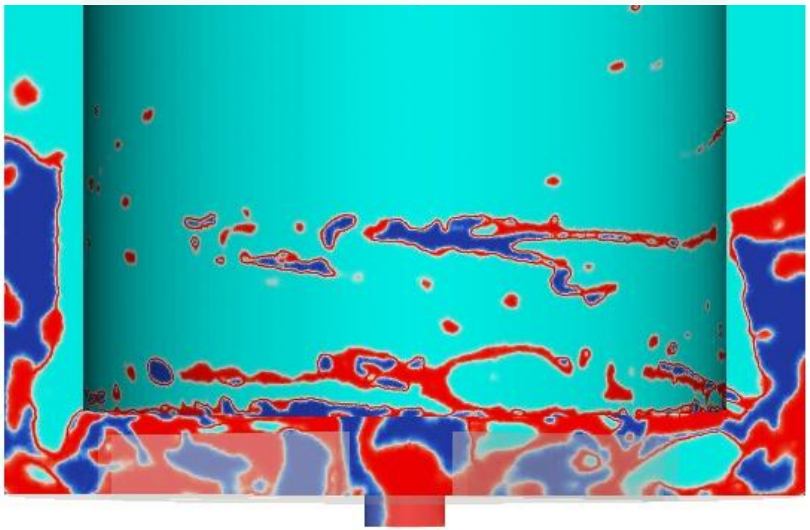
CFD of Centrifugal Contactors

Three-phase Water-Oil-Air Annular Mixing Simulation Using VOF-type Solver

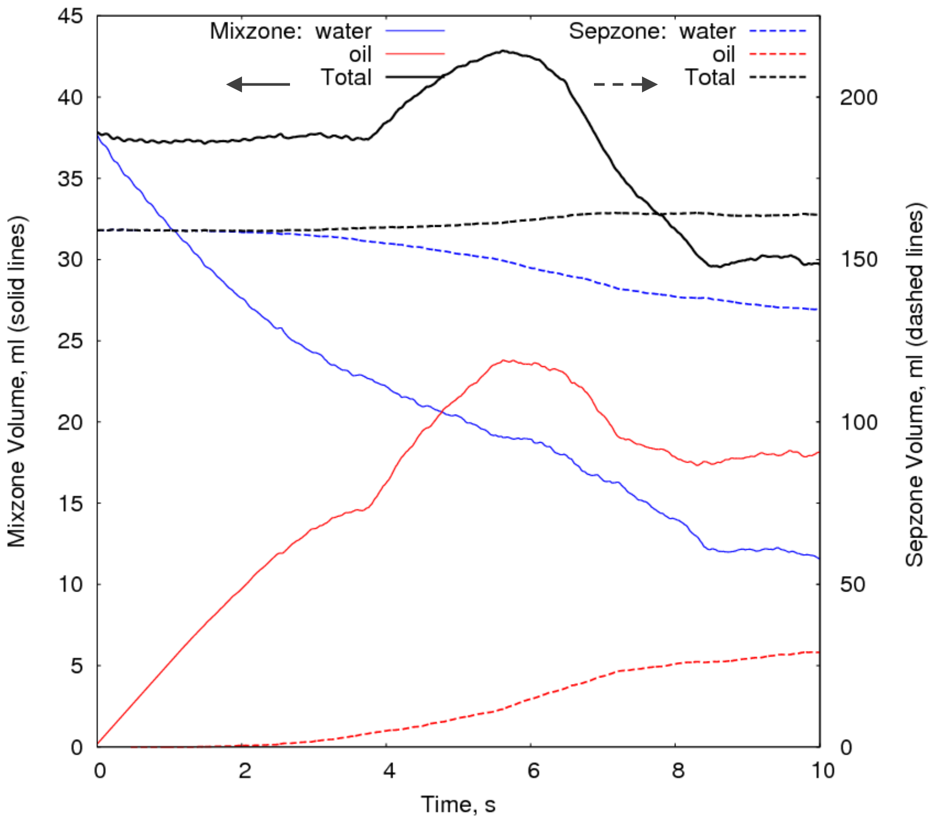


- Only 'large' droplets are resolved (~1mm)
  - Actual droplet size, ~25 µm
  - ~5 µm mesh (Δx, ~50x smaller)
    - N ~ 1×10^{11} cells
    - Δt ~ 1×10^{-7} s
    - Cr limit, as Δx ↓, Δt ↓

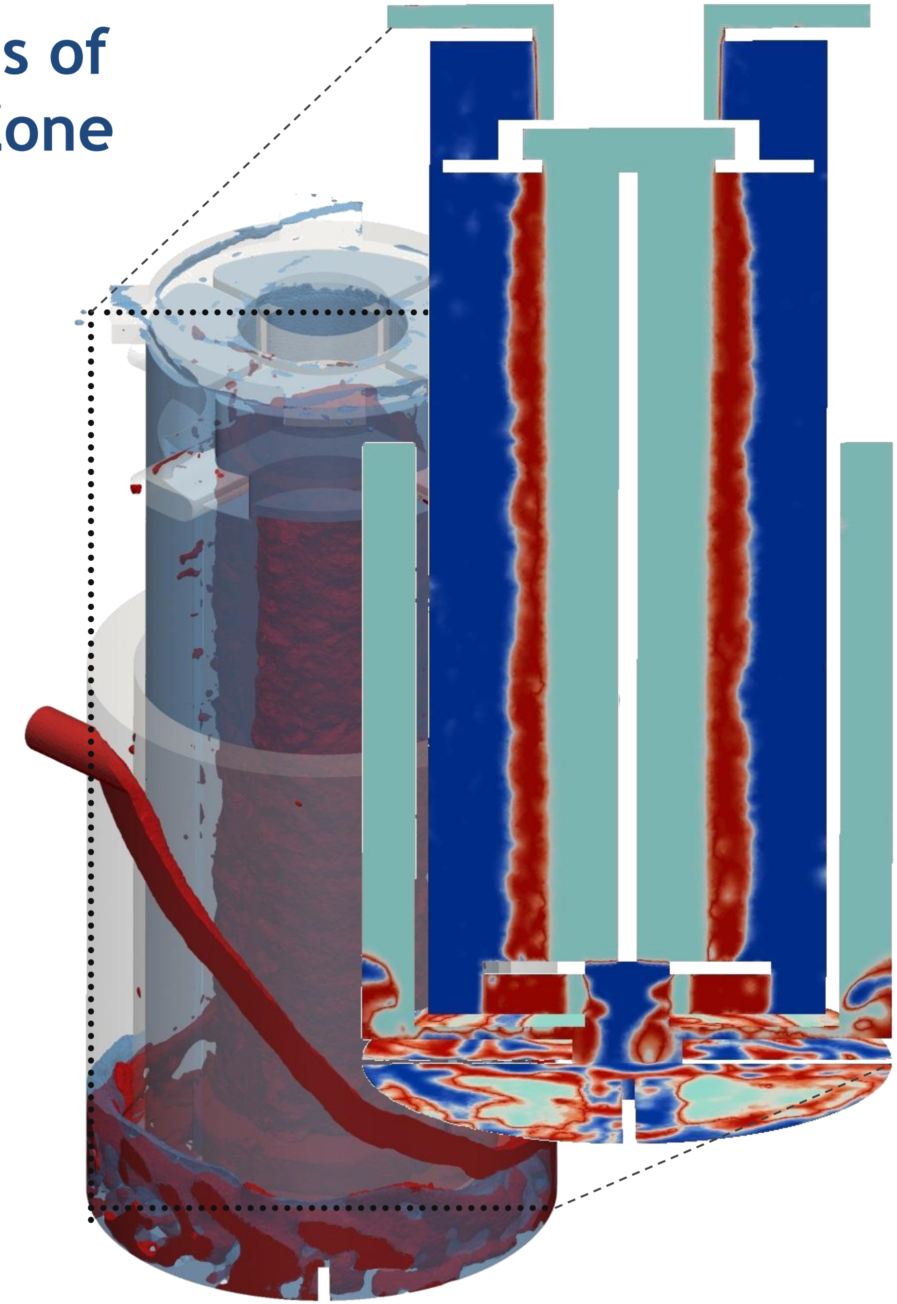
$$\boxed{Cr = \frac{u\Delta t}{\Delta x} \approx 0.25}$$



