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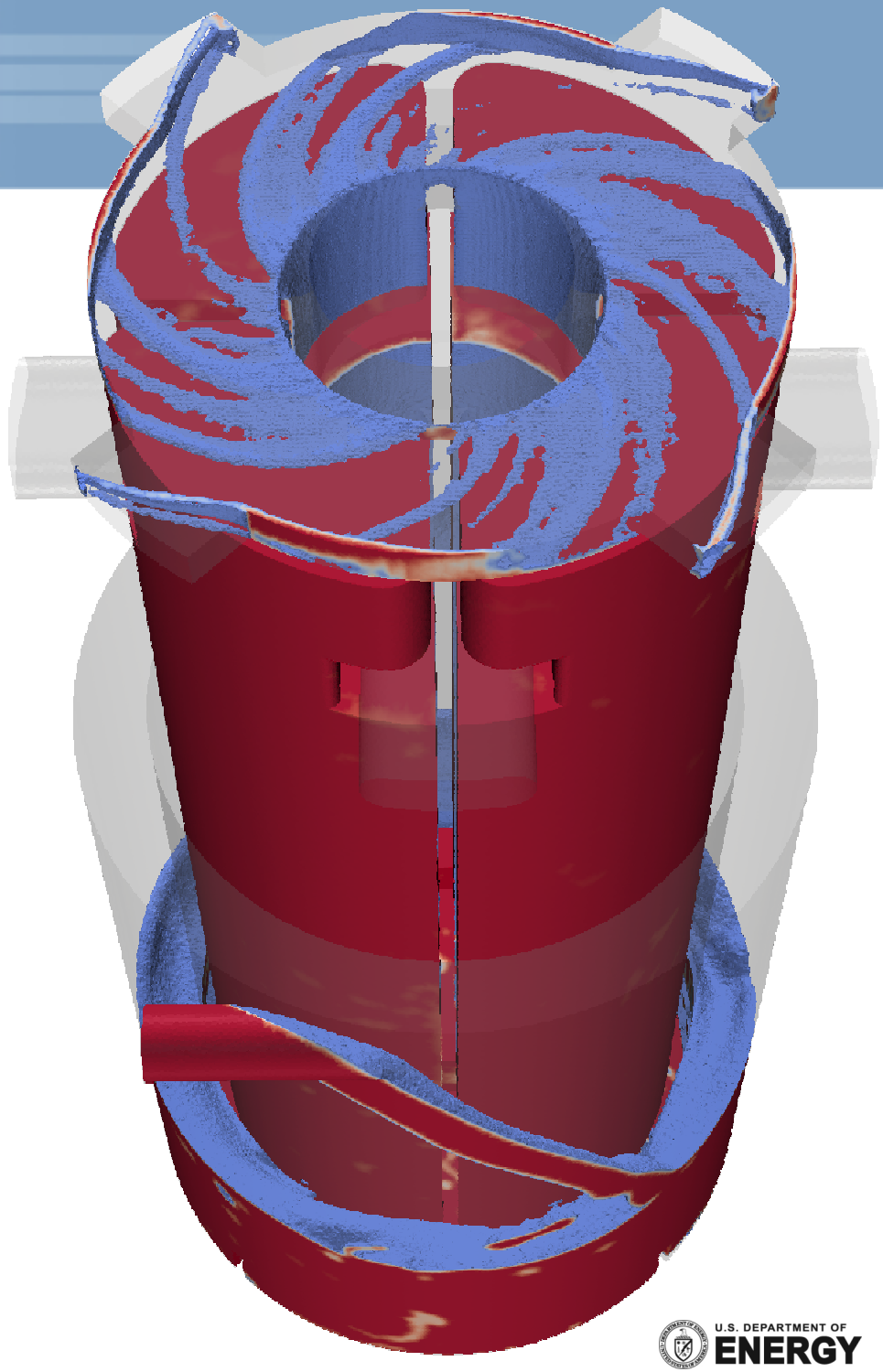
Advanced Multi-Fluid Simulations and Experiments of Flow in Liquid-Liquid Contactors



