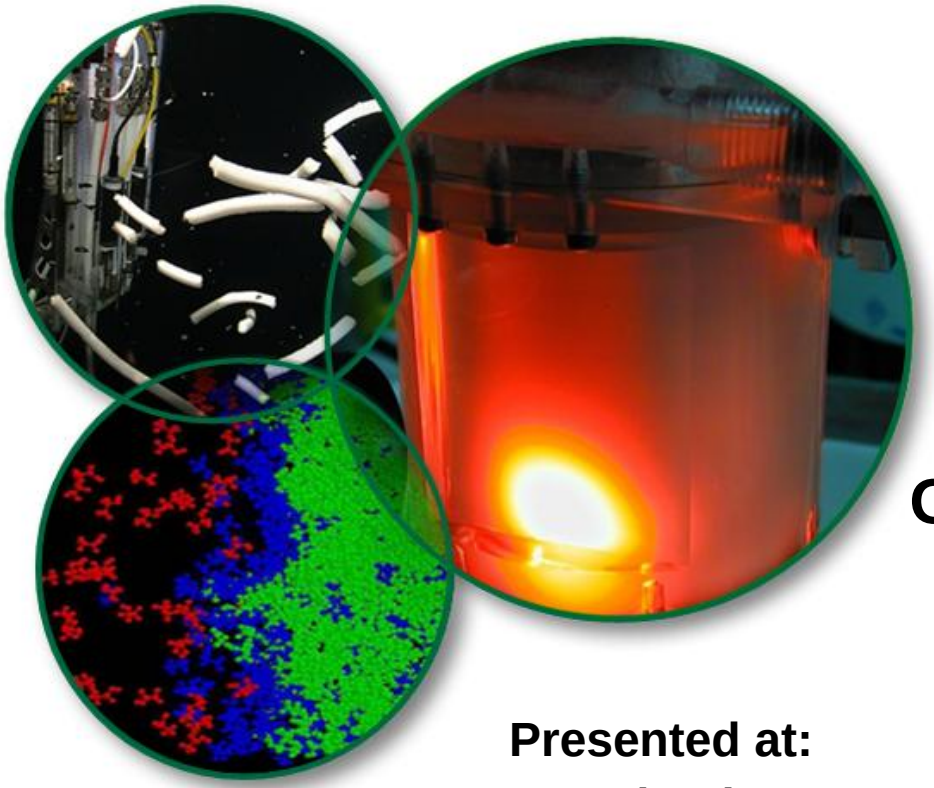
Modeling and Simulation of Nuclear Fuel Recycling Systems



David DePaoli

Oak Ridge National Laboratory

Presented at:

Introduction to Nuclear Chemistry and Fuel Cycle Separations

North Las Vegas, Nevada

July 20, 2011

Outline

- Introduction
- Some applications to date
  - Solvent extraction
  - Plant-level modeling
  - Agent design
- Key research needs
- Advancing to the future
  - NEAMS vision
  - Separations M&S development

Used Nuclear Fuel Recycling Entails Many Interconnected Steps

Used fuel
varied composition
(burn-up, cooling time)

Products
meeting stringent specifications

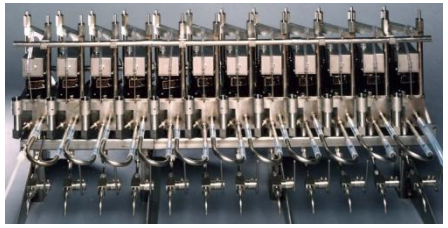
Environmental, safety, accountability constraints

shearing

dissolution

voloxidation

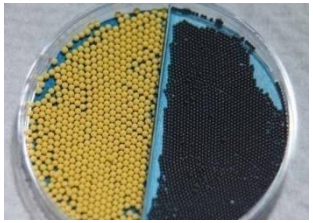
feed & accountability



solvent extraction cycles

solidification

waste treatment



Fuel

Waste forms

off-gas treatment

recovery systems

- **Need new processes to meet future goals**
- **Emerging modeling and simulation capabilities can improve development and implementation** (better, cheaper, faster)

Benefits of modeling and simulation of nuclear reprocessing systems

- Reduced cost of process development by guiding and minimizing the amount of experimental and piloting work required
  - Compare different separation and fuel cycle strategies
  - Develop new chemical processes with lower cost and waste generation
- Optimized system designs, with reduced design margins
  - Scale up with confidence
  - Reduce hot-cell footprint (surge capacity, throughput)
  - Process control
- Increased safety and acceptance of regulatory bodies
- Reduced risk of material diversion by providing accurate predictions of materials streams

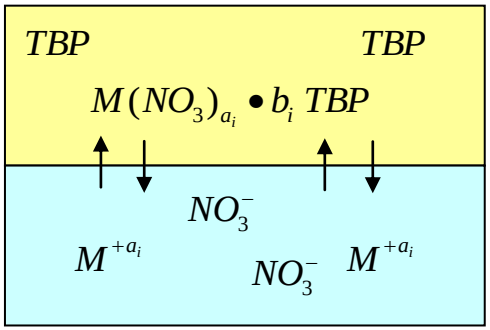
Modeling and simulation

- **Modeling is the development of an approximate mathematical description of physical and chemical processes at a given level of sophistication and understanding.**
- **Simulation utilizes computational methods to obtain predictions of process perform**
- **"Together modeling and simul**
  - **enhance understanding of l**
  - **provide qualitative/quantitative insights and guidance for experimental work, and**
  - **produce quantitative results that replace difficult, dangerous, or expensive experiments."**

Important Note: ***Advanced modeling and simulation do not replace the need for experiments!!!***

(*Basic Research Needs for Advanced Nuclear Energy Systems,* http://www.sc.doe.gov/bes/reports/abstracts.html#ANES)