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:*

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

drag force

surface tension force

Volume fraction transport:

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

Interface compression velocity [1]:

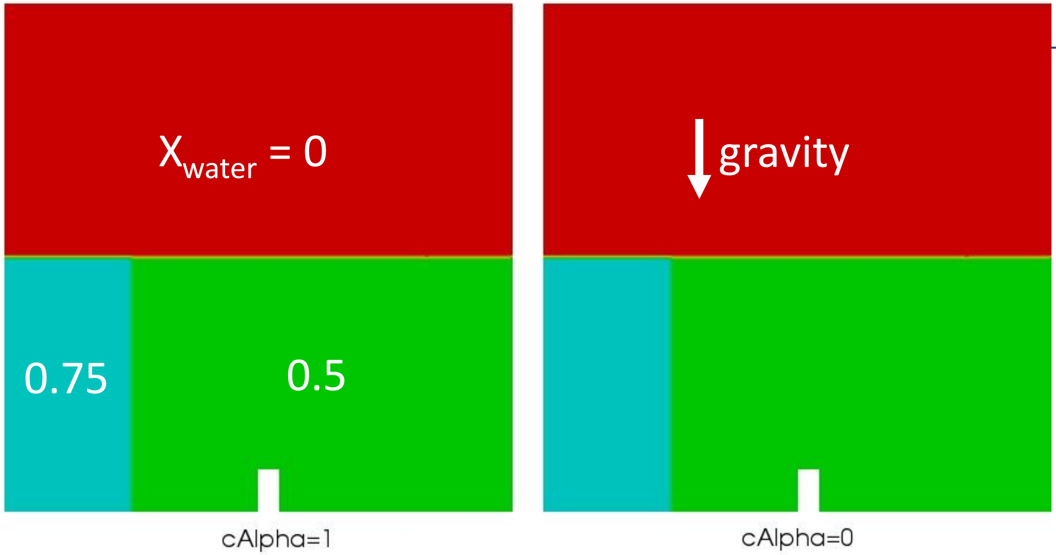
$$\vec{u}_c = C_\alpha \, |\vec{u}| \, \frac{\nabla \alpha}{|\nabla \alpha|}$$

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

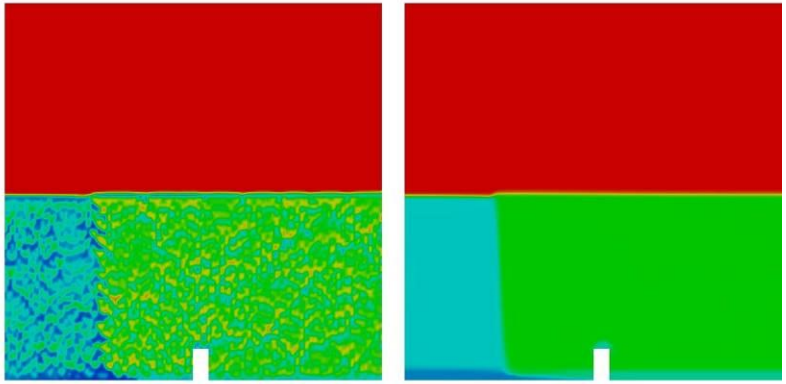
[1] Weller, H.G., A New Approach to VOF-based Interface Capturing Methods for Incompressible and Compressible Flow. Technical Report. OpenCFD (2008).

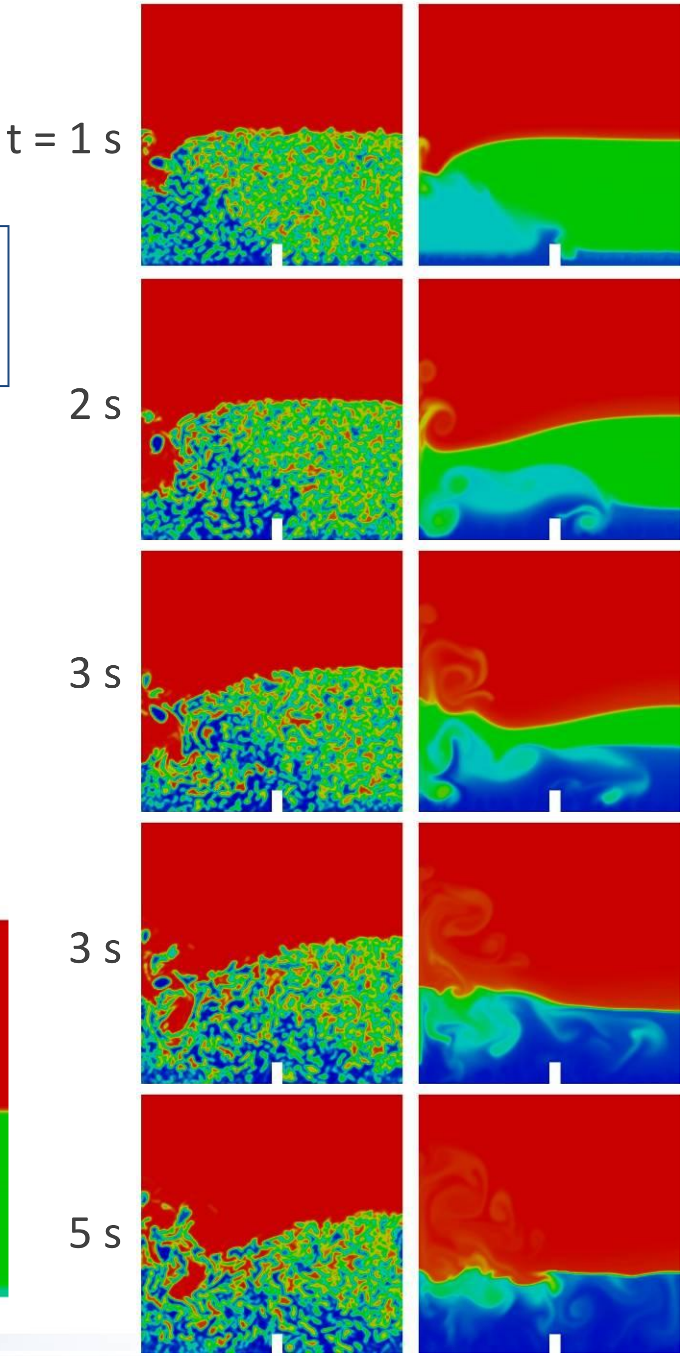
Multifluid-VOF Coupling Example: Collapsing Liquid-Liquid Column

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



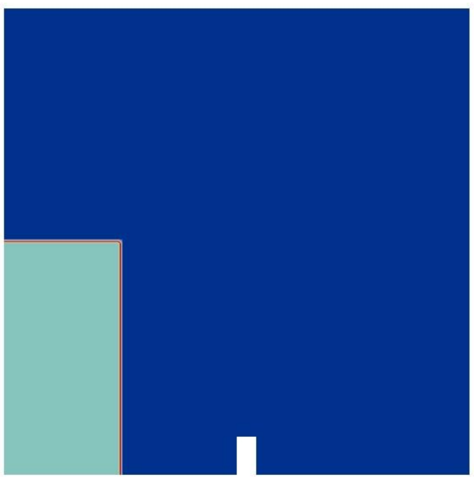


Ex: Collapsing Water Column, w/ cAlpha Switching [2]