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Argonne National Laboratory

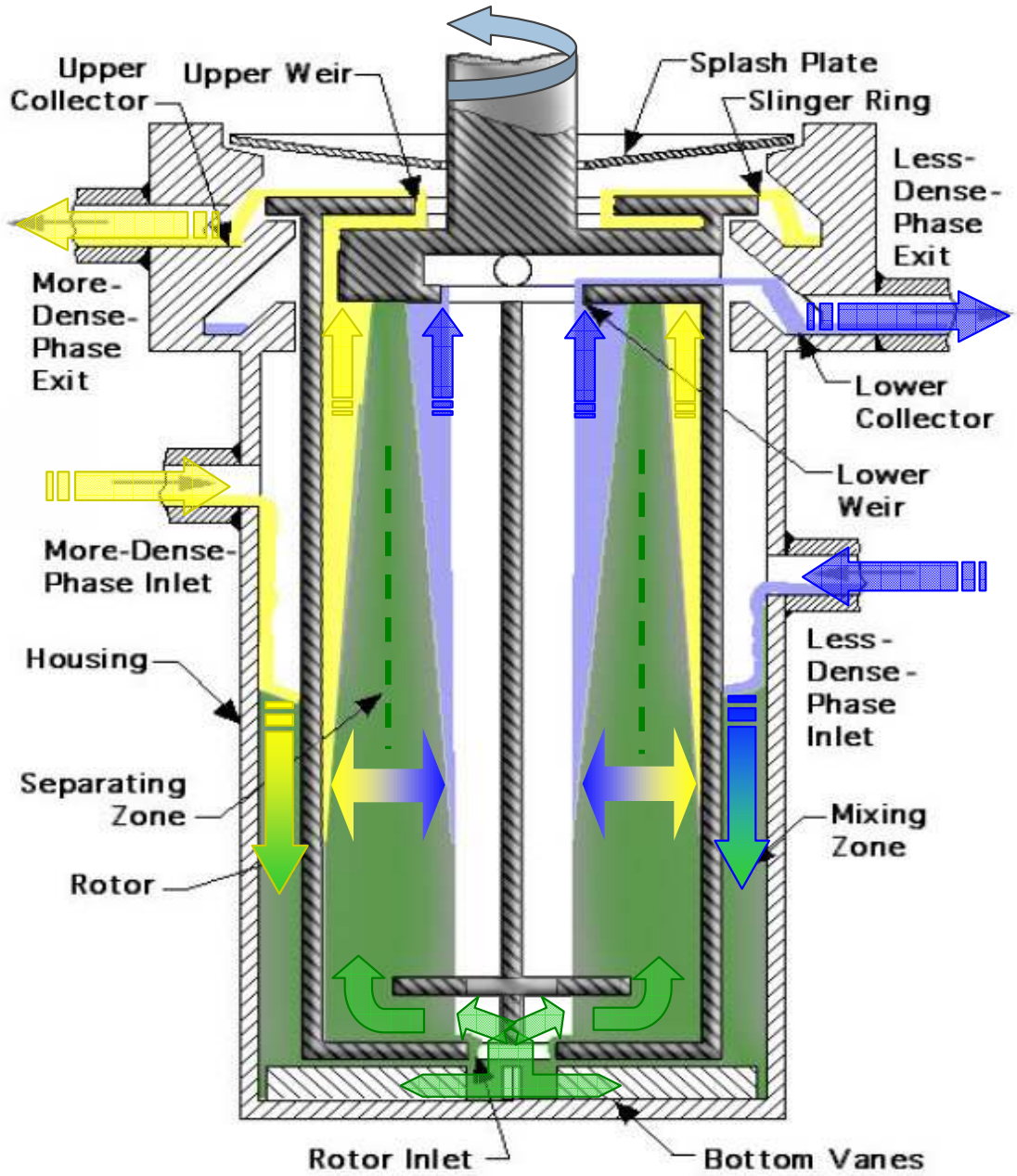
ANS Annual Meeting 2011
30 June 2011

U.S. DEPARTMENT OF ENERGY

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

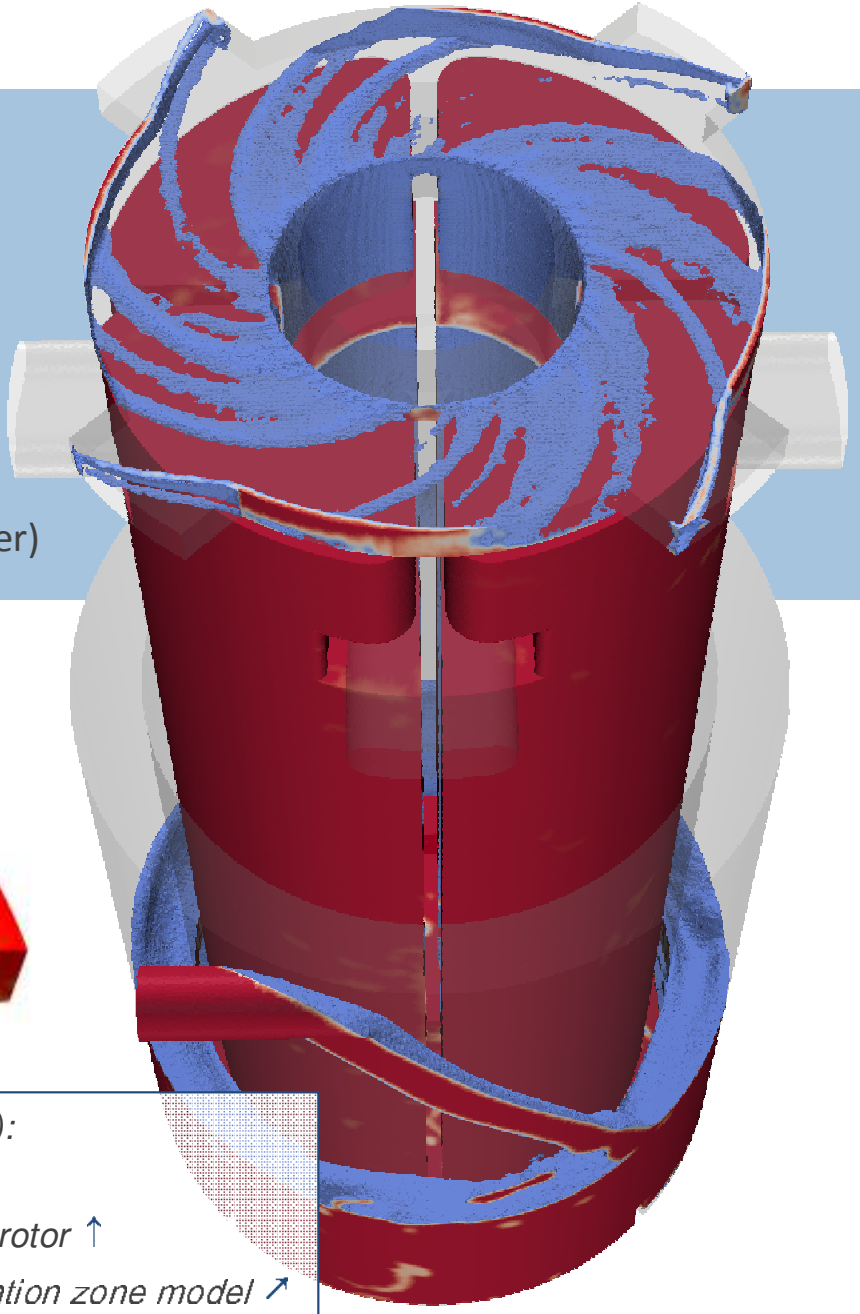


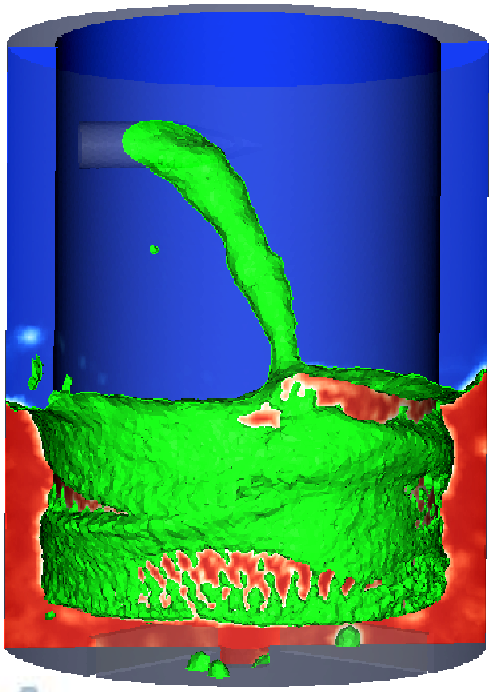
CFD of Centrifugal Contactors

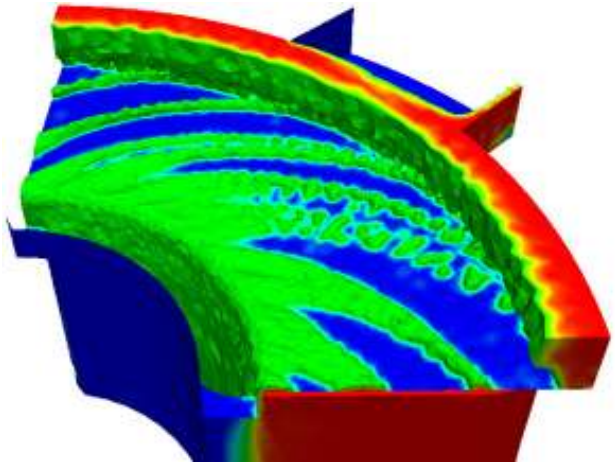
Centrifugal Contactor Simulations Using Open-Source CFD

OpenFOAM® (www.openfoam.com)

- Open-source toolkit - collection of libraries and solvers
- Capable of wide variety of physics
  - Multiphase, turbulent, moving boundary, etc.
- Good parallel performance
  - >2-4 times faster than comparable commercial CFD
  - Scales down to ~5K polyhedral cells/processor (Linux cluster)







Free surface flow examples (water/air):

← *flow in mixing zone*

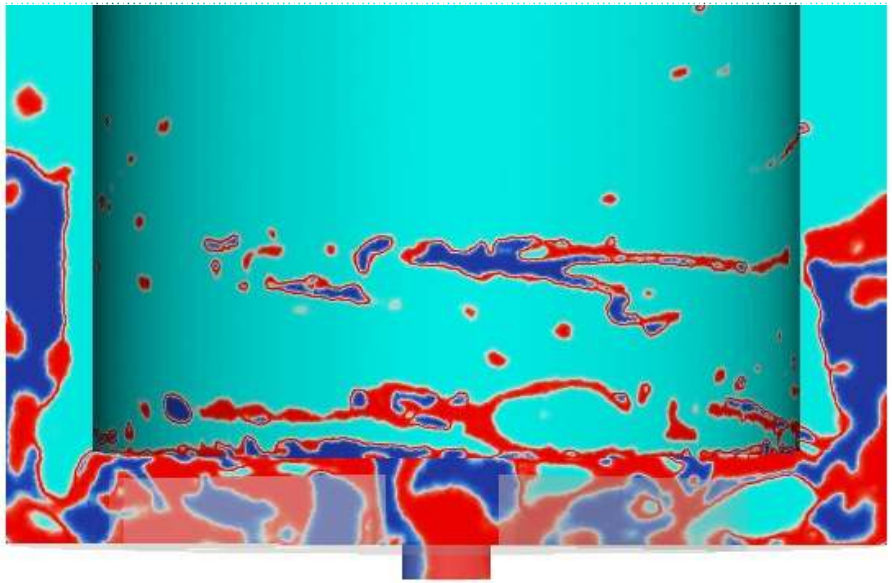
flow in the upper section of the rotor ↑

flow in coupled mixing/separation zone model ↗

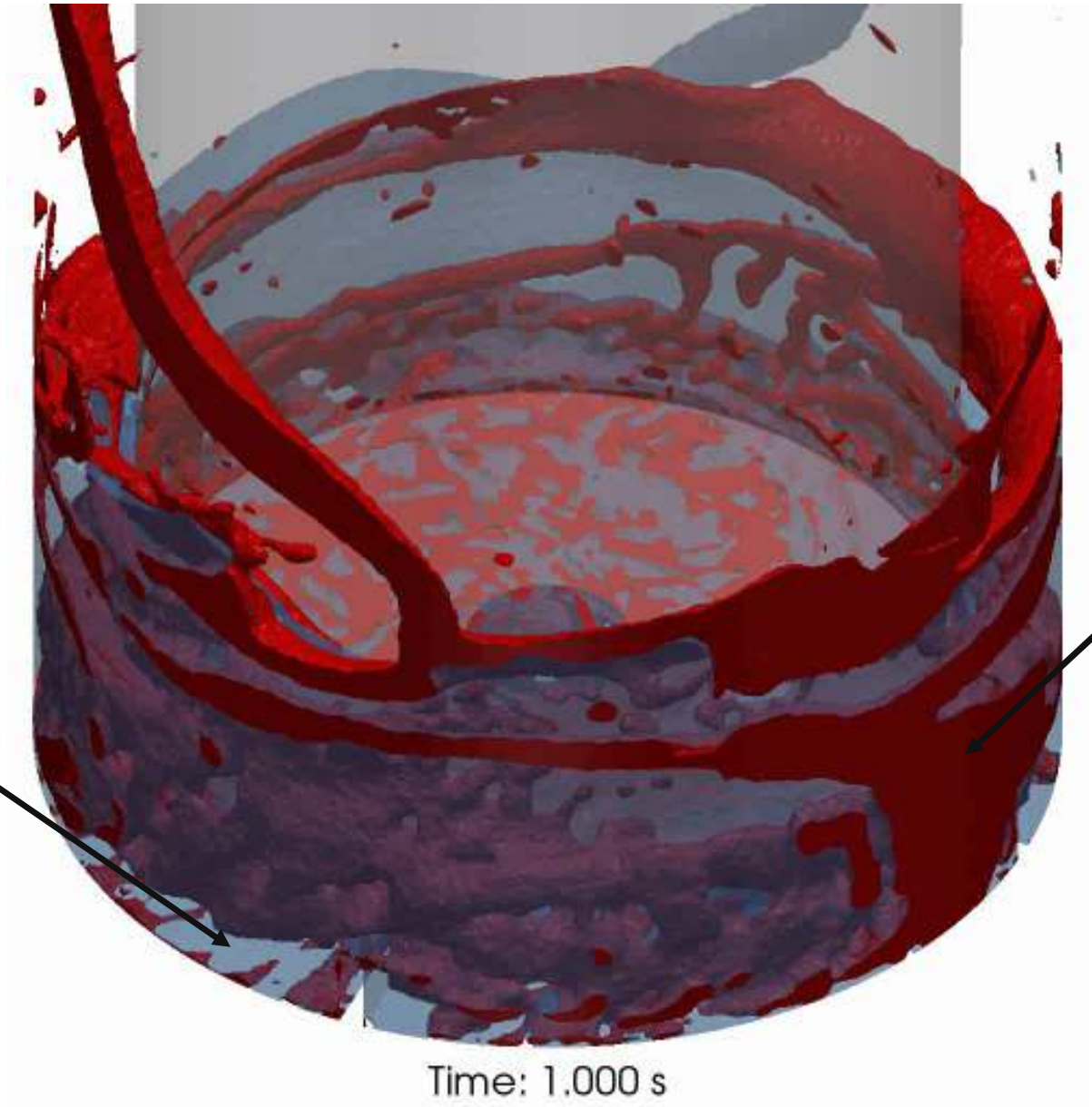
Three-phase Water-Oil-Air Annular Mixing Simulation Using Open-source CFD (OpenFOAM)