Modeling and simulation of nuclear separations has primarily focused on solvent extraction



$$M^{+a_i}_{(aq)} + a_i\, NO^-_{3(aq)} + b_i TBP_{(org)} \Leftrightarrow M(NO_3)_{a_i} \bullet b_i\ TBP_{(org)}$$

$$K_i = \frac{\left[M(NO_3)_{a_i} \bullet b_i\ TBP\right]_{org}}{\left[M^{+a_i}\right]_{aq}\left[NO_3^-\right]^{a_i}_{aq}\left[TBP\right]^{b_i}_{org}}$$

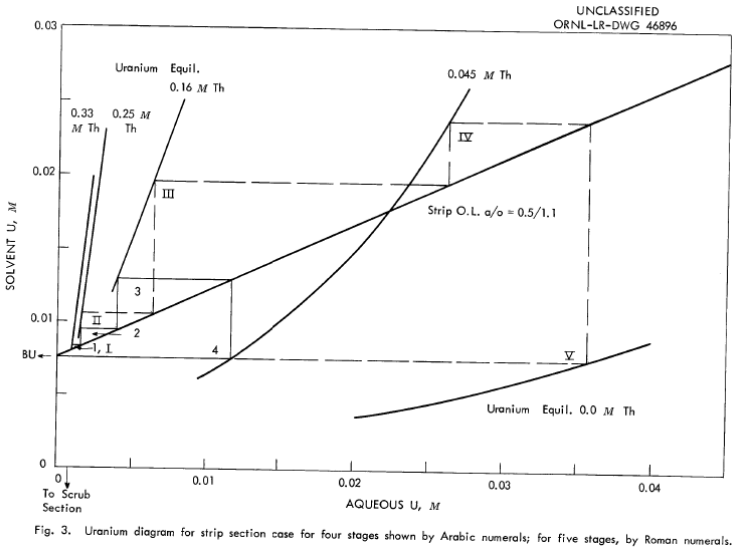


Fig. 3. Uranium diagram for strip section case for four stages shown by Arabic numerals; for five stages, by Roman numerals.

A. D. Ryon, ORNL-3045, 1961

- **Original predictions:**
  - **Graphical stage calculations using experimental equilibrium data and operating lines**

Existing models are based on empirical fits to experimental data

$$K_U^{'} = \frac{\left[UO_2(NO_3)_2 \bullet 2\ TBP\right]_{org}}{\left[UO_2^{2+}\right]_{aq}\left[NO_3^-\right]_{aq}^2\left[TBP\right]_{org}^2}$$

$$K_{Th}^{'} = \frac{\left[Th(NO_3)_4 \bullet 3\ TBP\right]_{org}}{\left[Th^{4+}\right]_{aq}\left[NO_3^-\right]_{aq}^4\left[TBP\right]_{org}^3}$$

$$K_H^{'} = \frac{\left[HNO_3 \bullet 3\ TBP\right]_{org}}{\left[H^+\right]_{aq}\left[NO_3^-\right]_{aq}\left[TBP\right]_{org}}$$

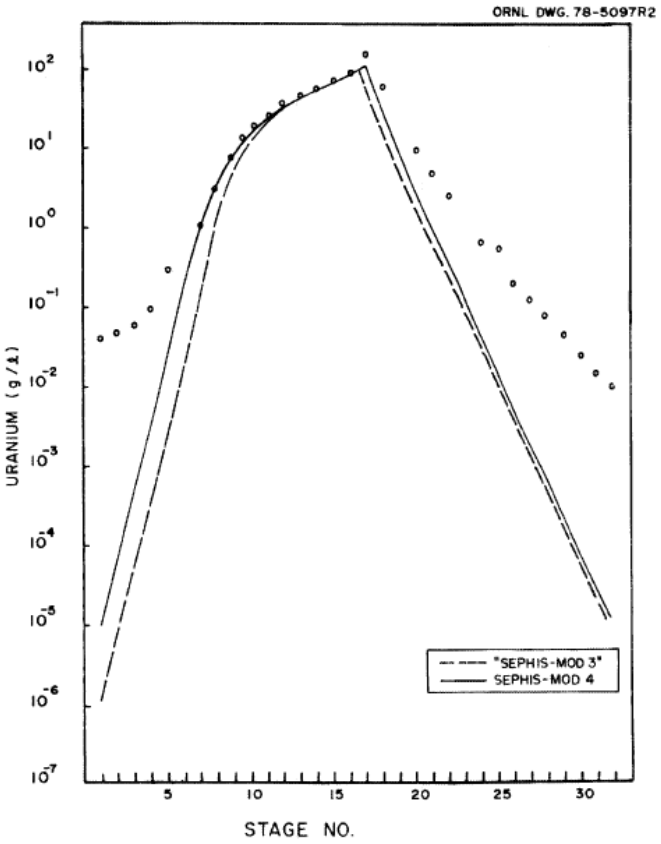
$$K_U^{'} = C_1 + C_2\,\mu + C_3\mu^2 + C_2\,\mu^3$$