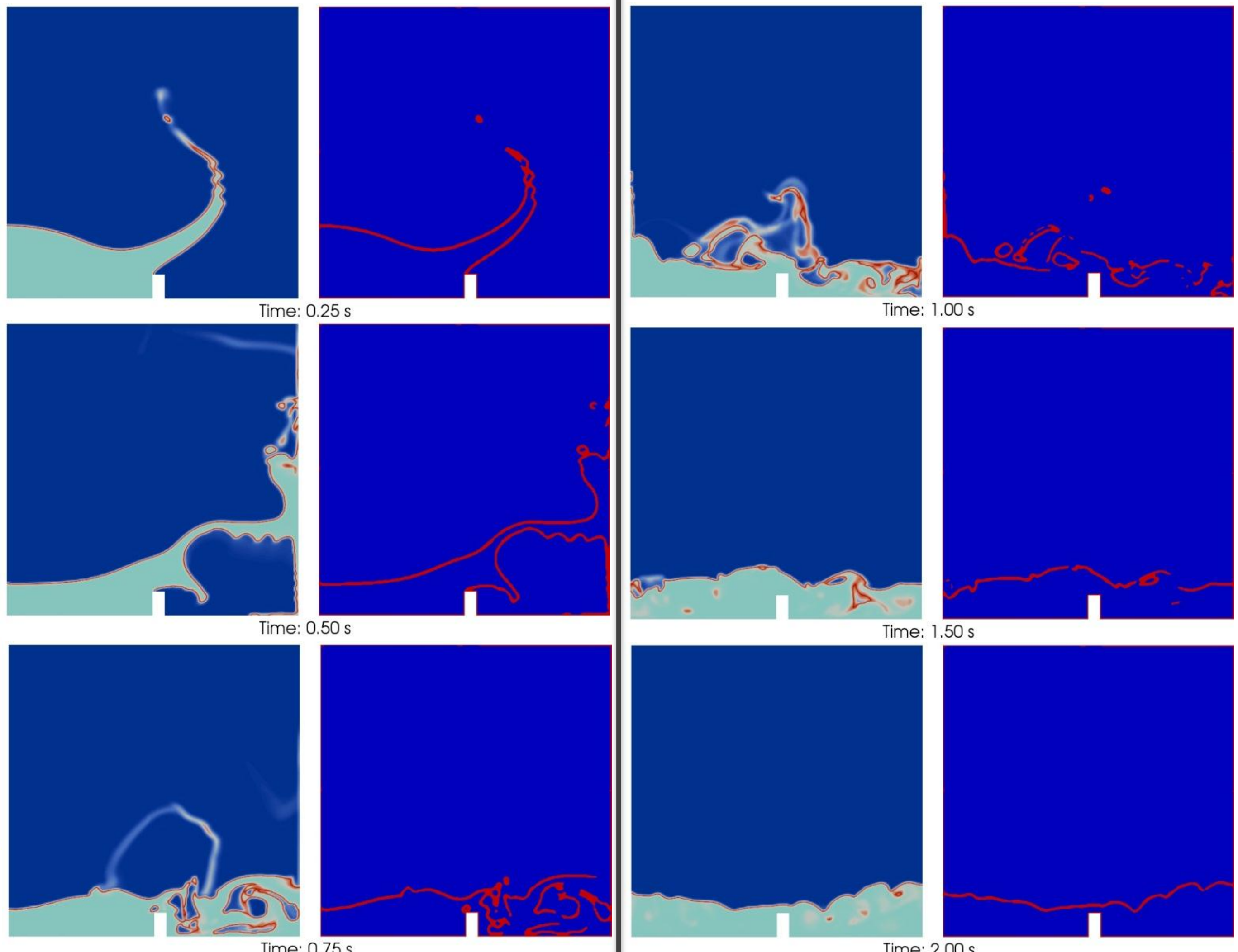
$$\gamma = \frac{|\nabla \alpha|}{max(|\nabla \alpha|)}$$

for $\gamma \geq \gamma^{\star}$

$$C_{\alpha} = 1$$



Time: 0 s



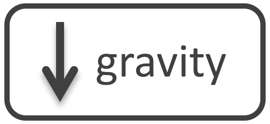
[2] Cerne et al. *J. Comput. Phys.* **171**, 776 (2001).

Three-phase (Water-Oil-Air) Examples

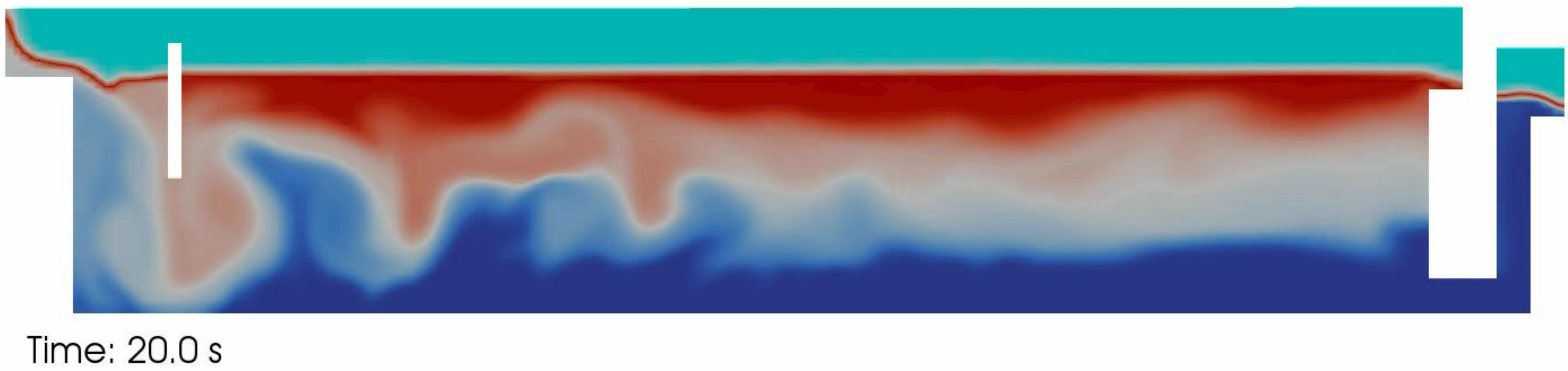
- No cAlpha switching -- interface compression applied for air/water & air/oil interfaces only
- Water/oil interface treated with multi-fluid model w/ interphase drag model of Schiller-Naumann (‘blended’ scheme)
- Fixed droplet sizes [3]
  - $d_{water} = d_{oil} = 0.150$ mm
  - $d_{air} = 1$ mm

[3] Padial-Collins et al. *Sep. Sci. Technol.* **41**, 1001–1023 (2006).

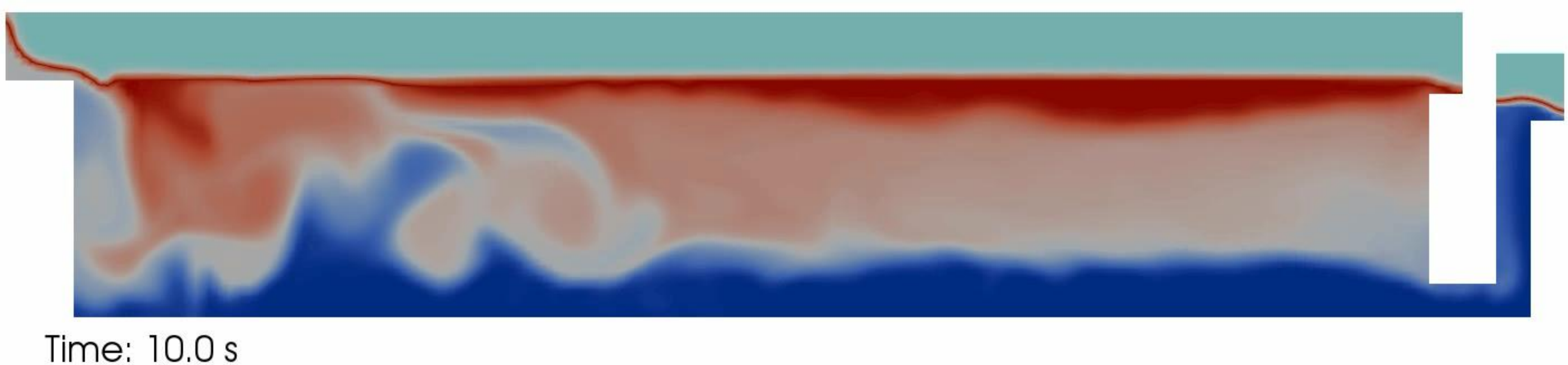
Three-phase 2D Horizontal Settler (Water-Oil-Air)