- 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 ↓

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

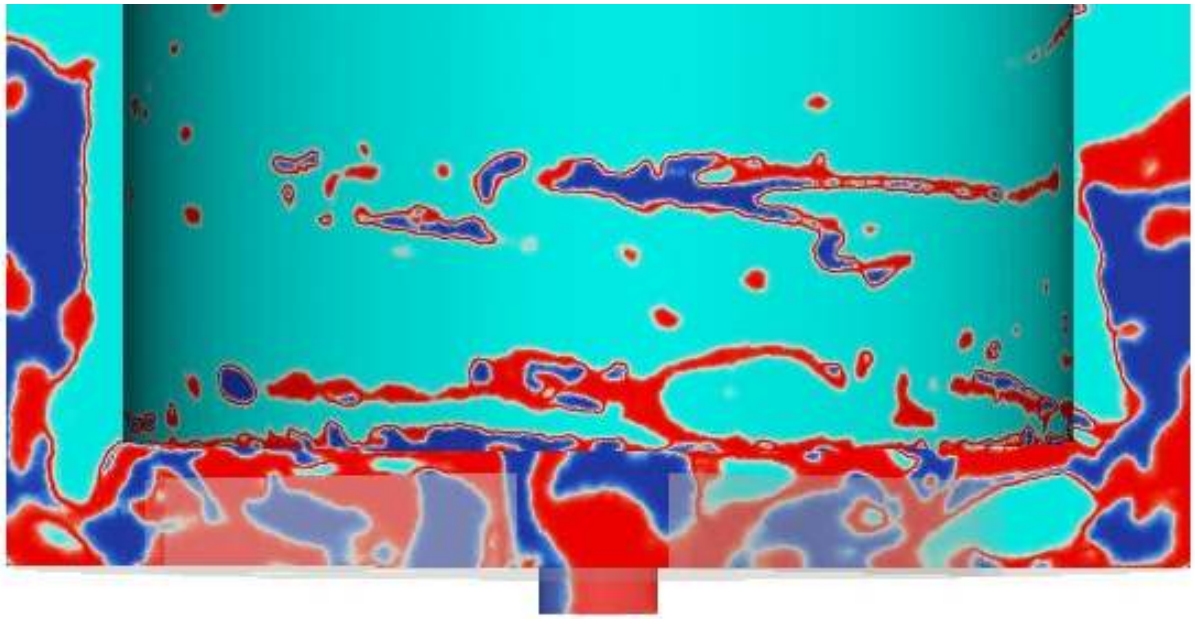


Animation of Liquid-Liquid Mixing



New Multiphase Models are Needed

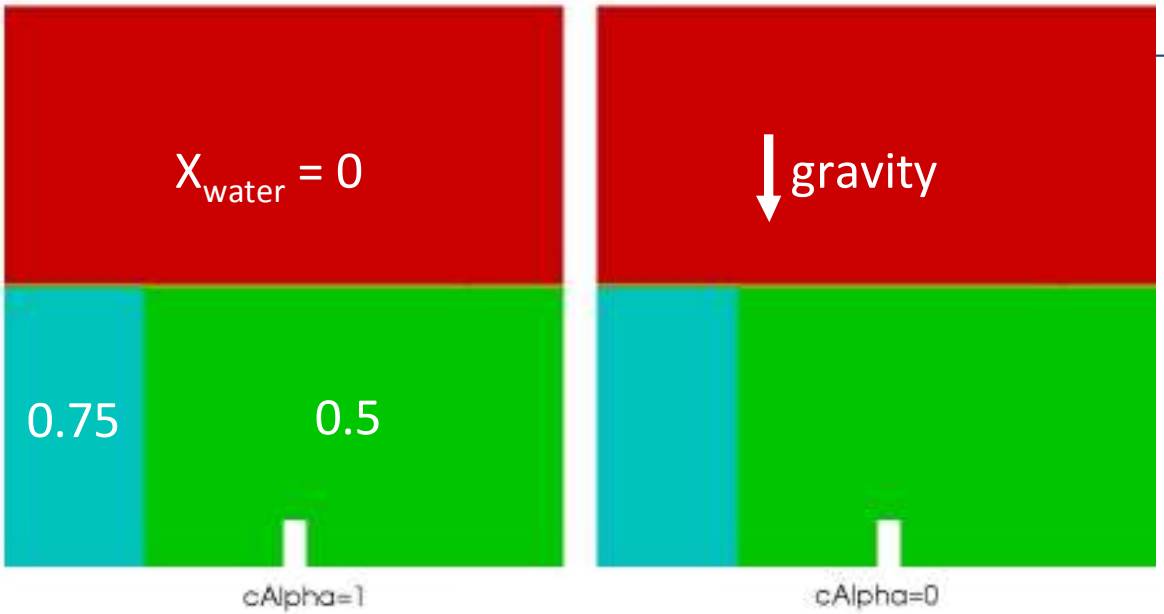
- Euler-Euler-VOF Coupled Multiphase Model
  - VOF (interface capturing/tracking) to capture liquid-air interface and fluid/rotor interaction
  - Compatible multiphase model for unresolved scales of liquid-liquid dispersion
    - Sub-grid models for droplet breakup/coalescence and mass/momentum transfer ← LANL
- Combination not available in existing commercial codes *(except ANSYS-CFX, in part)*
- Proposed progression of methods to be implemented in OpenFOAM VOF solver
  - Euler-Euler with fixed dispersed phase droplet size and characteristic drag model (as in Padial-Collins et al. 2006) ← completed for 2 phases, extending to 3
  - Droplet size distribution capturing – interfacial area, identification of unresolved scales



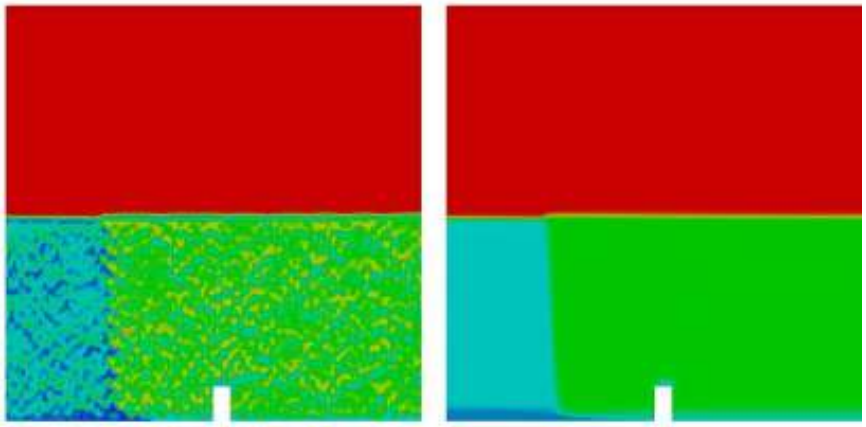
Multifluid-VOF Coupling Example: Collapsing Liquid-Liquid Column

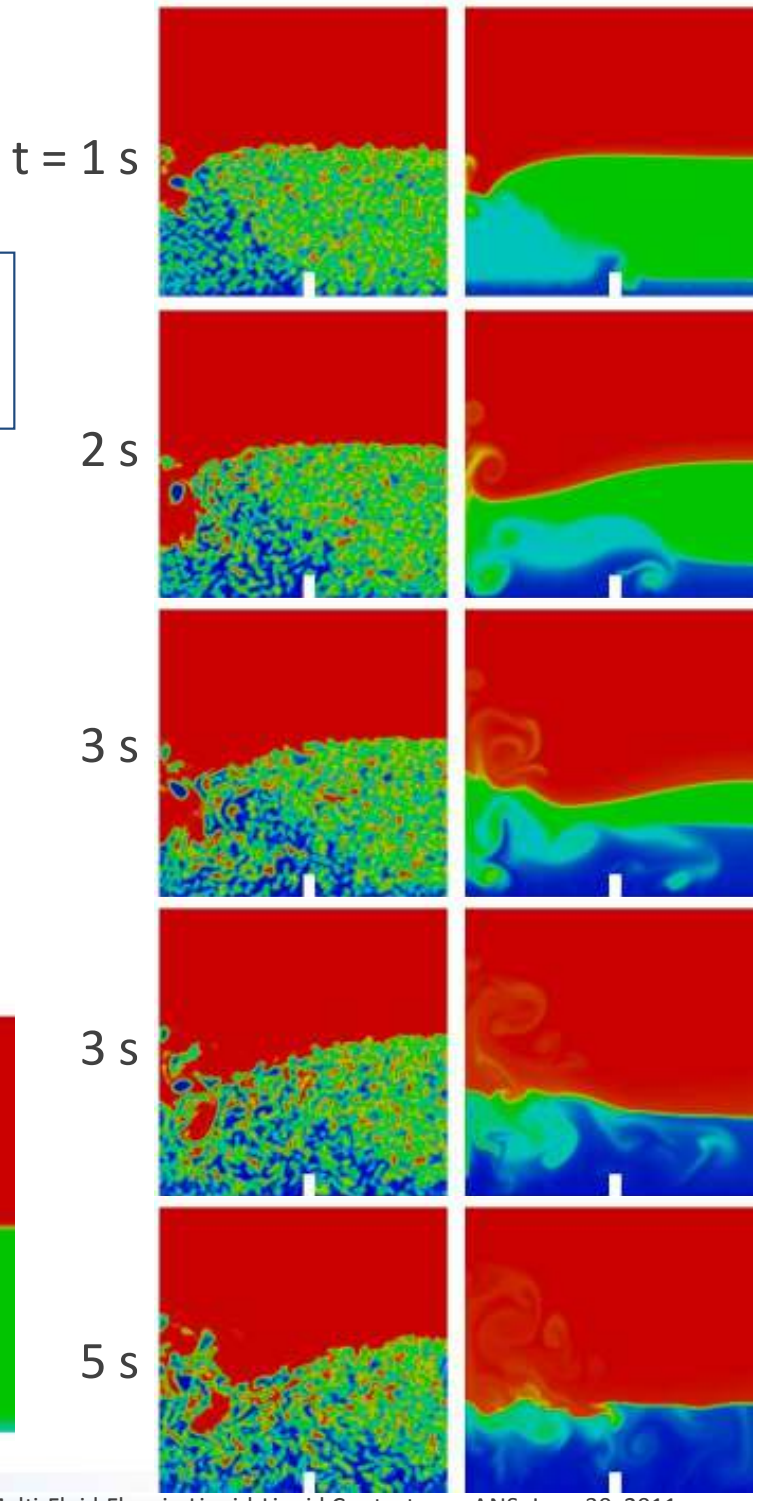
cAlpha parameter controls interface compression for multifluid solver

Interface capturing ON (left, cAlpha=1) vs. OFF (right, cAlpha=0)