$$K_{Th}^{'} = C_5 + C_6\,\mu + C_7\mu^2 + C_8\,\mu^3$$

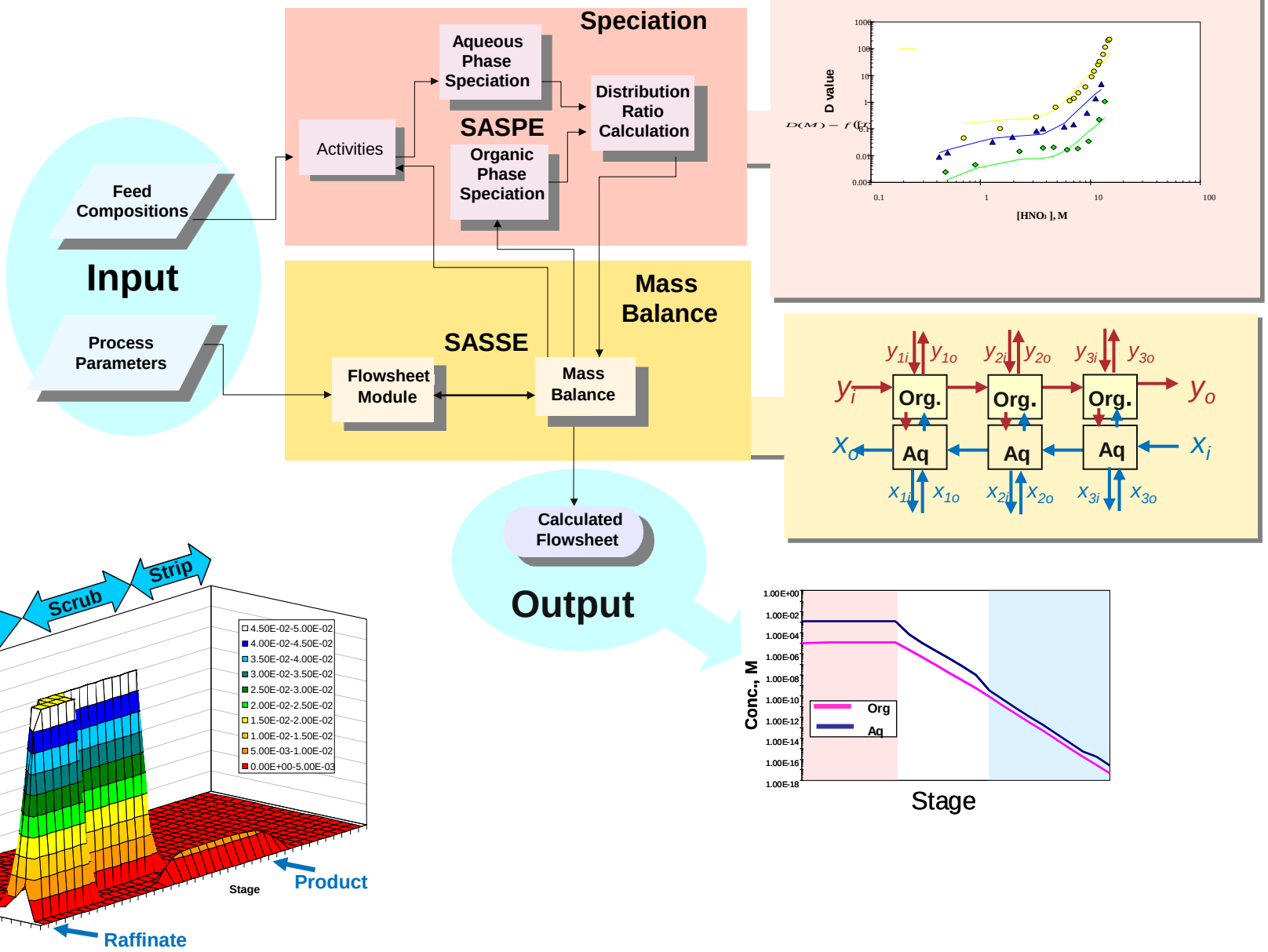
$$K_H^{'} = C_9 + C_{10}\,\mu + C_{11}\mu^2 + C_{12}\,\mu^3$$

$$\mu \equiv \left[H^+\right] + 3\left[UO_2^{2+}\right] + 10\left[Th^{4+}\right]$$

Rainey and Watson, 1975



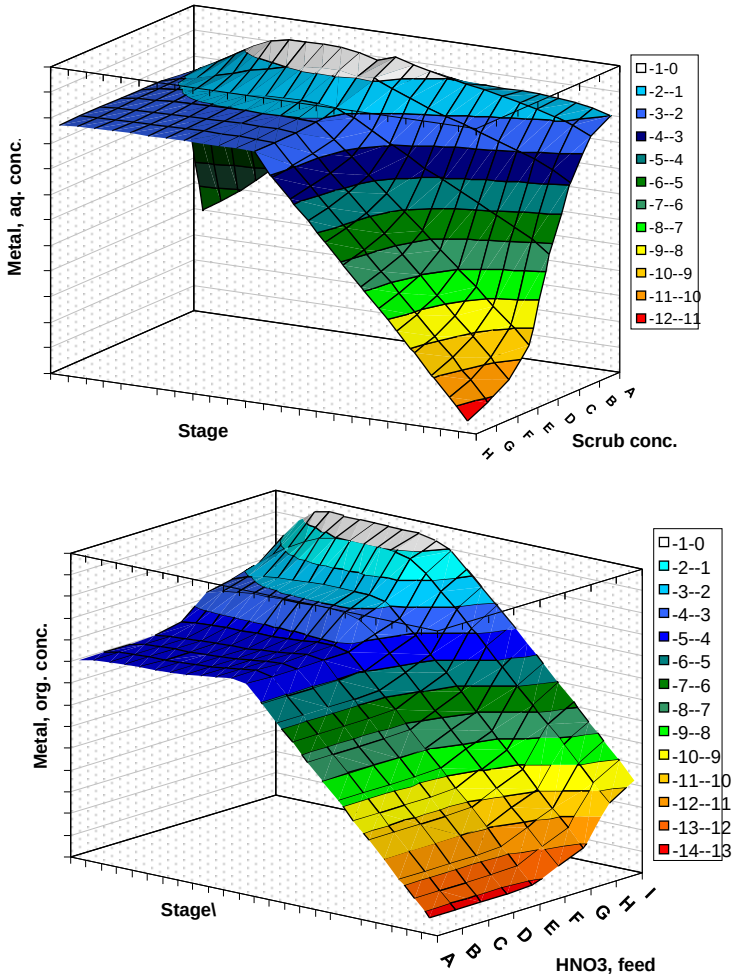
AMUSE Models Solvent Extraction



M. Regalbuto and C. Pereira, ANL

AMUSE has been used for process upset and product diversion analysis

- AMUSE was used to bracket the operational window for a plant conceptual design
  - Four fuel compositions were used as the initial process feed
    - *High and low burn-up; long- and short-cooled fuels*
  - Results showed little difference with cooling time but stronger effect due to burnup differences
- More recently AMUSE has been used to examine the effect of changing specific process parameters on the behavior of different elements
  - Design of instrumentation to track material
  - Process control
  - Product purity determination
  - Product diversion detection