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

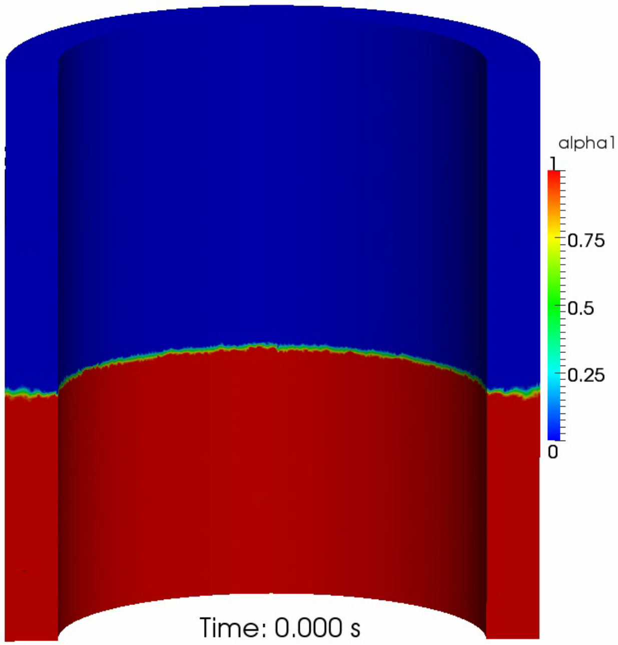


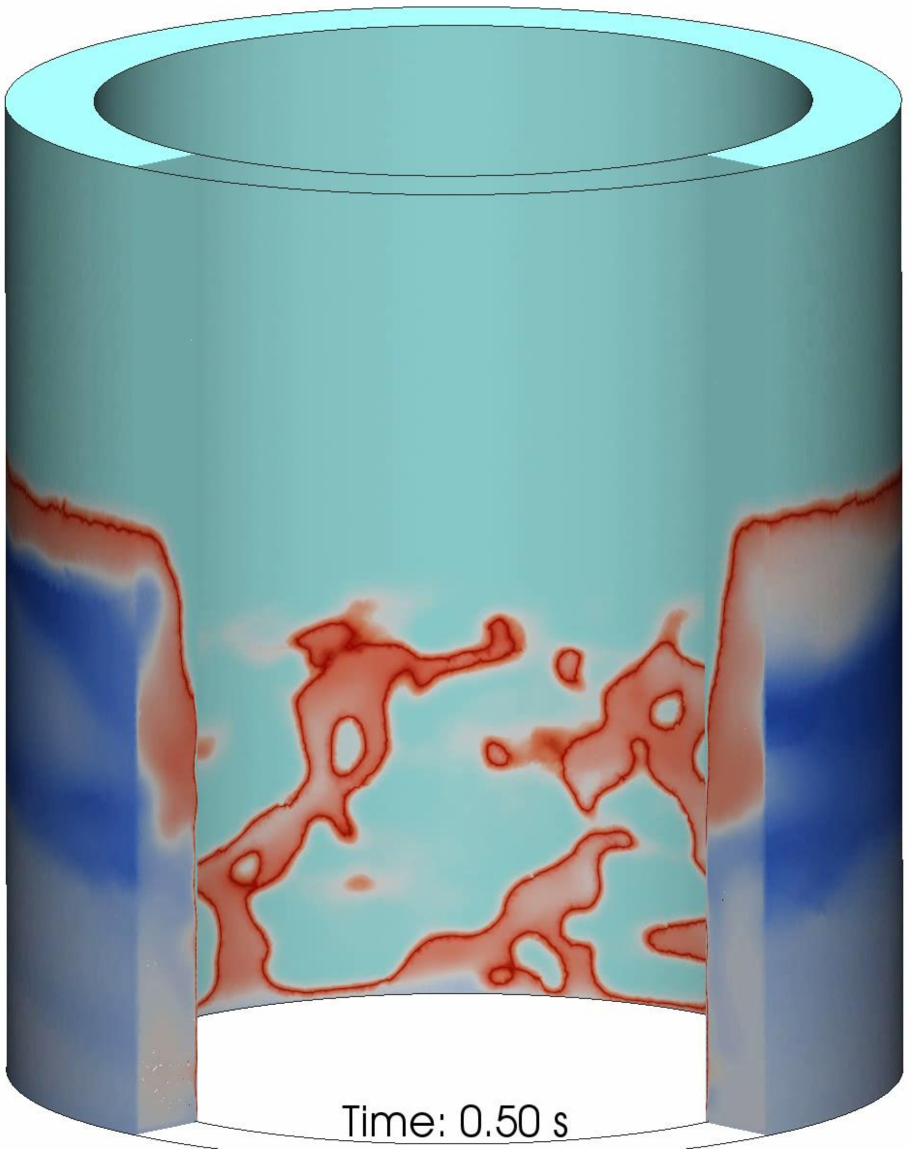
- No diverter disk - inlet flow O/A = 1, initial gravity = 2g, @ t=10s gravity = 3g



3D Annular Mixer

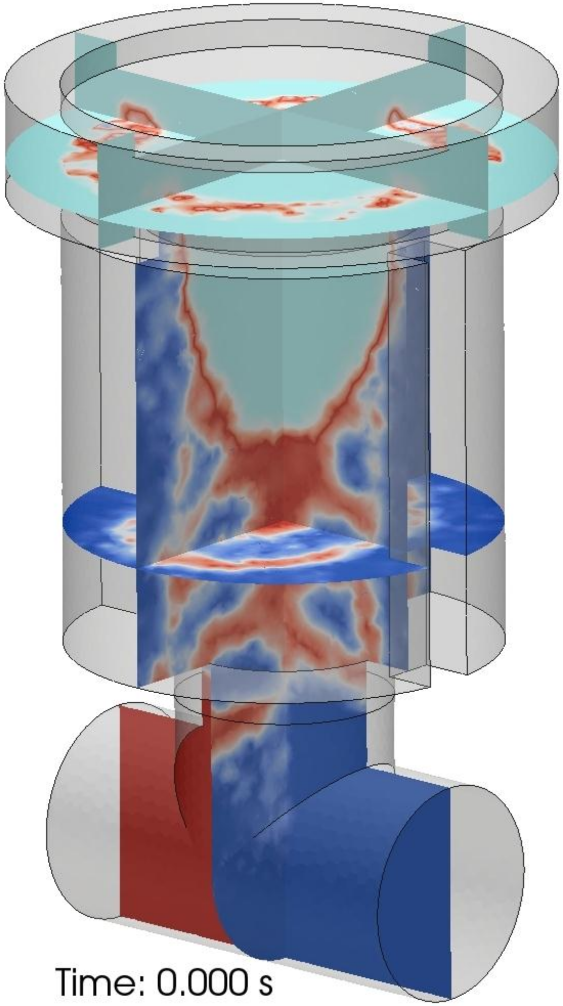
- Geometry similar to CINC-V2 mixing zone
  - r_{in} = 2.54 cm, r_{out} = 3.17 cm
  - height: 7 cm
  - initial liquid height: 2 cm water/oil
  - Rotor speed: 3600 RPM
- High shear at rotor surface requires interface sharpening to maintain liquid (multi-fluid only, two-phase ↙)