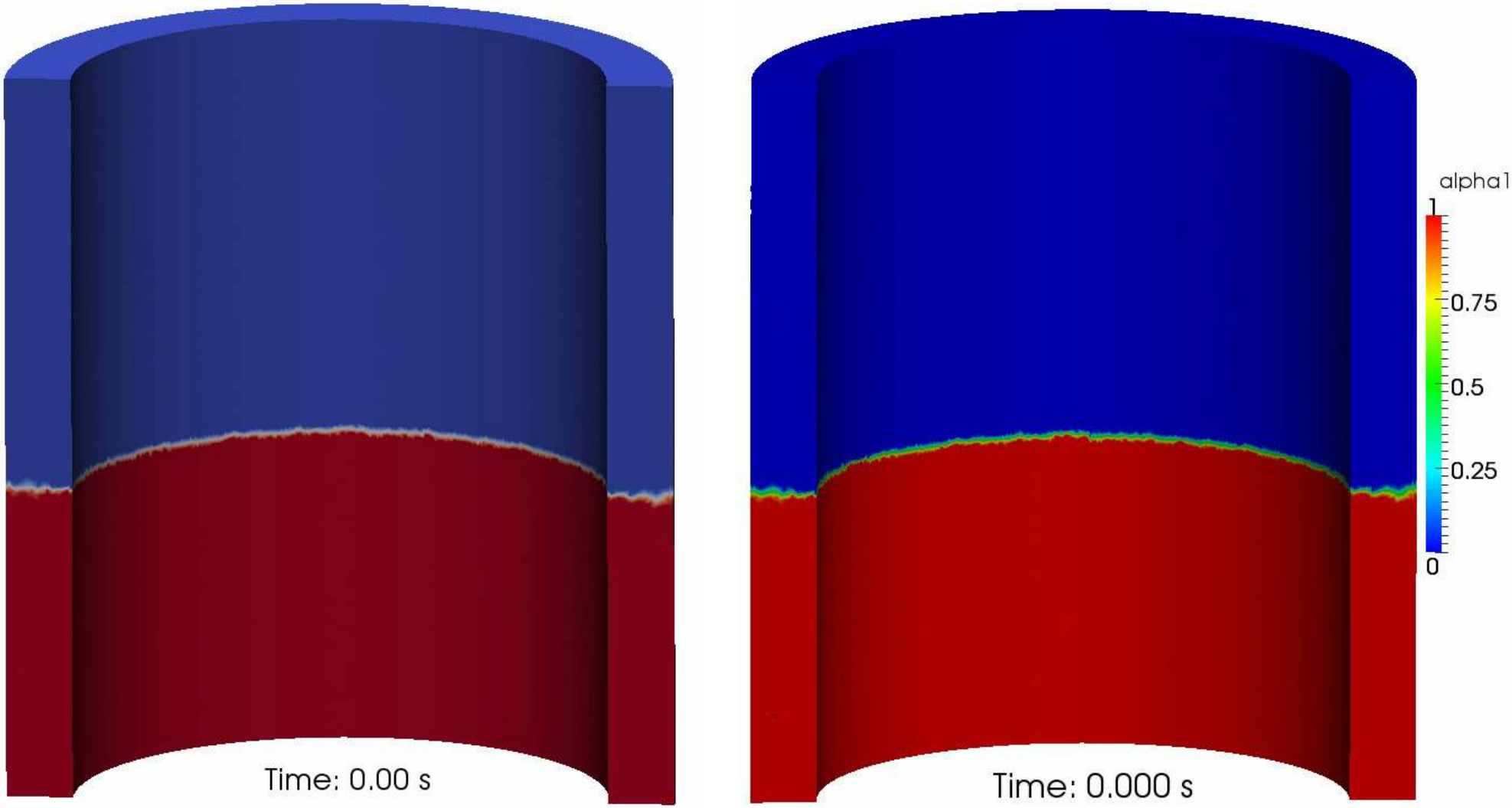
With interface compression on (left), 'droplets' form immediately (t=0.25 s →) at resolvable scale based on mesh spacing





Multifluid-VOF Coupling Example: Annular Mixer

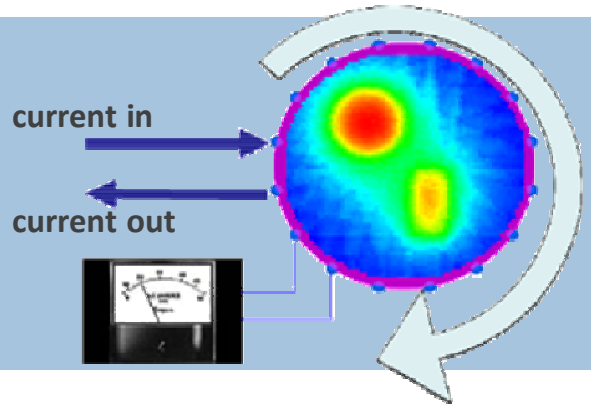
3D annular mixer with no inlets. Water (red) and Air (blue).
LEFT: Multifluid-VOF w/ interface capturing ON (cAlpha is field w/ switching as in Cerne et al. 2001)
RIGHT: Multifluid-VOF w/ interface capturing OFF (cAlpha=0)



Cerne et al. *Journal of Computational Physics* 171:776 (2001). See also Strubelj and Tiselj *Int. J. Numer. Meth. Engng.* (2010).

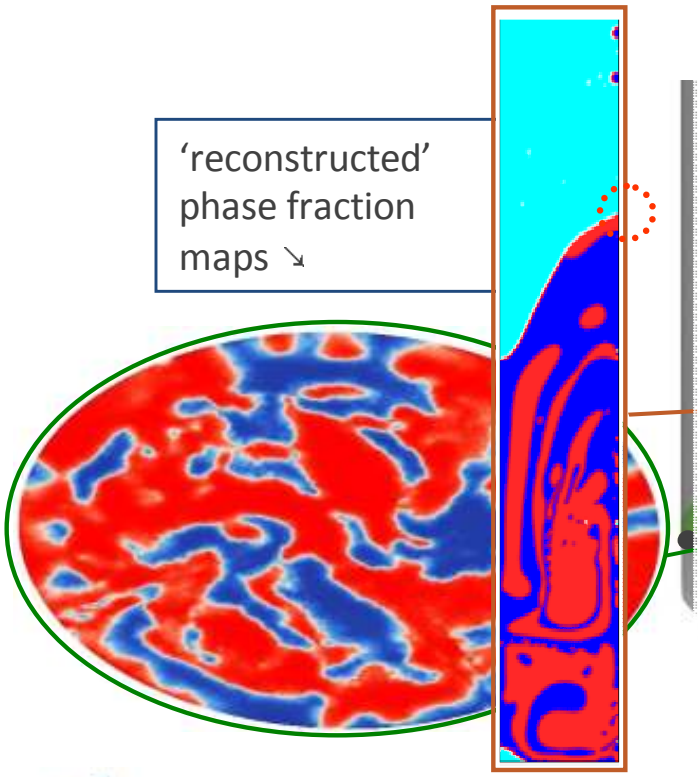
CFD Validation and Experimental Support of Model Development Efforts

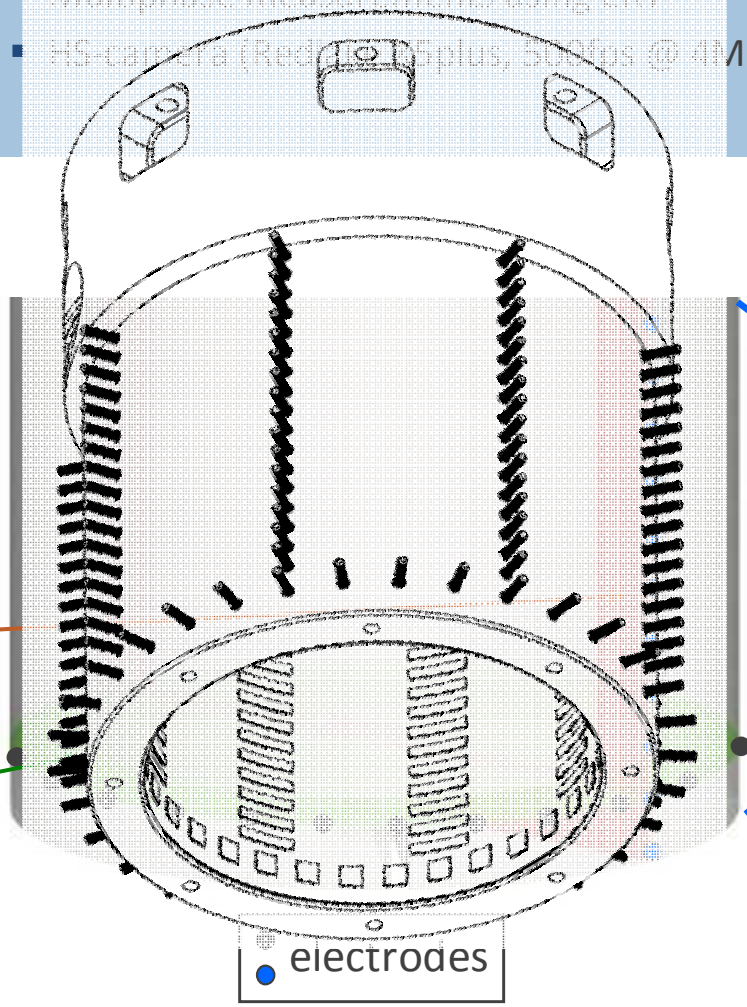
Contactor CFD Validation Using Electrical Resistance Tomography (ERT)

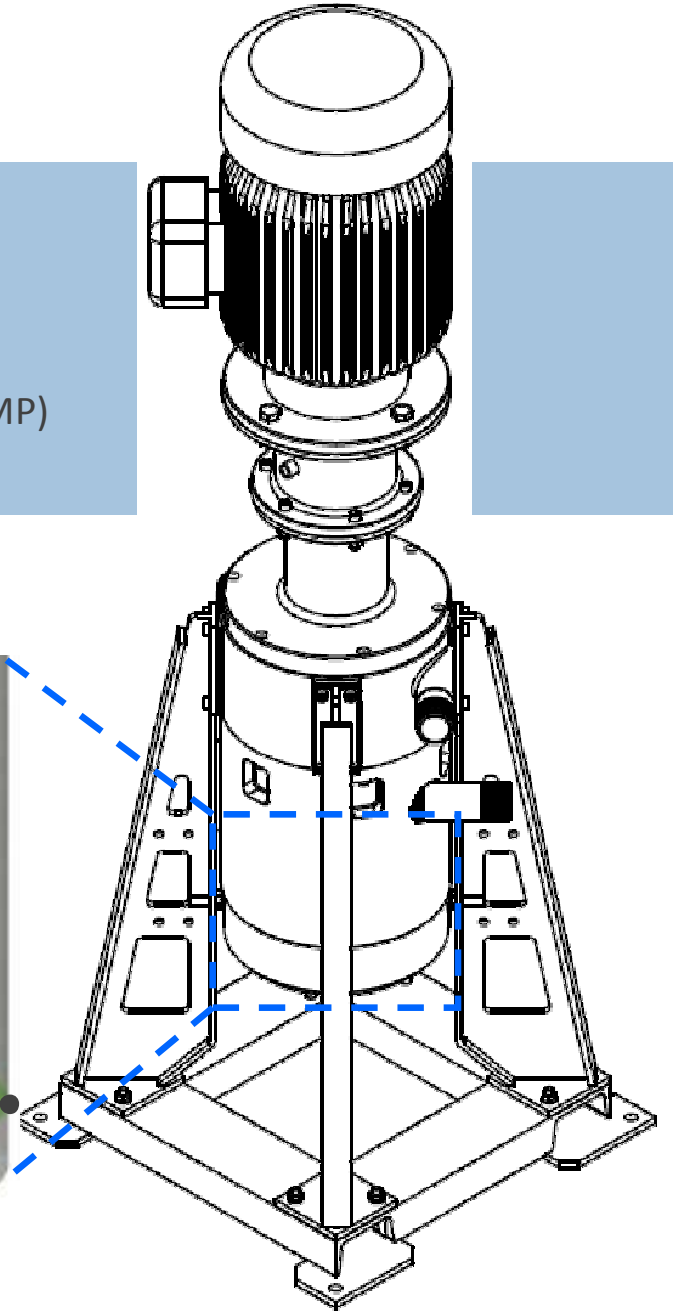


Contactor ERT (CERT) Facility

- Engineering-scale contactor (CINC V-5)
- Multiphase measurements using ERT
- [illegible] (HP)