Changes in feed composition lead to changes in the concentration profiles in the aqueous and organic phases

Recent work – Linkage of AMUSE to plant-scale flowsheet in ASPEN

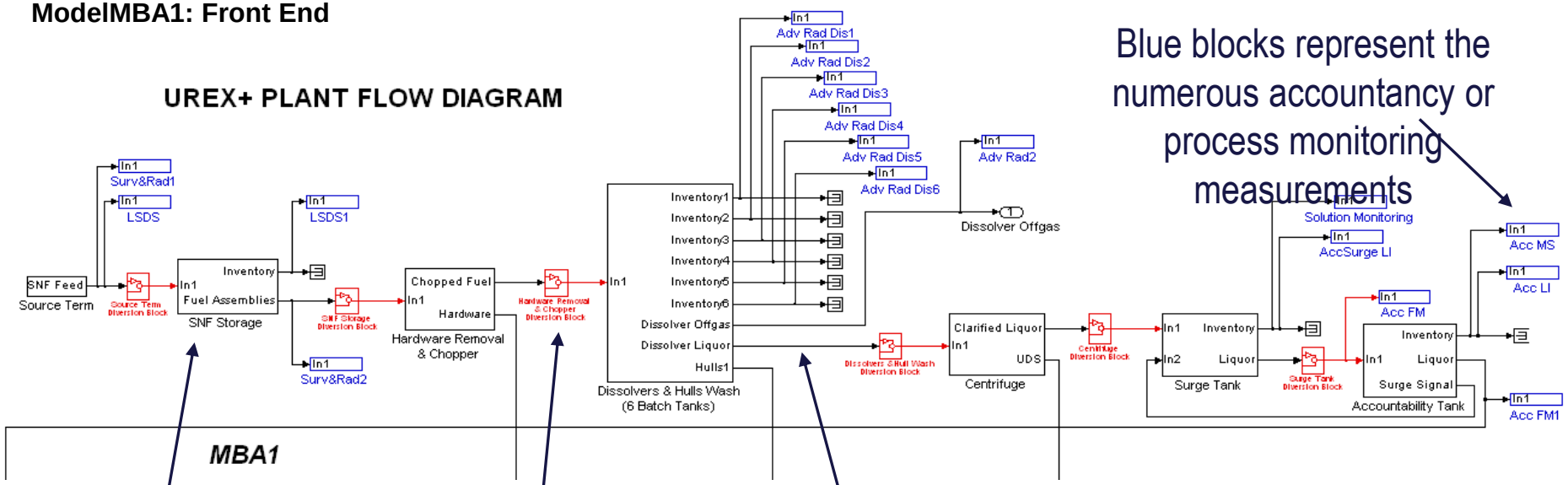
M. Regalbuto and C. Pereira, ANL

1980's – a full plant model

- **Consolidated Fuel Reprocessing Program - a complete plant simulation run in the Advanced System for Process ENgineering (ASPEN) simulator**
- **52 components tracked throughout a preconceptual design of a plant containing 32 systems and approximately 700 streams, including:**
  - **fuel cleaning and storage**
  - **disassembly and shearing**
  - **dissolution and feed preparation**
  - **hulls drying**
  - **feed clarification**
  - **feed preparation and accountability**
  - **solvent extraction**
  - **solvent extraction ancillary systems (concentration, backcycle, storage, high-activity waste concentration, solvent recovery)**
  - **process support (acid and water recovery and recycle, process steam, and sump)**
  - **product conversion**
  - **cell atmosphere cooling and purification**
  - **process off-gas treatment**
  - **vitrification**
  - **vitrification off-gas treatment**
- **Large simulation for computers of the time**
  - **broken down into three segments that were executed separately to achieve a steady-state material balance for the complete plant.**

Sandia Safeguards Performance Model

ModelMBA1: Front End



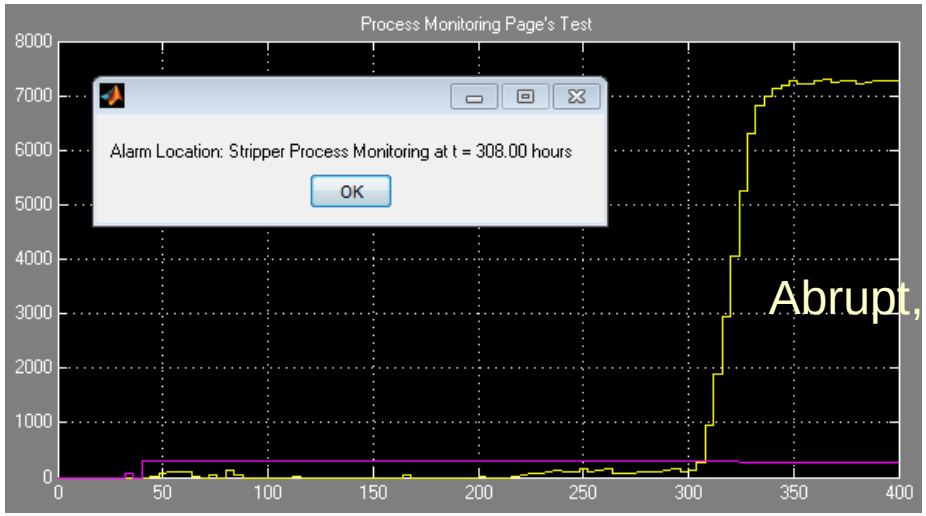
Blue blocks represent the numerous accountancy or process monitoring measurements