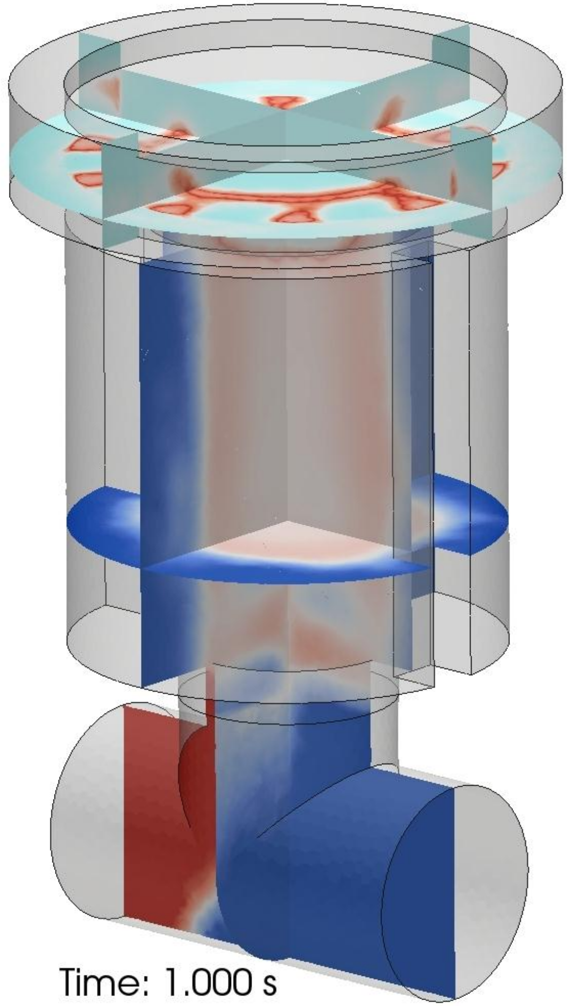




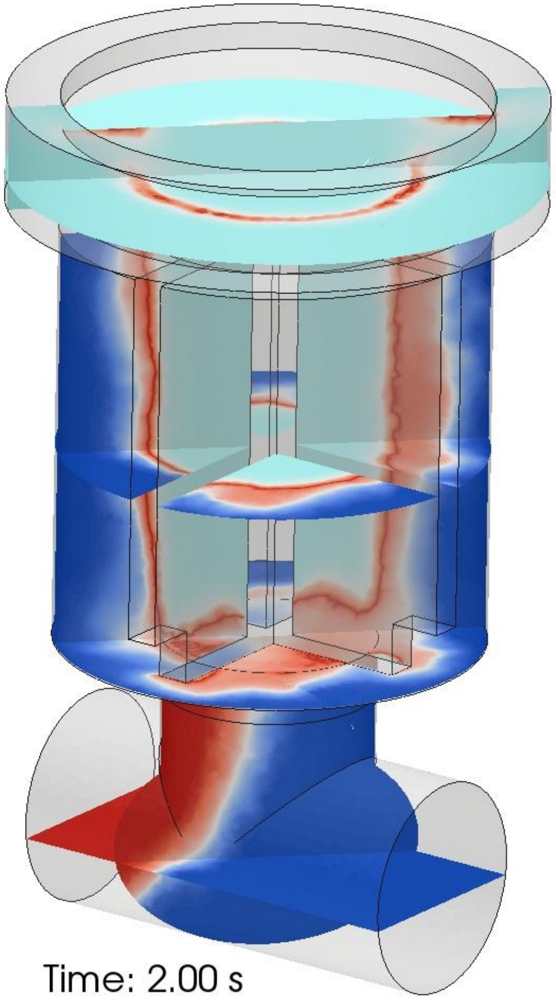
Tee-fed Rotating Centrifuge with Baffles (Water-Oil-Air)

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

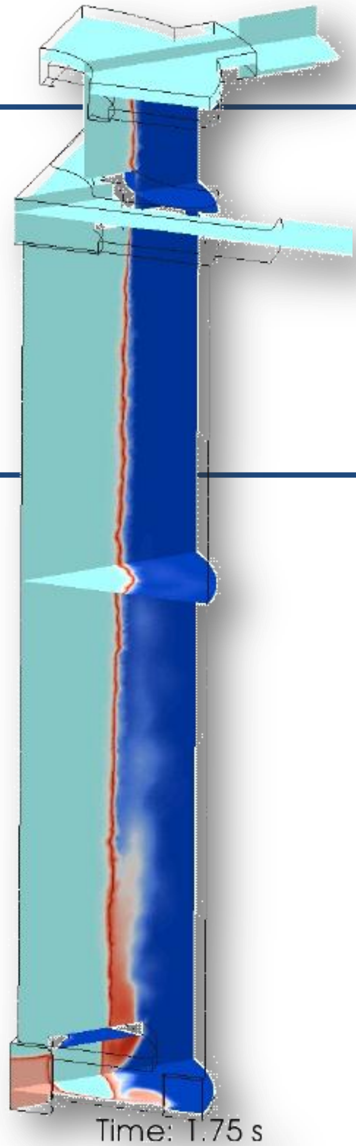




Full Baffles (4)

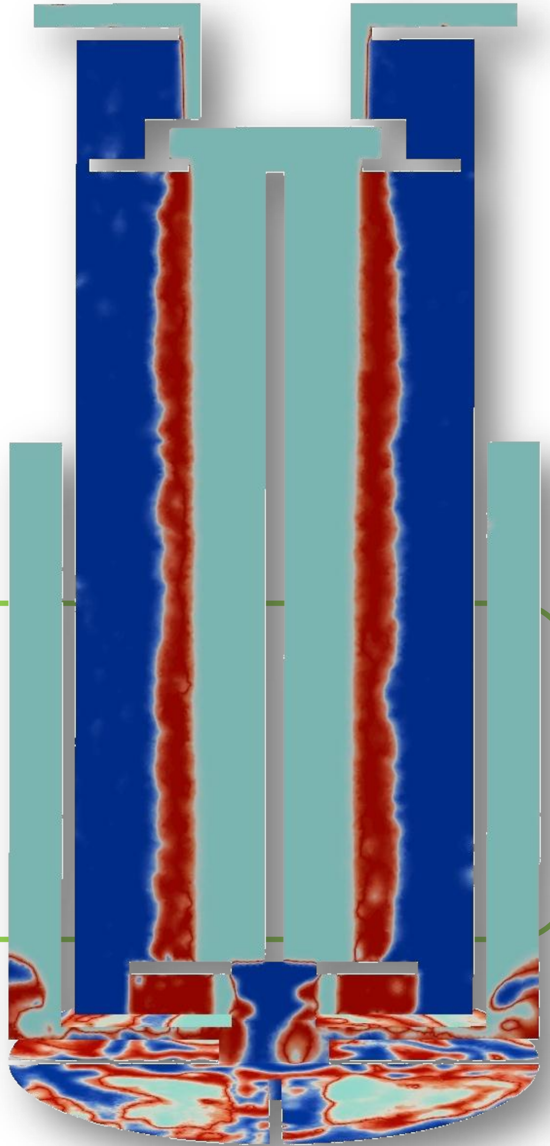


Annular Centrifugal Contactor (underway)



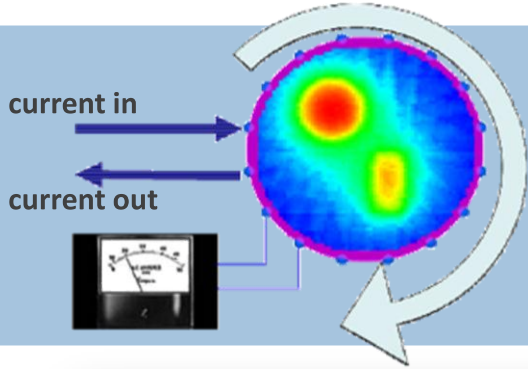
One-quarter section of contactor rotor
Initialize from two-phase, VOF-only solution
(t=1.75s shown)

Coupled mixing-, separation-zone
Initialize from VOF-only solution (t=0 shown)