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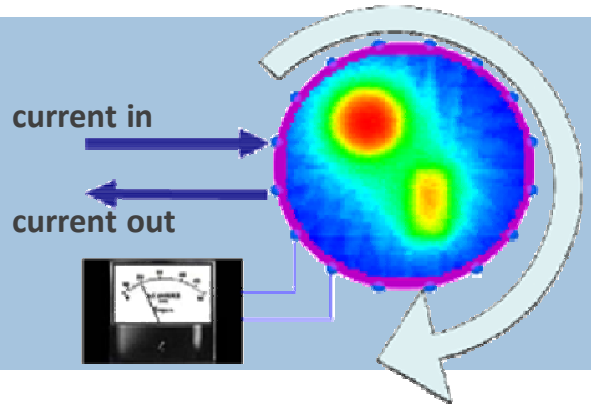
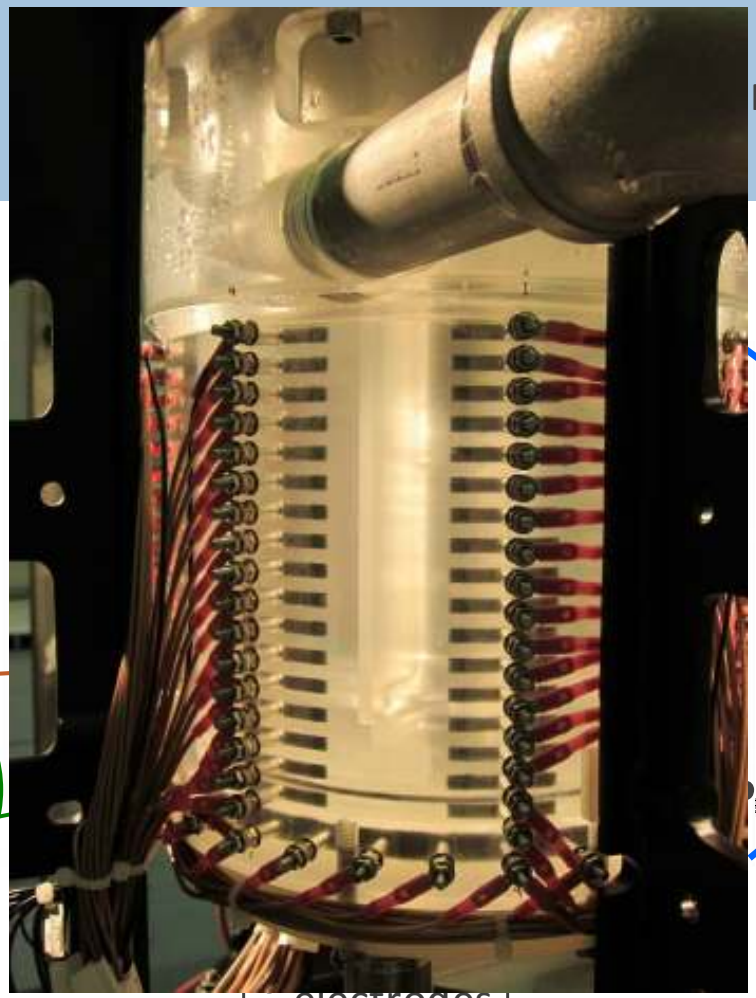
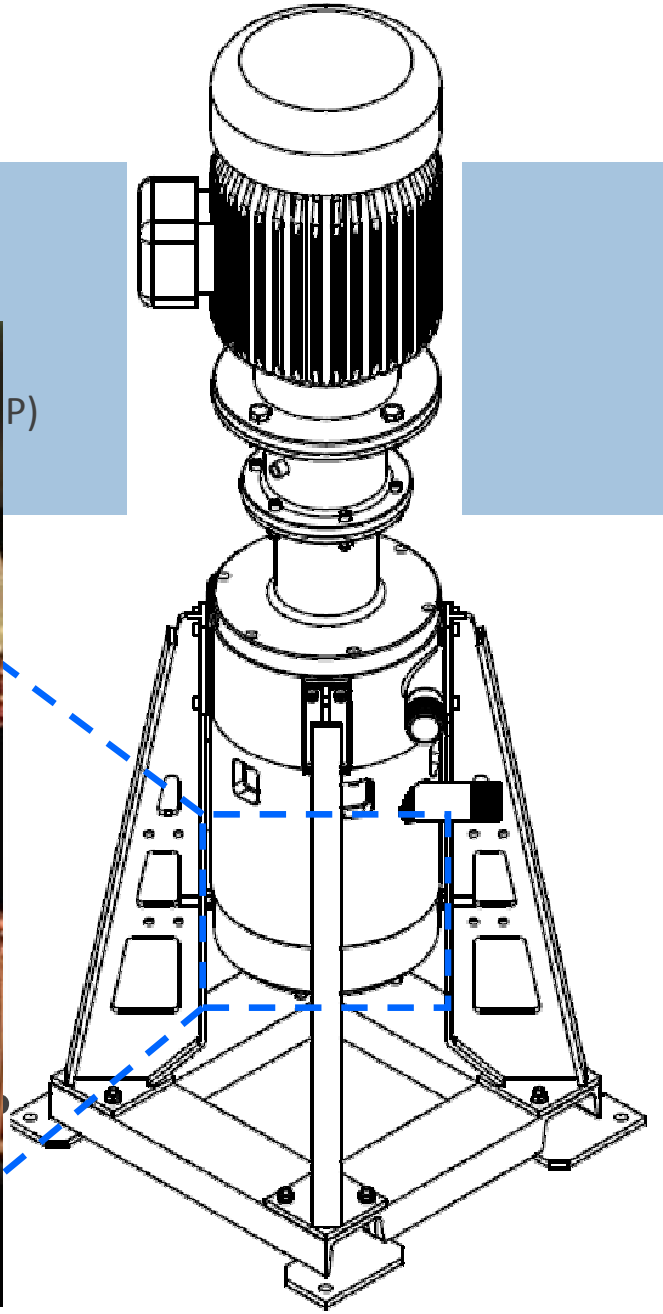


Contactor ERT (CERT) Facility

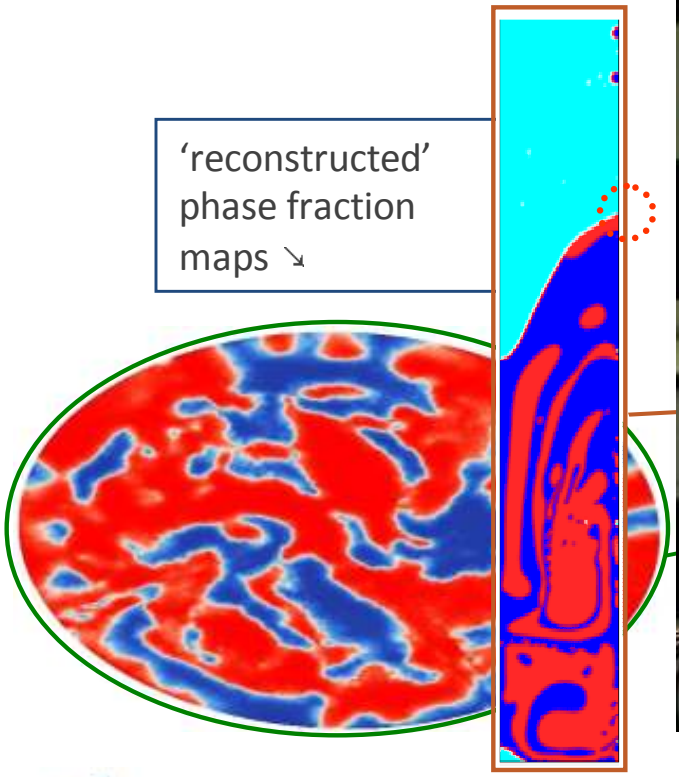
- Engineering-scale contactor (CINC V-5)

P)