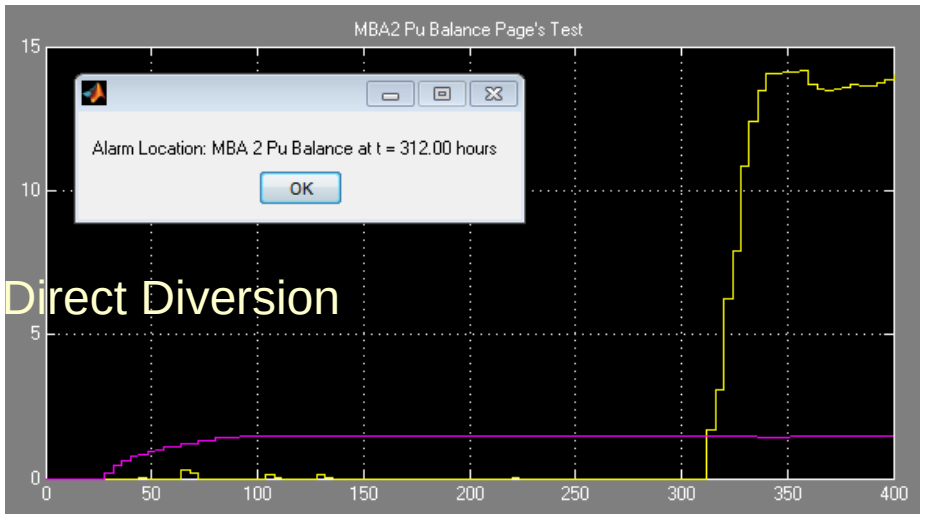
Each unit operation is a subsystem that models the process

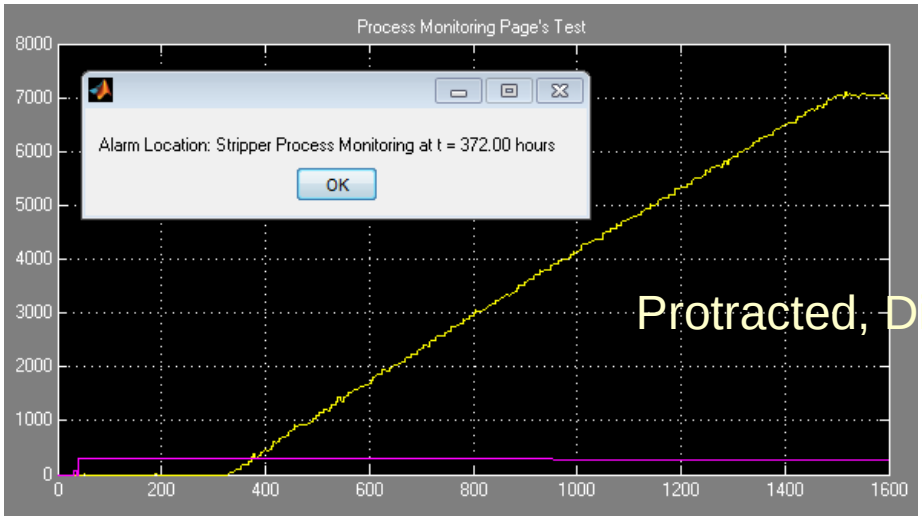
Red blocks are potential diversion points that can be turned on by the user

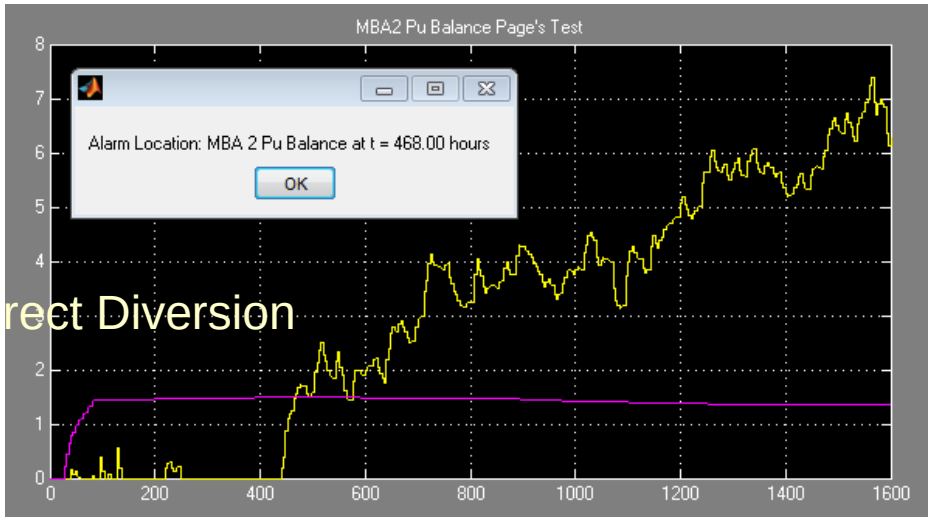
Each signal is an array that contains the mass flow rate of each element as well as bulk liquid and solid flow rate—arrays are expandable