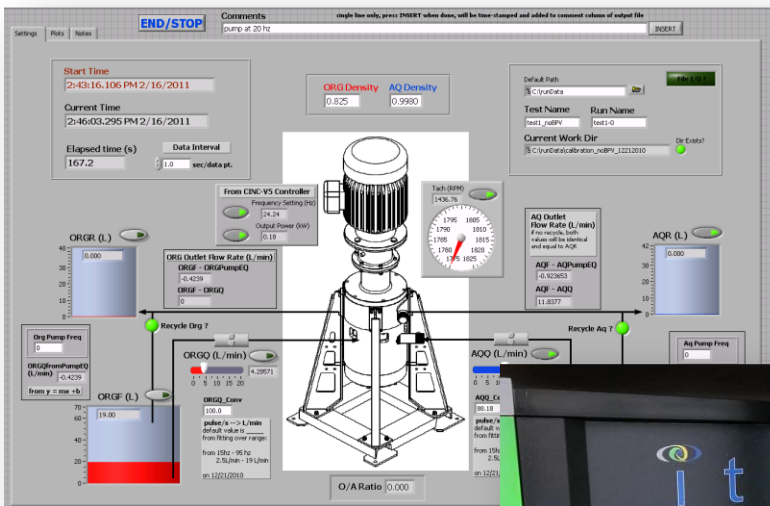
Companion Experimental Effort: Multiphase Measurements in Solvent Extraction Equipment for CFD Validation

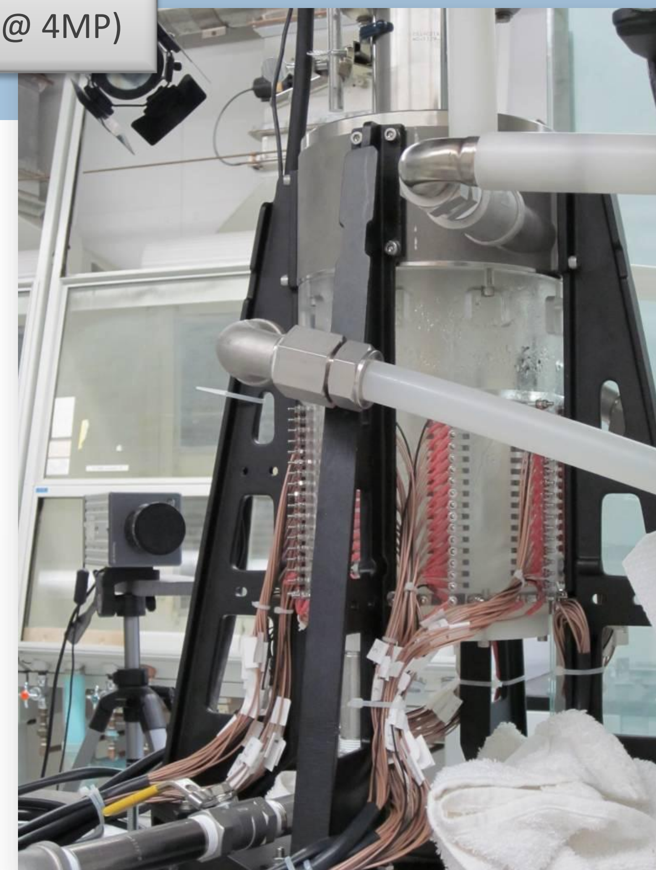
Contactor CFD Validation Using Electrical Resistance Tomography (ERT)



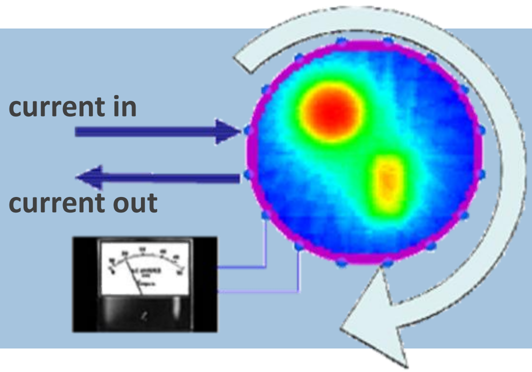
<u>Contactor ERT (CERT) Facility</u>

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





Contactor CFD Validation Using Electrical Resistance Tomography (ERT)



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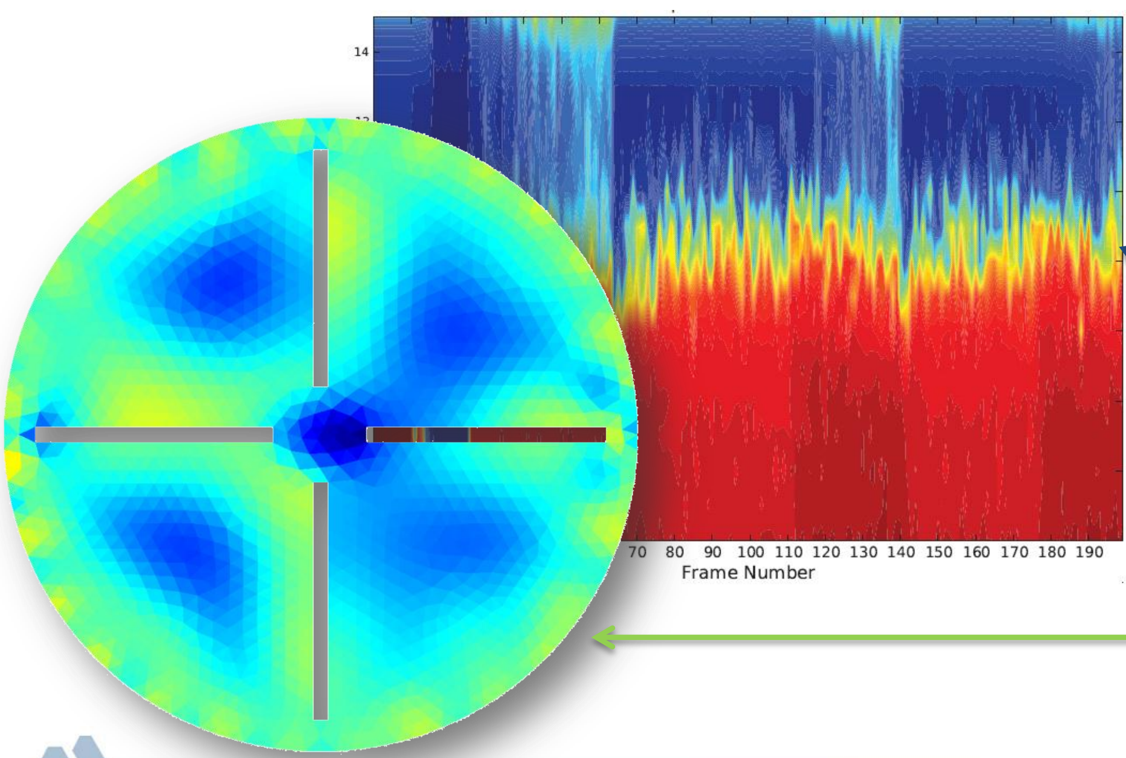
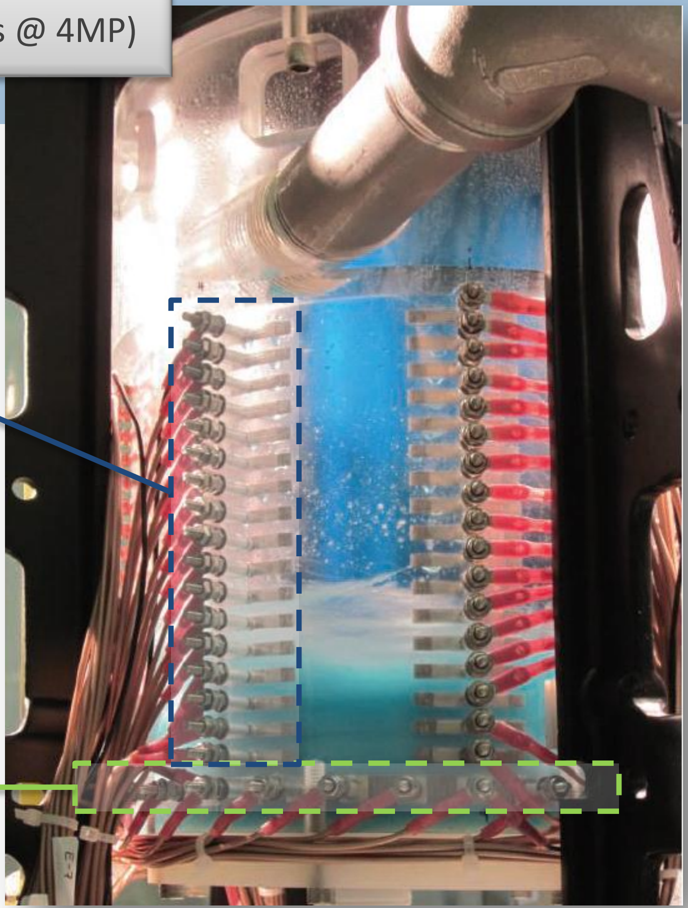
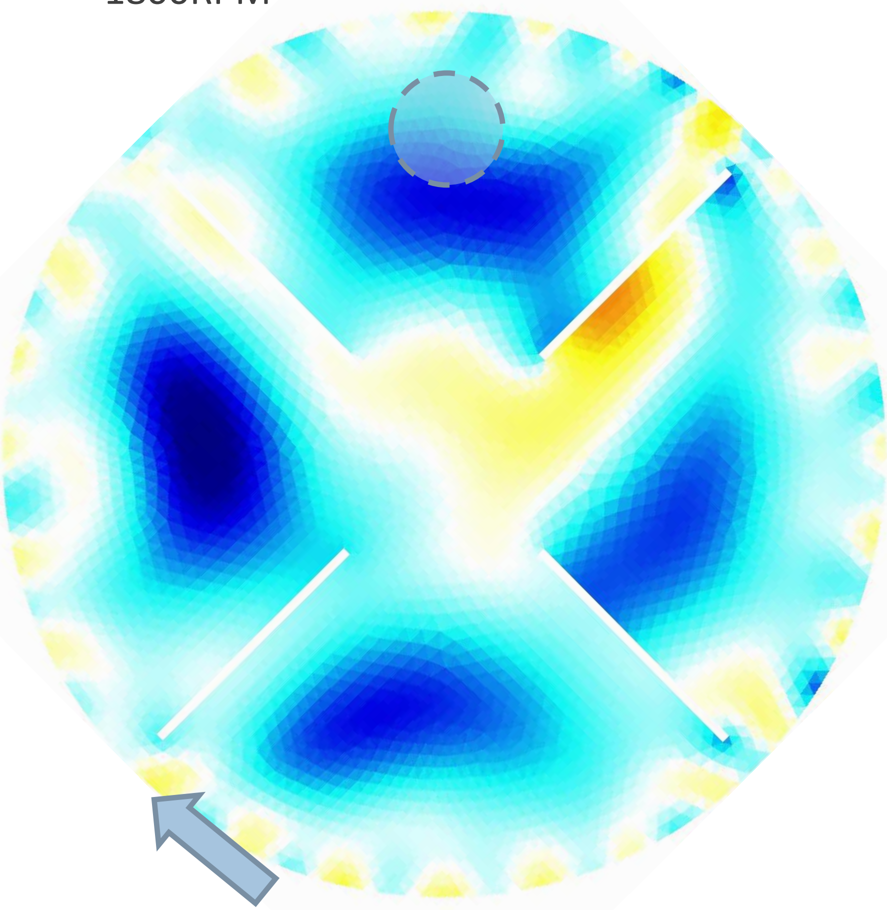