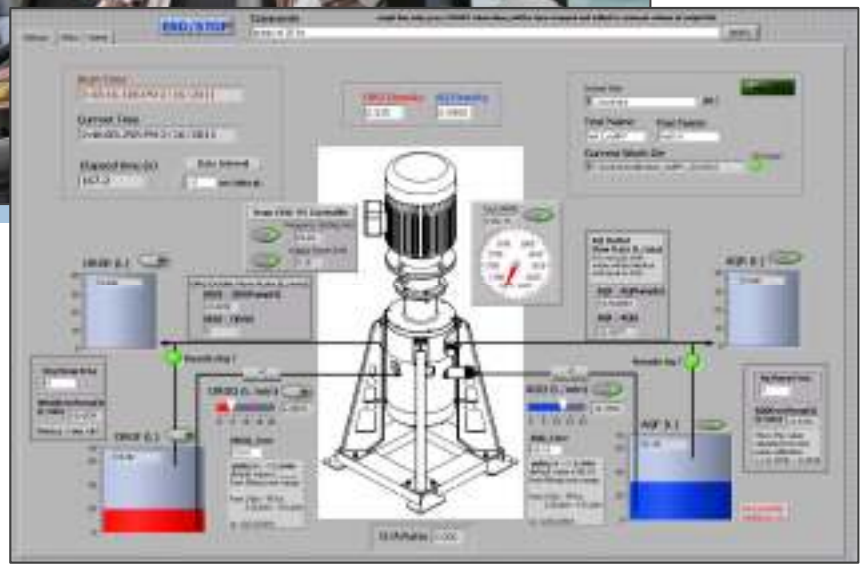


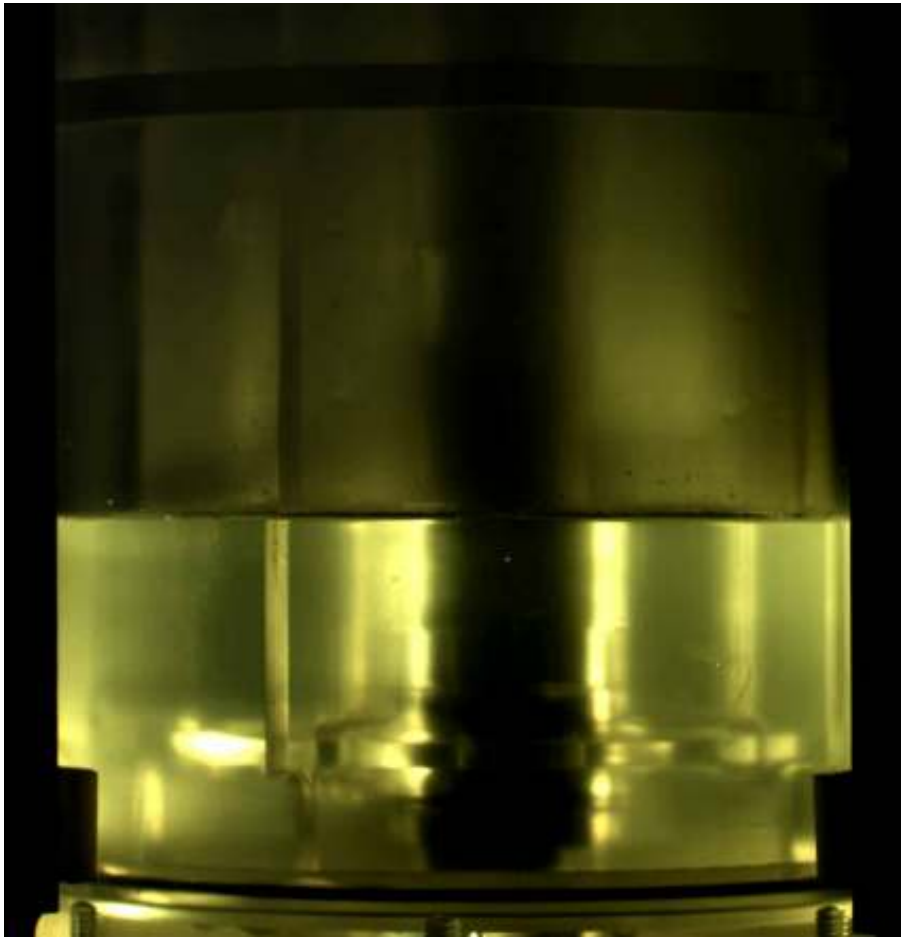
‘reconstructed’ phase fraction maps ↘



electrodes

Contactor ERT (CERT) Facility





Mixing Vane Effect on Mixing Zone Holdup (single-phase): HS-Imaging (1800 RPM, 10 LPM), time-average

4V | 6V | 8V | CV

- Decreasing liquid height with increasing number of vanes, lowest height for curved vanes
  - Same trends as seen previously for CINC-V2 (2inch rotor) [Wardle et al. 2010]
- ***Assuming that single-phase trends hold for liquid-liquid operation***, should affect efficiency
  - Curved vanes are "standard" configuration from manufacturer (CINC)
- Such CINC contactors are in use for CSSX process at Savannah River (CINC-V5 and -V10)

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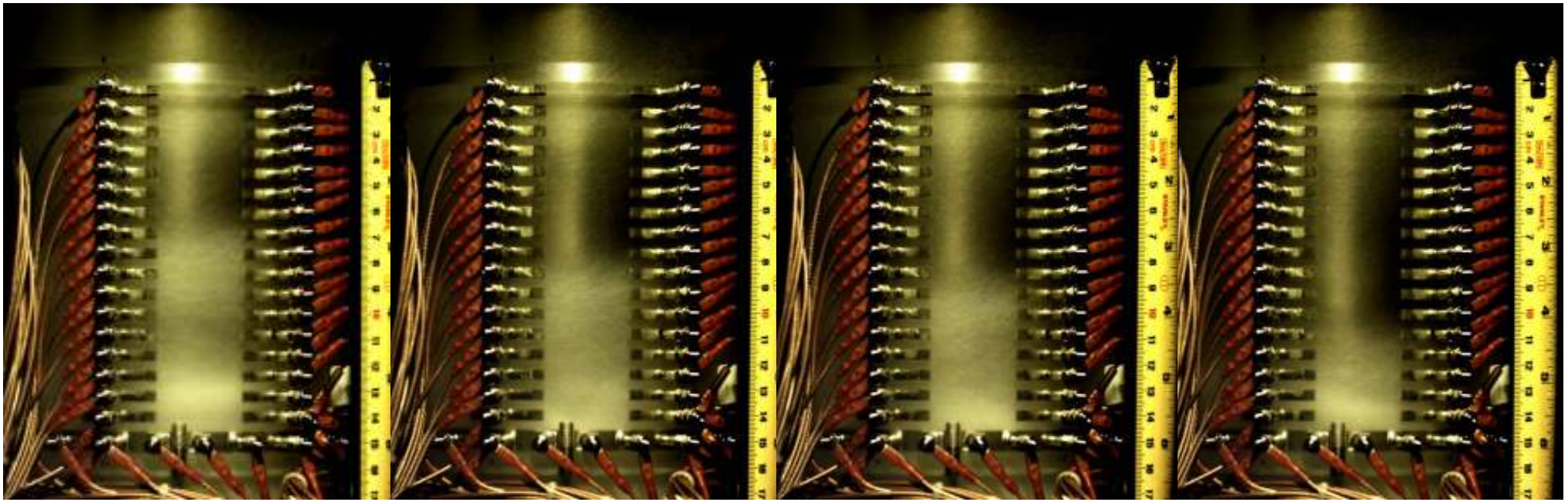