Advanced Monitoring System Results:
Direct Diversions of 8 kg of Pu







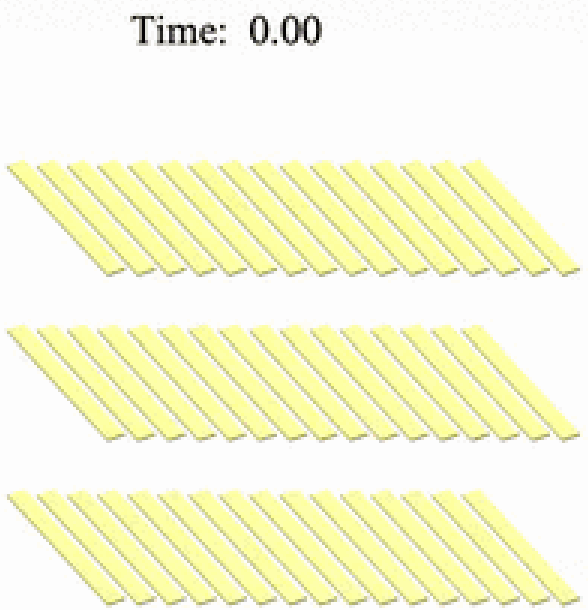


B. B. Cipiti, SNL

Current state of separations process modeling

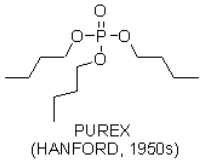
- **Solvent extraction most developed**
  - **Useful aid in process development and analysis**
  - **Semi-empirical fits**
  - **Many species not modeled well, or not at all**
  - **Leading codes use equilibrium stages**
  - **Current codes do not predict well:**
    - **Mass transfer and reaction kinetics effects**
    - **Effects of micellization, third-phase formation, radiolysis, etc.**
  - **Few transient codes**
- **Other important processes not well modeled**
  - **Legacy modules for some important unit operations are available**
    - **e.g., dissolver, acid recovery**
- **Full plant models are crude**
  - **Simple descriptions of important unit operations**
  - **Not fully transient**

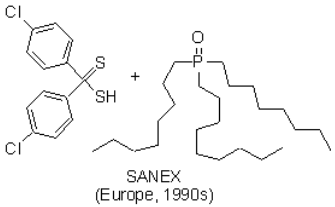
Example of transient output from SEPHIS process model for U/Pu solvent extraction step.

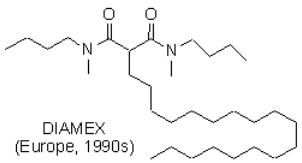


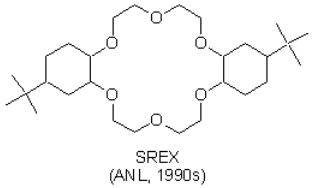
Height of bars indicates concentration of uranium in organic (top) and aqueous (bottom) phases in a 48-stage mixer settler bank. Time indicates the time in minutes from the start of operation with zero concentration throughout the system.

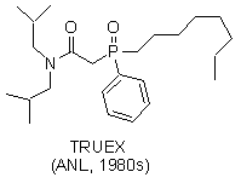
Sequestering agents are the basis for separations

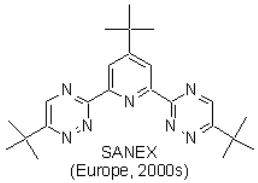






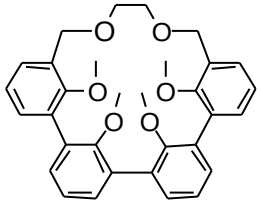




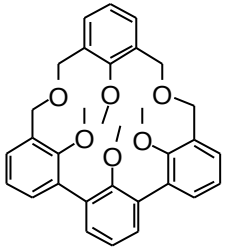


Influence of ligand architecture

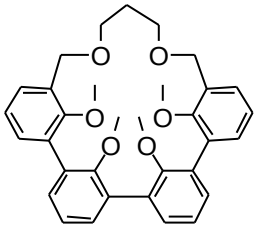
Large effects on binding affinity:



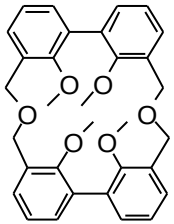
10^{10}



10^{6}

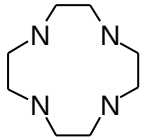


10^{5}

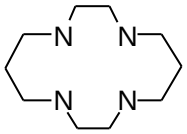


10^{3}

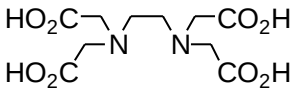
and significant impacts on selectivity:



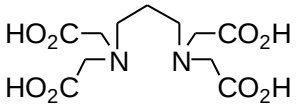
$Hg^{2+}/Cu^{2+} = 5$



$Cu^{2+}/Hg^{2+} = 10^{4}$



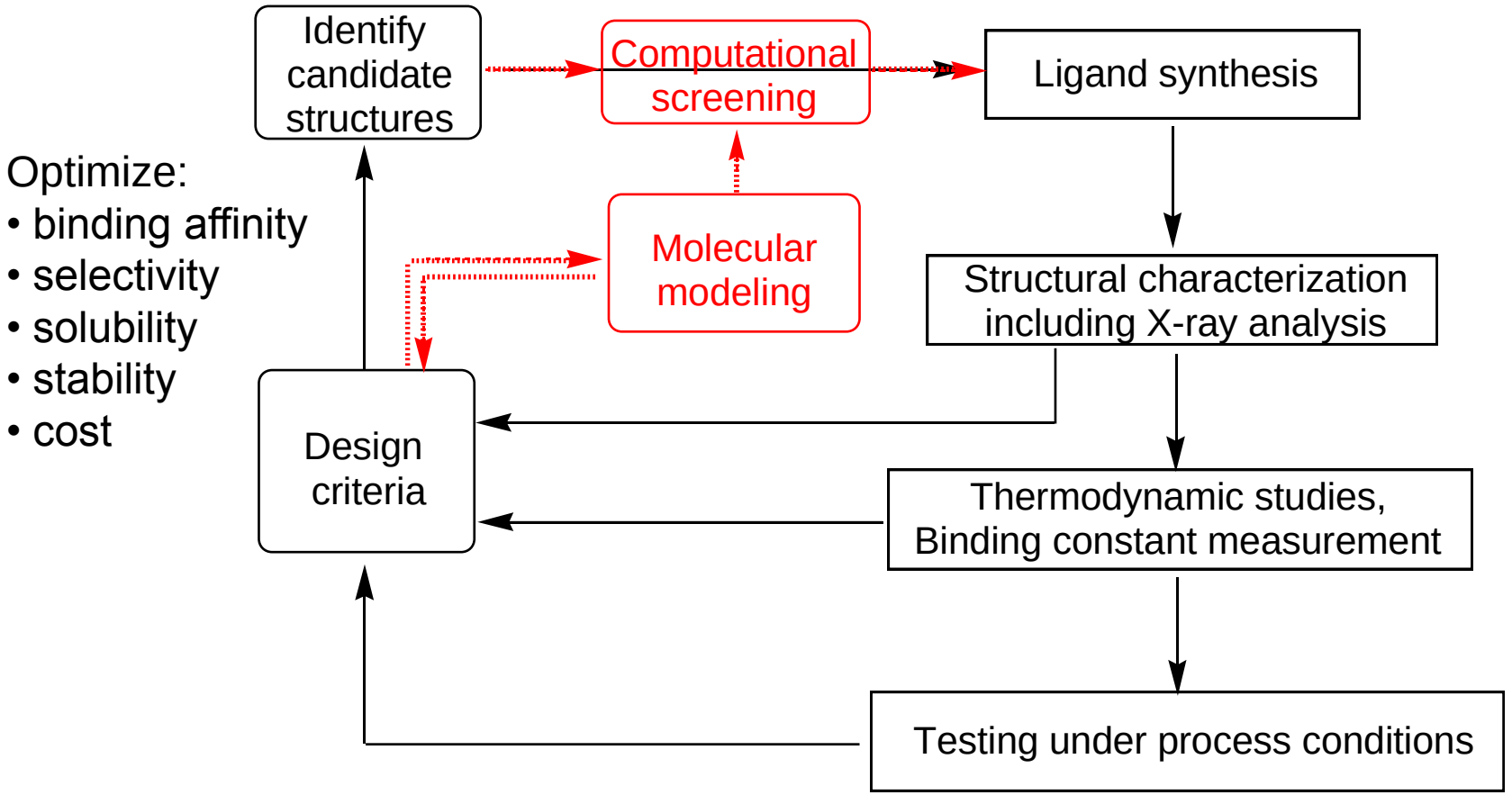
$Eu^{3+}/Al^{3+} = 13$



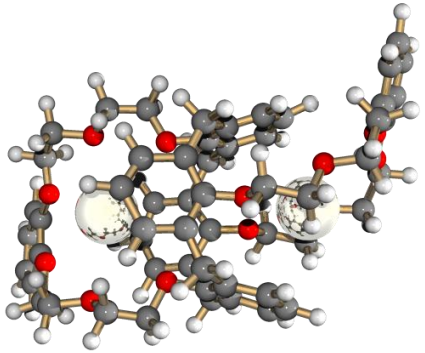
$Al^{3+}/Eu^{3+} = 500$

B.Hay, ORNL

Experimental development is slow and expensive



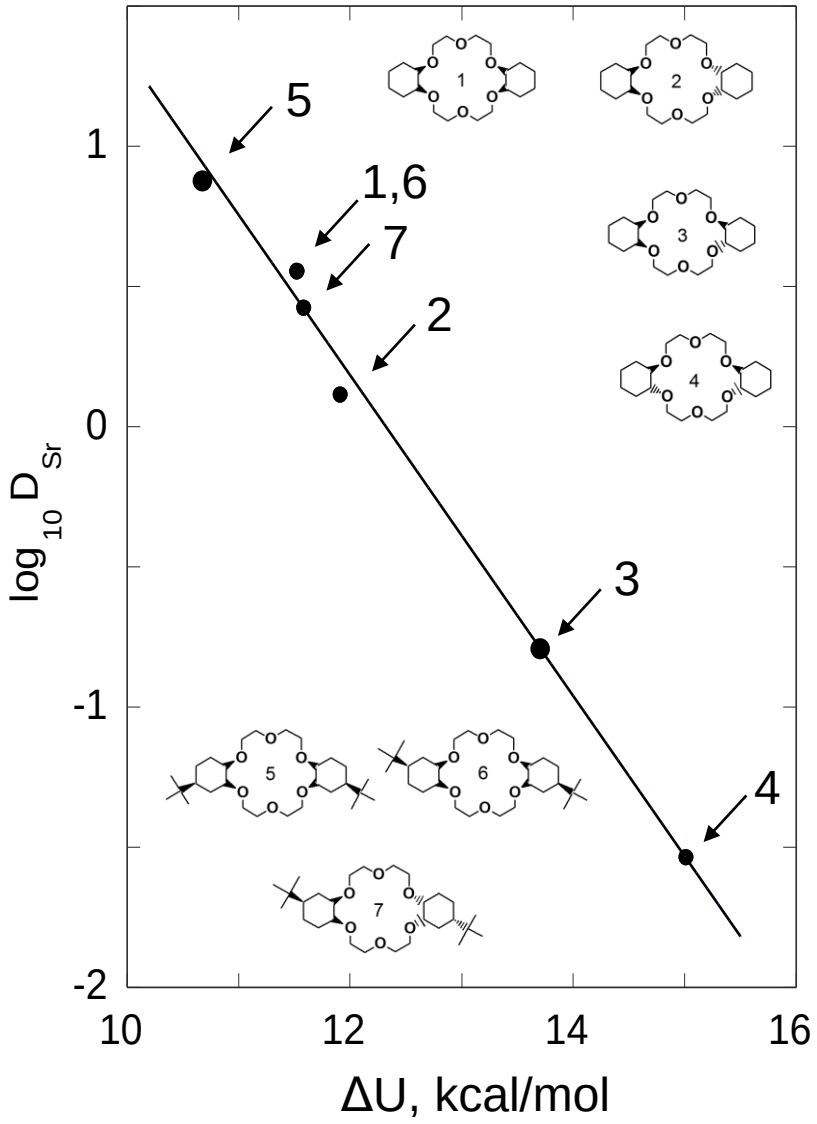
Computer-aided ligand development can acclerate progress



