Simulation of Microfluidics and Droplet Statistics in a Contactor

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Microflows of Solvent Extraction, PI: James Glimm, Stony Brook University

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Title: Sharp Interface Tracking in Rotating Microflows of Solvent Extraction

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Approach to achieve objectives:

Modeling: Microcontinnum theory for viscous, incompressible, two-phase flows with sharp interface tracking.

Software: Parallel front tracking and fluid flow solver adapted for liquid-liquid immiscible micromixing simulation. Resolution of micrometer and microsecond scales of mixing.

Simulation: Direct simulation of interfacial dynamics on parallel architectures using the MPI library. Tested up to 4,000 cores on Idaho Nat. Lab. Center for Advanced Modeling and Simulation clusters.

Purpose: Enable modeling and simulation of micromixing of aqueous-organic fluids used in nuclear solvent extraction.

Importance: Predict detailed information of the dynamics of immiscible, liquid-liquid interfacial flows in vigorous mixing.

Objective of project:



Specific interfacial area Phase distribution Velocity field

Statistical data analysis

Potential Impact: Enable first-principles-based subscale calibration for new modeling of nuclear solvent extraction

Sample Results: Micromixing simulation of aqueous-organic fluids in an annular sector for nuclear solvent extraction based on tri-butyl-phosphate.

Status of Deliverables:

 Year I and II: Simulation code to resolve two phase droplet microphysics.
 Year III: High resolution simulations and statistical data analysis

Publications: Development of a Front Tracking Method for Two-Phase Micromixing of Incompressible Viscous Fluids with Interfacial Tension in Solvent Extraction, ORNL/TM-2012/28.







AFCI, AFM-12

The Problem

Fuel separation for spend fuel rods

Seek processes with lower proliferation risk (no purified plutonium)
Actinide chemistry, many stages
Contactor (high speed rotating flow) gives high contact between
organic and acqueus phases
Chemistry occurs at interface between phases (between two chemicals,
each dissolved in one of two phases.

Research focus: understand chemical reaction rates, to optimize processes

Method 1: understand the statistical distribution of droplet sizes, surface areas, geometrical location within the contactor; assess chemical reaction rates

Method 2: solve the two phase incompressible flow equations with sharp interface in the high speed contactor and collect, analyze, understand the statistics of the droplets.

The Physical Process



Flow regimes near the outer wall of mixing annular gap. **Left:** Centrifugal contactor (5cm-diameter rotor) with clear housing; rotor speed at 2500 rpm. Feeds are TBPdodecane 30% by volume, and 1 M nitric acid. **Middle:** organic-rich 5:1 O/A flow rate ratio. **Right:** aqueous-rich 1:5 O/A flow rate ratio. Exposure time: 24 ms; spatial resolution: 7μ m; field of view cropped to 1 mm x 1 mm.

Theory: droplet stable to breakup has Weber number

$$We = 6 = \frac{\rho U^2 D}{\sigma}; U =$$
 velocity change over droplet size

For flow in question, stable size = 300 microns; current grid 100 microns

Numerical Method

Numerical code: FronTier

Supports sharp interfaces by method of front tracking Interface = organic-acqueous contact surface Moves through 3d Eulerian grid Method is thus mixed Eulerian-Lagrangian

Multiphysics capabilities: compressible, incompressible MHD, combustion, turbulence, fluid-solid interactions boundary layers, fluid-structure interactions

Multiple tests for validity, verification, explanation of methods: Development of a Front Tracking Method for Two-Phase Micromixing of Incompressible Viscous Fluids with Interfacial Tension in Solvent Extraction. ORNL Tech Report TM-2012/28

Numerical tests for solutions (a sample out of many)

Manufactured solutions convergence test in L1, L_infty (u_theta)



Goals

- 1. Build a robust code usable by ORNL scientists in future studies of solvent extraction
- 2. Demonstrate value through a sample study of droplet statistics
- 3. Simulate to late time, to achieve statistical steady state for droplet population
- 4. Expect: Stable droplets with about 300 micron diameter

Progress

- 1. Organic phase has formed dispersed phase, acqueous phase is continuous
- Two or so generations more of droplet splitting still needed to achieve a statistically stationary flow
- 3. Statistical analysis software of droplet surface area and volumes developed
- 4. Organic phase is light, hence prefers inner portion of contactor
- Droplets tend to clump, so that surface area is not a good indicator of chemical reactivity
- 6. New diagnostics needed to assess chemical reactivity of droplet flow



Organic phase is dispersed, droplets about 2 mm diameter. Stable size: about 0.3 mm









Final time step interface and a movie of the slices at theta = constant.

Initially all oil on outside (unstable). Oil is moving to inside and has broken up into 2 mm diameter droplets. Eventual size = 0.3 mm diam.

Plans for next 6 months

End view of computational domain, showing unstable cluster of (light) oil near the outside of the contactor. When fully broken up (at a stable droplet size of 300 microns), there will be some 20,000 oil droplets. Such a calculation is hardly feasible. For statistical convergence, 200 to 500 droplets will be easily sufficient. So the simulation domain should be 3x smaller in z and in theta directions. Initial simulations should be done on a coarse grid, and after a stable distribution on that grid is achieved, successive grid doubling applied until the statistically stable droplet size is achieved.

In this way the computation will be feasible and will be fast enough to allow multiple simulations, variation of parameters, study of statistical convergence issues and analysis of chemical reaction rates.