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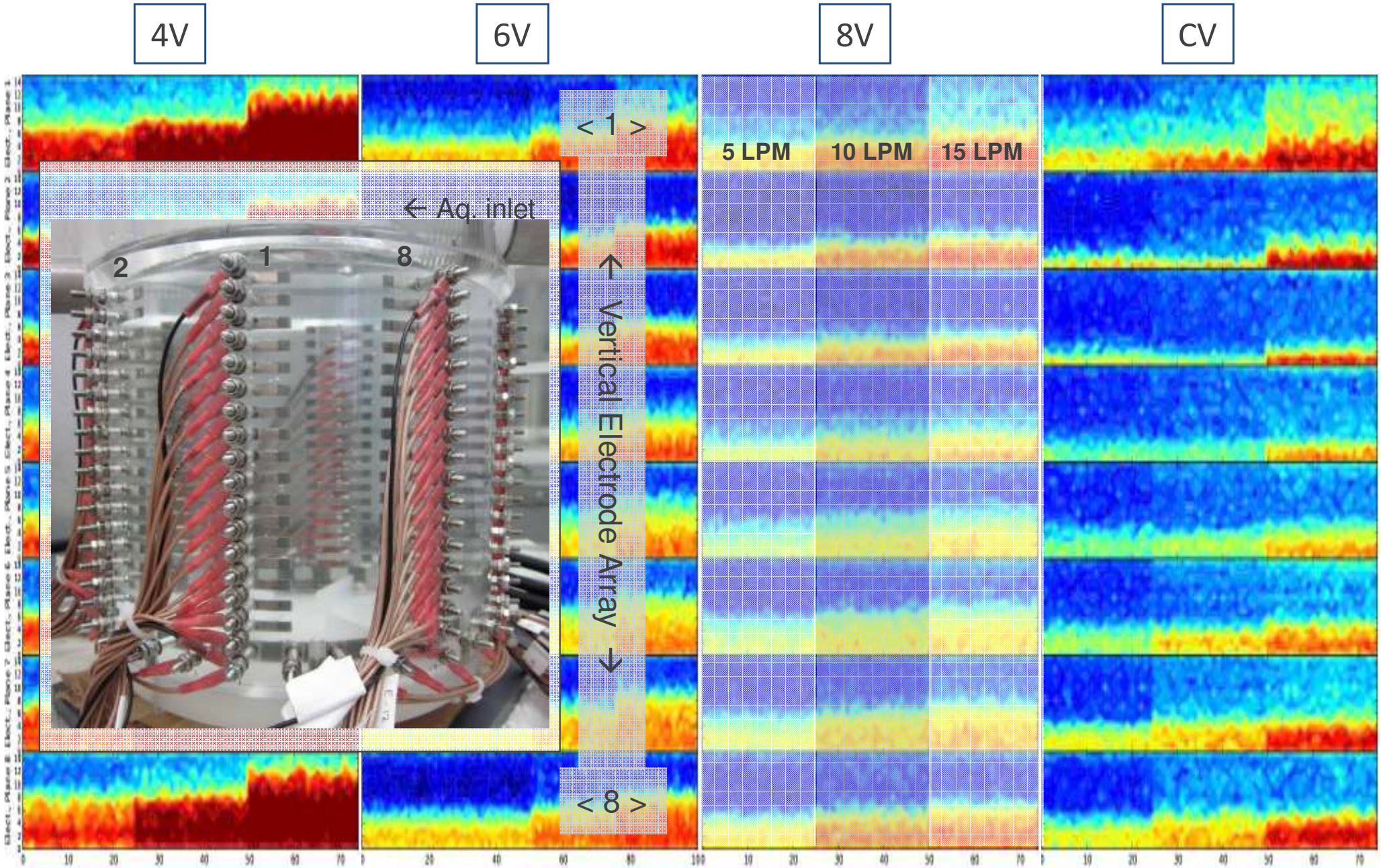
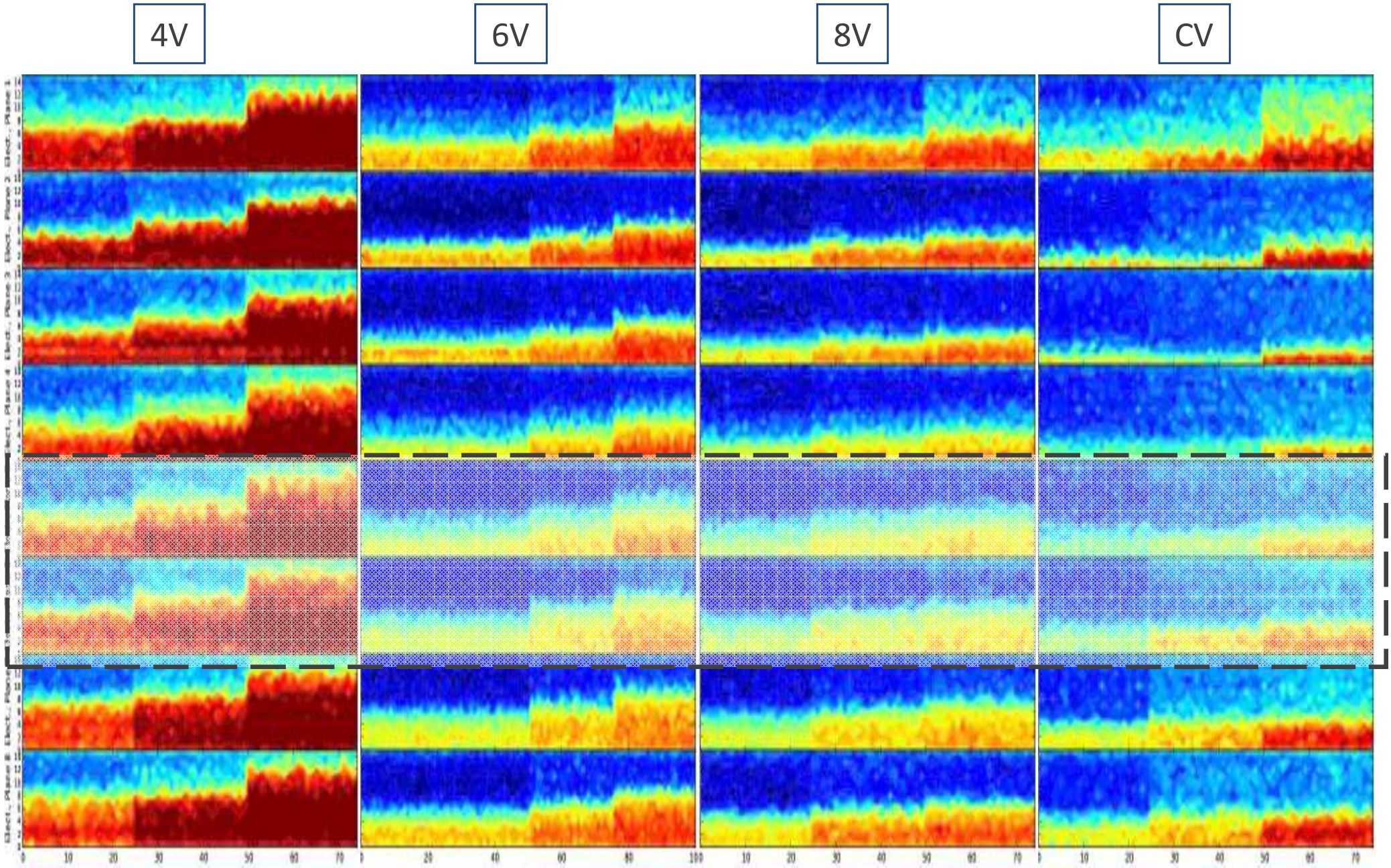
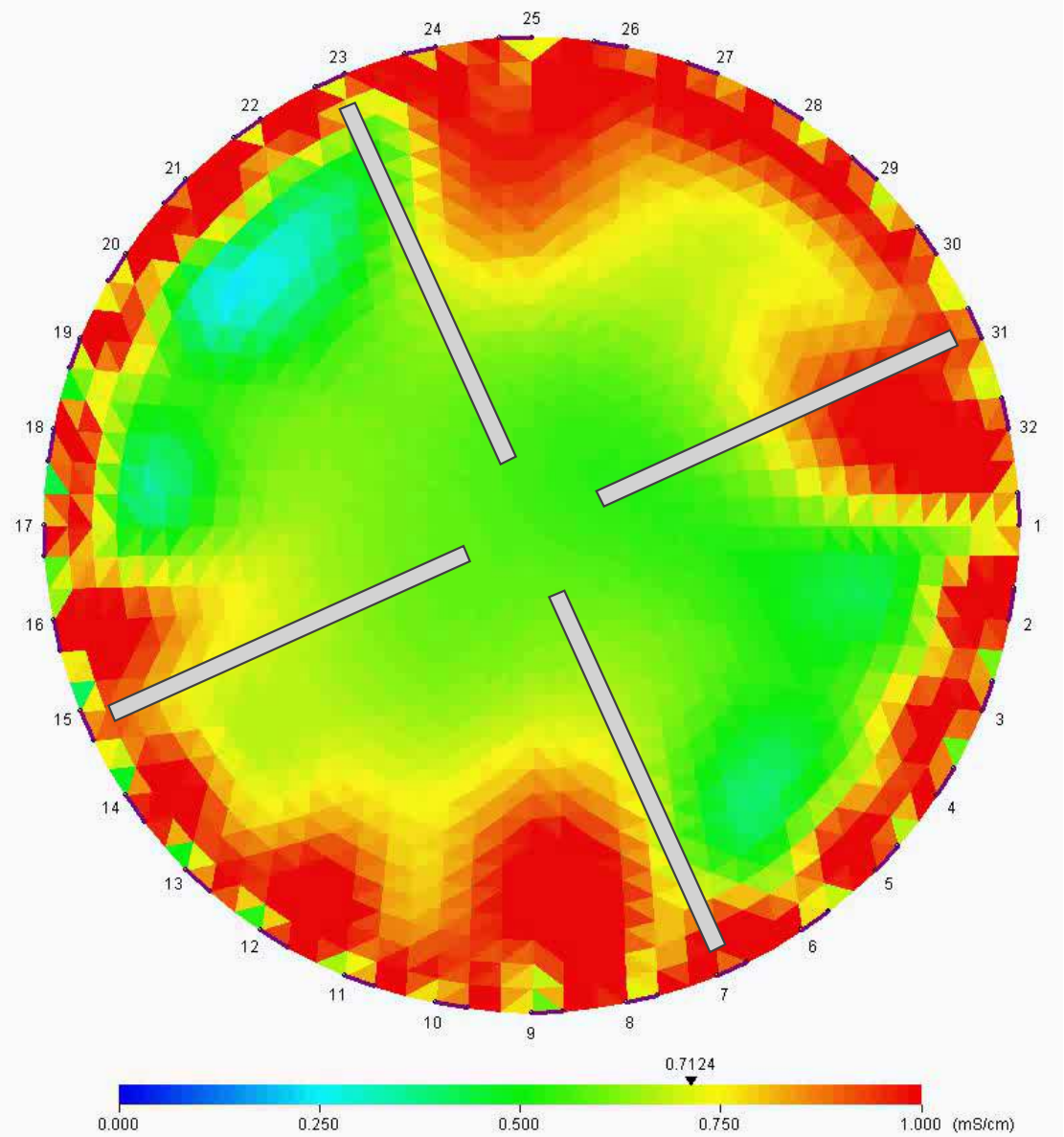
Annular Conductivity Data: Liquid Height (volume fraction = 0..1)

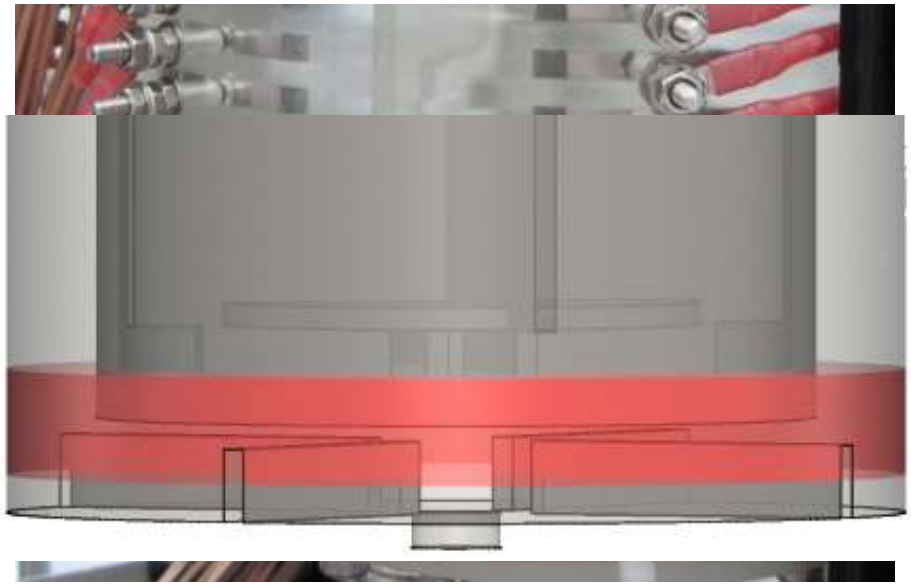


Annular Conductivity Data: Liquid Height (volume fraction = 0 - 1)



Circular 32-Electrode Array Tomography Data: 4-Vane





- Acquired data is a temporal and spatial average
  - Temporal: ~0.75 s (overall rate of ~1.4 Hz)
  - Spatial:
    - Out of plane: electrode size, 7.6mm x 7.6mm
    - In plane: ITS quotes 5% of vessel diameter (5% of 6" = 0.3" = 7.6mm)
- Approximate vane location is shown
  - Measurements are relative to a reference measurement (avg of 100 frames)
  - Effect of internals is masked
- Tomographic "reconstruction" based on Sensitivity Conjugate Gradient (SCG) method [Wang 2002]
- Result is generally asymmetric
  - This was unexpected, but feed is also asymmetric
  - Addition of windows to vane plate could visually verify this result

Wang, M. *Meas. Sci. Technol. 13:101* (2002).