Qualitative ERT Validation

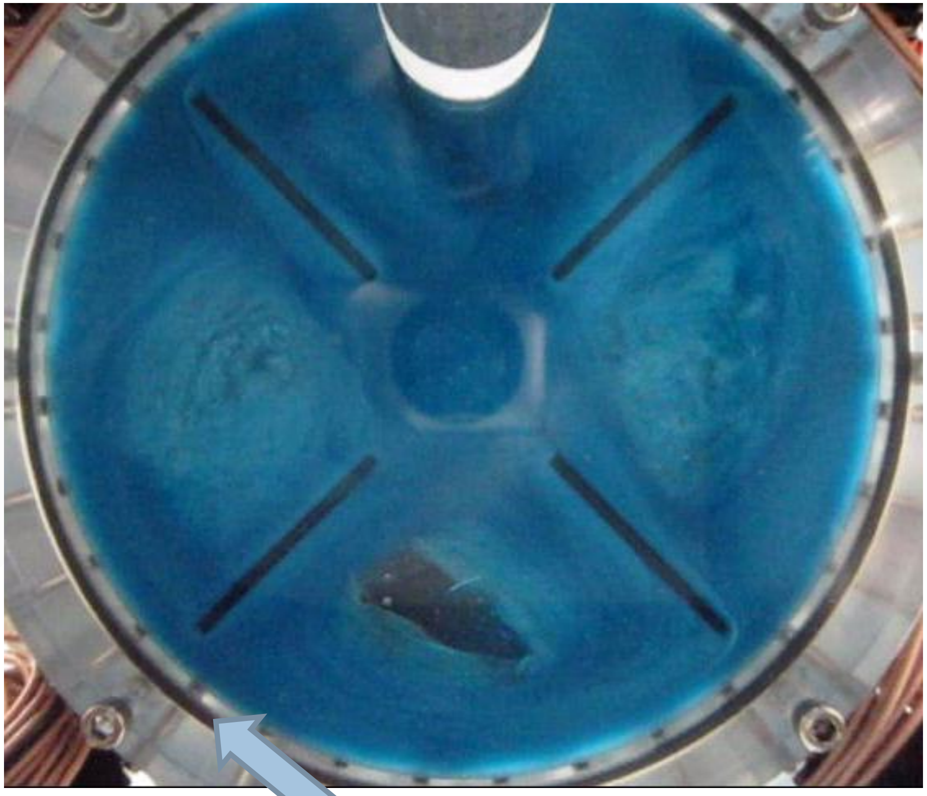
ERT (array at TOP of vanes):

tap water (ρ = 1),
10 L/min,
1800RPM



Video (through vane plate):

aqueous phase (ρ = 1.17),
10 L/min,
1800RPM



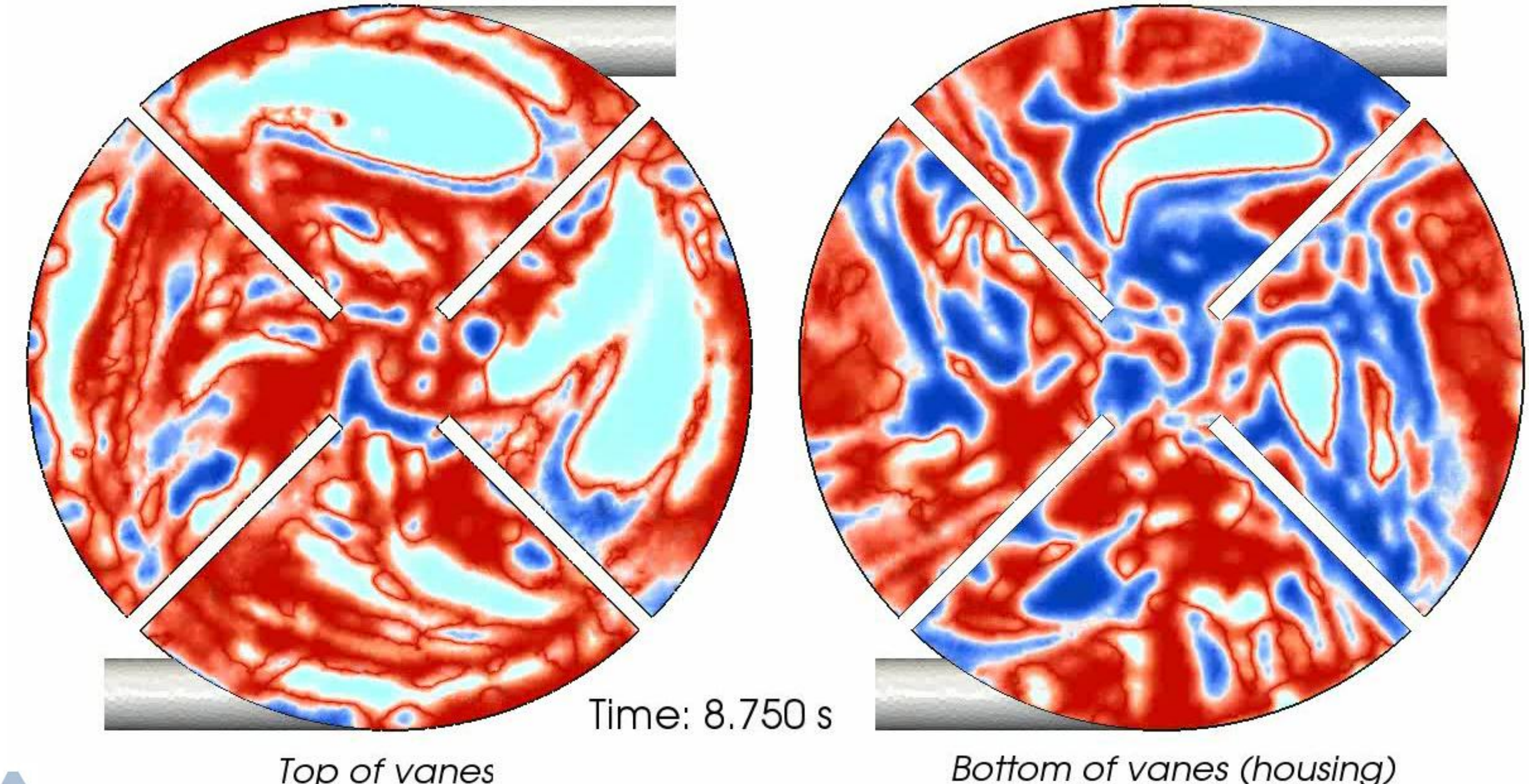
(has been mirrored match rotation of ERT measurement)

