Multiscale Models of Nuclear Waste Reprocessing: From the Mesoscale to the Plant-Scale

LDRD
LABORATORY DIRECTED RESEARCH & DEVELOPMENT

Sandia National Laboratories

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Problem

Imported oil exacerbates our trade deficit and funds anti-American regimes. Our president has called for the "end of the tyranny of oil."

- Nuclear energy (NE) is a demonstrated technology with high efficiency
- NE's two biggest political detriments are possible accidents and nuclear waste disposal. For NE policy, proliferation is the biggest obstacle
- Nuclear waste can be reduced through reprocessing, where fuel rods are separated into various streams, some of which can be reused in reactors

Current process developed in the 1950s and is dirty and expensive

- U/Pu separation is the most critical ⇨ PUREX

Fuel rods are sheared and dissolved in acid to extract fissile material in a centrifugal contactor. Plants have many contactors in series with other separations.

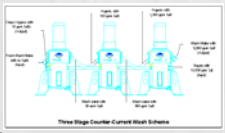
Approach

Science and simulation-based approach to develop a modern reprocessing plant
•Models of reprocessing plants are needed to support nuclear materials accountancy, nonproliferation, plant design, and plant scale-up
•Utilize high performance computing and ASC codes for energy apps
•Multiscale modeling with validation at all scales

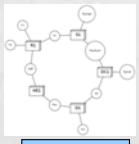
Missing Physics Models Are Being Developed at Multiple Length Scales

Droplet-scale

Contactor-Scale



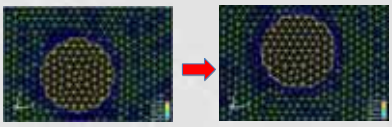
Column-scale



Plant-scale

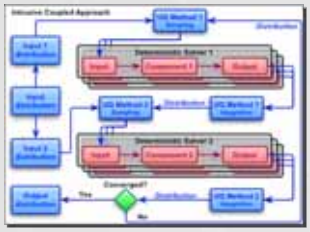
•Leverage Sierra Mechanics developed and supported through ASC for the Weapon's Program as modeling framework for turbulent flow and novel free surface algorithms (CDFEM) for droplet-scale and contactor-scale modeling

Conformal decomposition finite element method (CDFEM) dynamically adds/deletes mesh on moving interfaces as shown for a particle moving with respect to the background fluid



- Leverage ASCR development of parallel, variable fidelity network model for column-scale and plant-scale modeling
  - o Scalable plant flow sheet design
  - o Uncertainty propagation built in

LDRD is populating the ASCR developed network modeler with critical unit operations and reduced-order models



•Advanced thermodynamics/transport properties available through Cantera

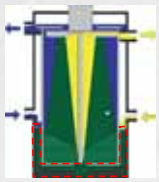
Results

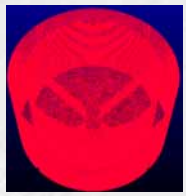
Validation Experiments for Droplet-Scale and Contactor-Scale

Microfluidic experiments developed to look at mass transport from a single drop

Centrifugal contactor experiments to determine droplet-size distribution and mass transfer

Contactor scale modeling in Sierra

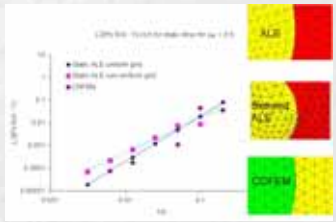




Sierra/Aria transient turbulence model of contactor – largest production Aria calculation to date

Droplet-scale CDFEM modeling in Sierra: verification journal article in progress

Testing showed issues with the algorithm for droplet break-up in shear flow and motivated verification study



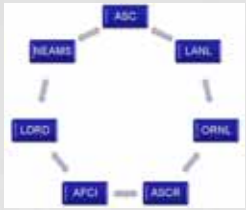
Static drop problem generates spurious currents depending on accuracy of the numerical method

•Thermodynamic modeling of uranyl transport to integrate into multiphase flow
•Network model furthered, with "units" developed for the front end of a plant
•Hybrid finite element method developed to allow for turbulent flow CDFEM coupling for multiphase flow models
•Collaborations /discussions with ORNL, LANL, Yale, NEAMS PI Meeting

Significance

•Enable cost-effective, commercially viable reprocessing while maintaining proliferation resistance

•State-of-the-art novel capabilities to attract new customers:
- •Multiscale models of turbulent concentrated-solution mass transfer for 3 to 5 phases
- •First-principles prediction of emulsion rheology, surfactant transport and phase behavior
- •Criticality assessment linked to separations
- •Plant flow sheet capability at Sandia



•Develop collaborations with experts at other labs and increase Sandia's footprint in NE for separations modeling

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