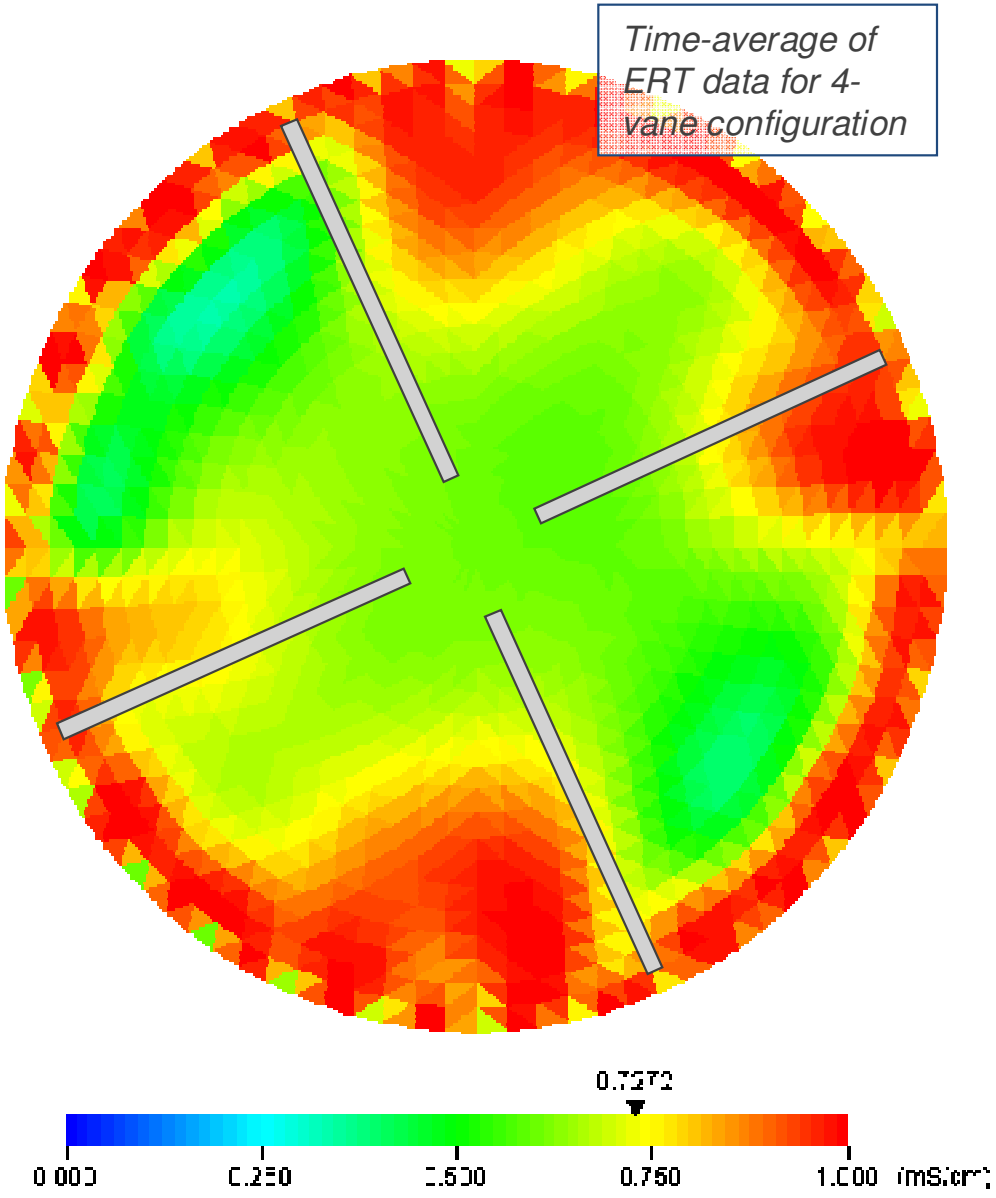
Challenges for CFD Validation Using ERT

Data Quality

- Electrode scans (point conductivity relative to ground, used in annular region)
  - Time resolution is limiting (hardware)
  - Faster with ERT, but uncovered electrodes are problematic
- Tomography
  - Time resolution (can perhaps be optimized)
  - Sensitive to tomographic reconstruction methods
    - Mesh-based reconstruction through solution of inverse problem
    - Various reconstruction algorithms available
    - Sensitive to number of reconstruction iterations
  - Open-source library (matlab or octave) for tomographic reconstruction available (Eidors)

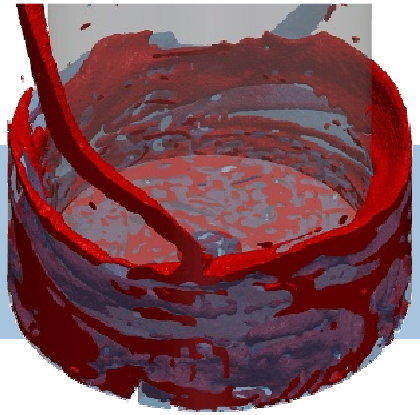
Comparison with simulations

- Comparison to equivalent temporally- and spatially-averaged CFD results
- Exp. data from V5 (large gap needed for ERT), simulations (so far) from V2



Summary and Path Forward

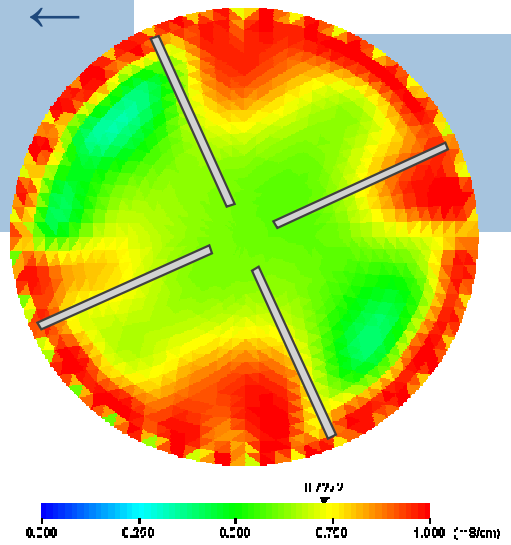
Summary



- Computational
  - Simulations of solvent extraction equipment require advanced multiphase coupling to account for both resolved (e.g. free surface flow) and unresolved (e.g. liquid dispersion) scales →
- Experimental

  - Experimental facility established to acquire data of multiphase flow in liquid-liquid contactors using high-speed imaging ←

    and electrical resistance tomography (ERT) →



Ongoing Work

- Development of coupled Eulerian-Eulerian-VOF solver for three phases is ongoing – phase momentum coupling term is a challenge (stability)
- Verify ERT results from 4-vane case and take ERT data for other vane types
- Data acquisition (HS-imaging, ERT) for liquid-liquid system

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

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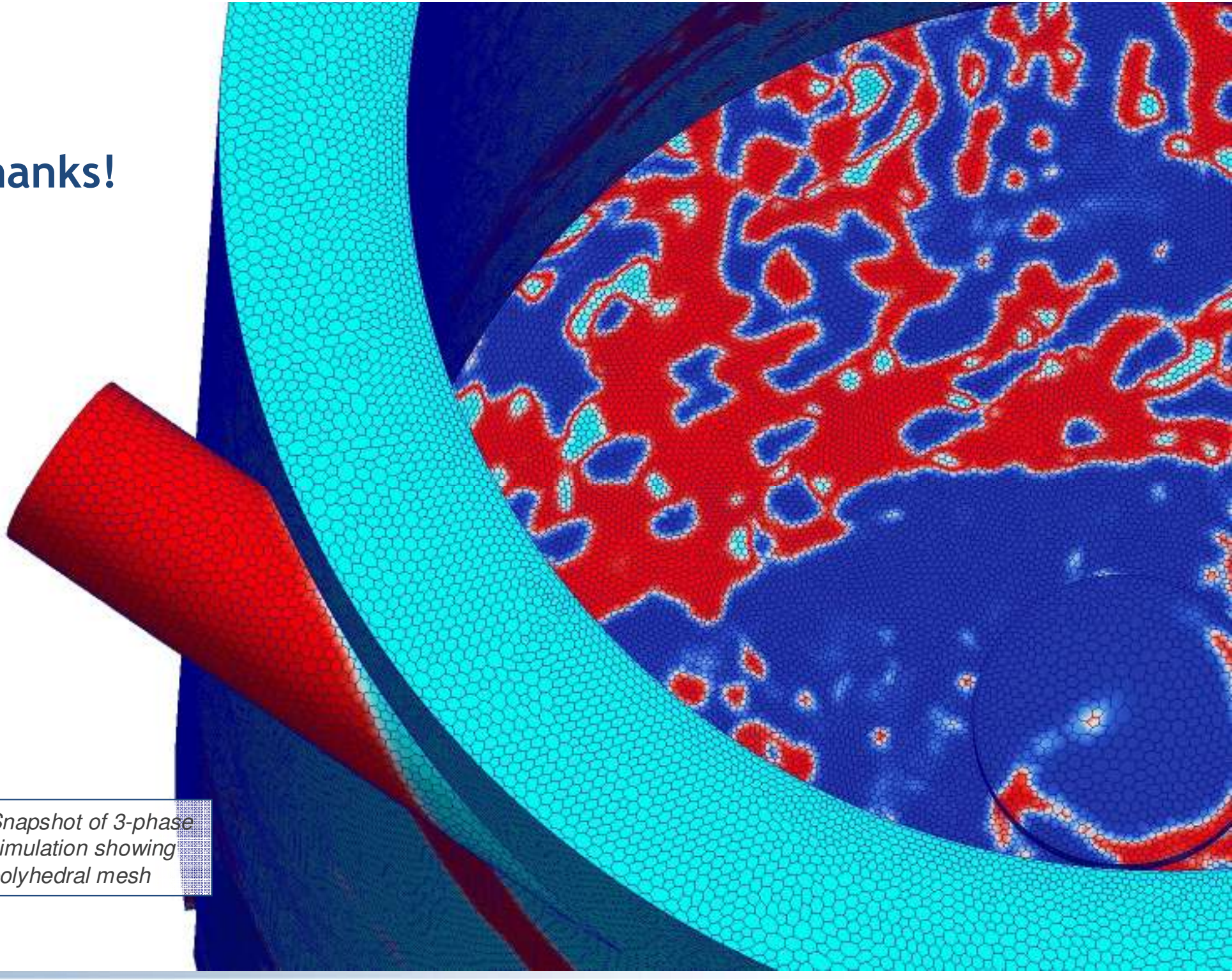
Thanks!



Snapshot of 3-phase simulation showing polyhedral mesh