shows inlet orientation

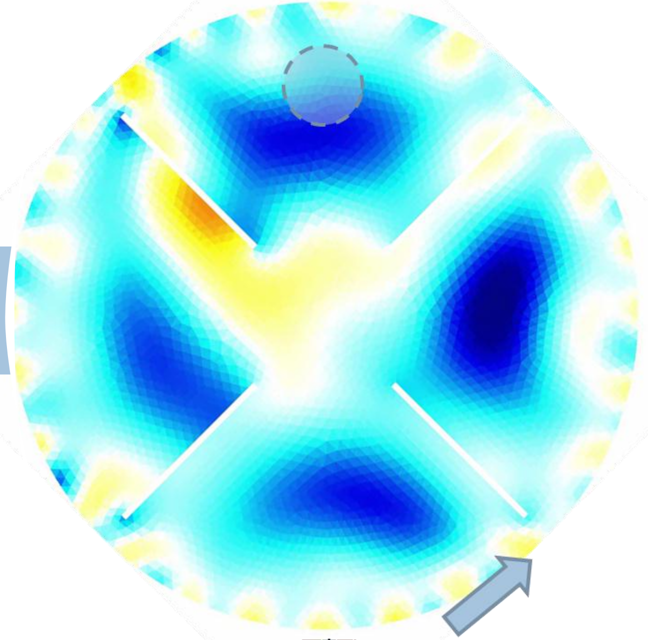
Comparison of Bottom/Top of Vanes Flow from CFD

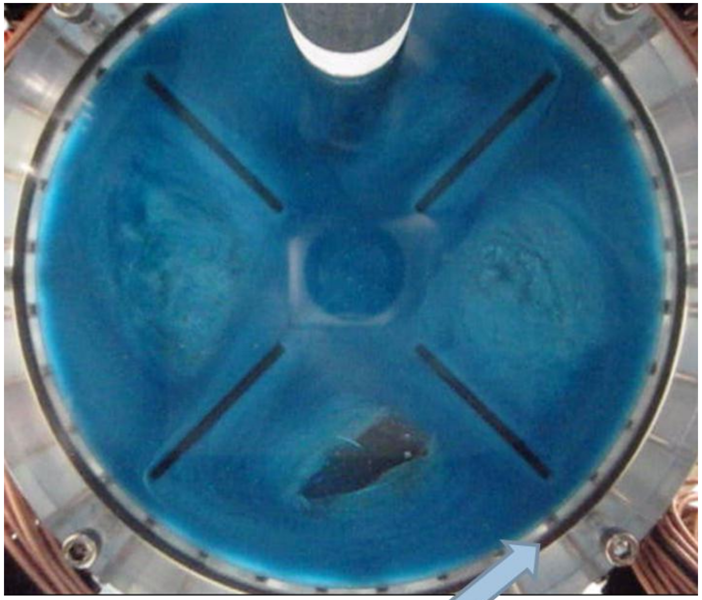
- 3-phase simulation (600 ml/min, O/A = 1), VOF-only solver
- CINC V2 geometry
  - vane orientation shifted 45º relative to inlets, vanes go to outer wall
  - slightly larger vane-to-rotor gap
  - low mixing zone volume (lower relative flow rate)

water
oil
air

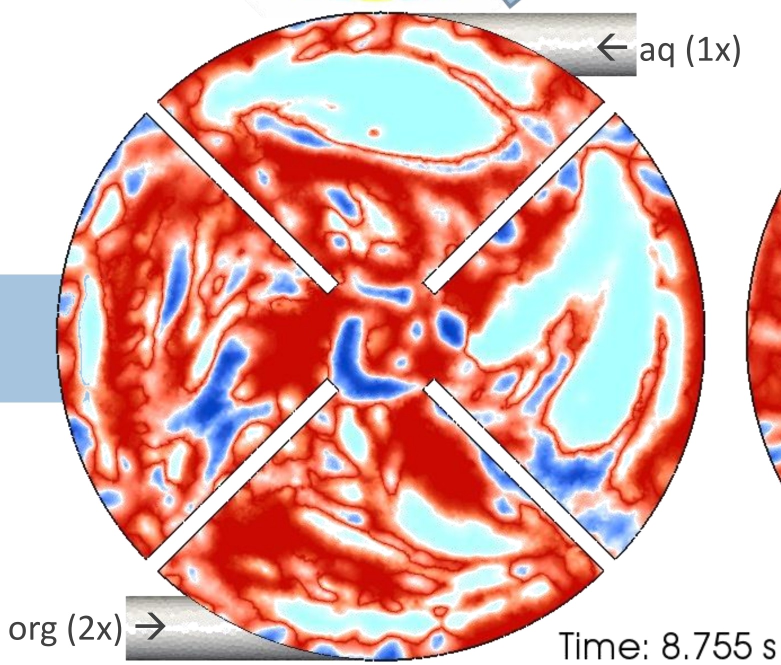


Experiment

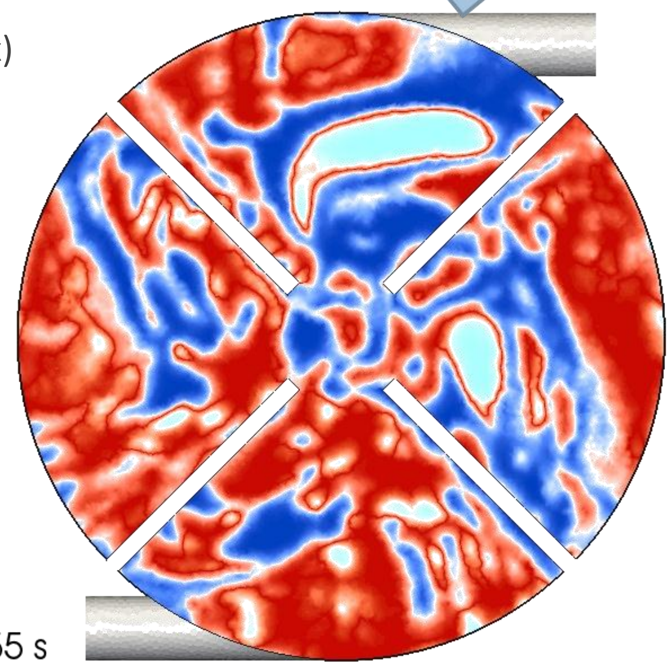




Simulation



Top of vanes



Bottom of vanes (housing)

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

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  - Candido Pereira and Ralph Leonard
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