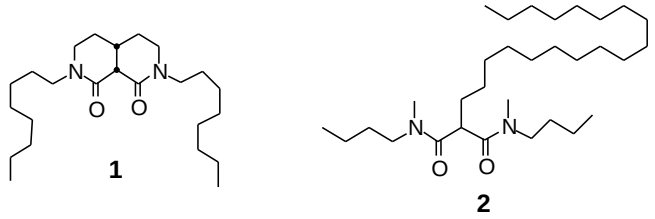
B.Hay, ORNL

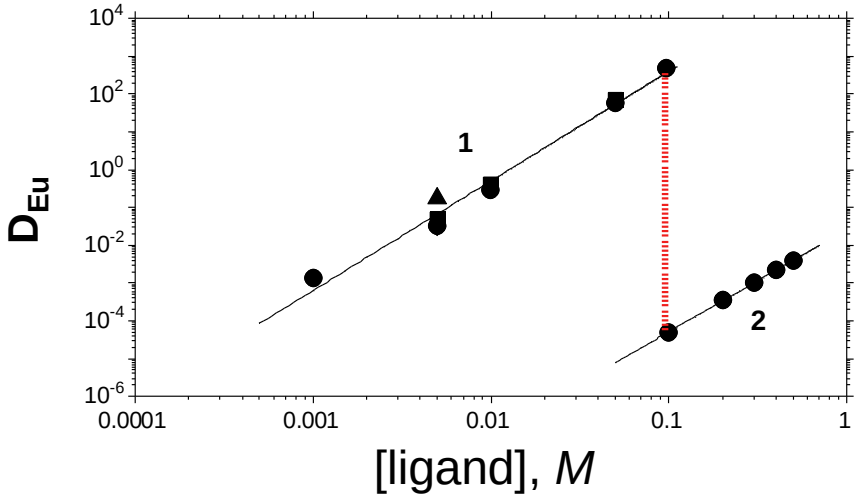
Experimental validation

Extraction of Sr^{2+} from 1M HNO_3 using 0.1 M ligand in n-octanol, 25 °C



Extraction into t-butylbenzene from aqueous solution containing 1 M $NaNO_3$, 1.5 mM HNO_3, 0.1 mM $Eu(N0_3)_3$, and 1-µL of ^{155}Eu tracer solution.





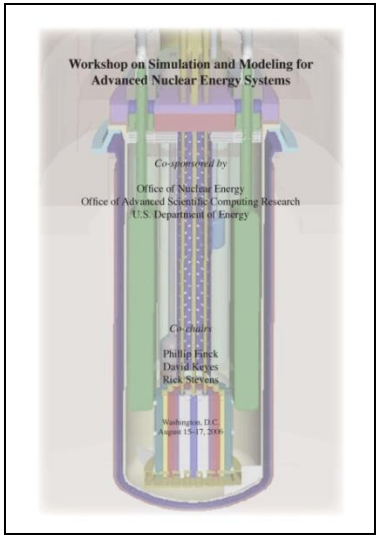
10 million times more effective

Lumetta, G. J.; Rapko, B. M.; Hay, B. P.; Gilbertson, R. D.; Weakly, T. J. R.; Hutchison, J. E. *J. Am. Chem. Soc.* **2002**, *124*, 5644.

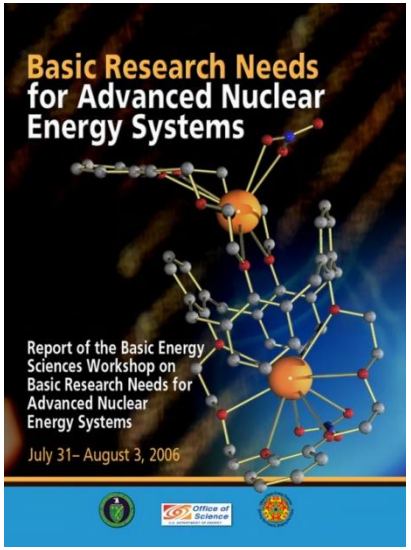
B.Hay, ORNL

Recent workshops have identified key needs for contributions by modeling and simulation

- **Separations Challenges**
  - **Plant-scale simulation**
    - integrated toolset to enable full-scale simulation of a plant – chemistry, mass transport, energy input, and physical layout
    - dynamic plant models
  - **Computational fluid dynamics**
    - Multiple fluid phases, fully developed turbulence, non-Newtonian flows, interfacial phenomena, radical chemical processes due to the presence of ionizing radiation
  - **Predictive methods for thermodynamics and kinetics data as input to process simulators**
    - extend currently limited thermodynamics data reliably into broader ranges of parameter spaces
    - incorporate limited experimental data and use computational chemistry approaches
  - **Rational design of the separations system from first-principles physics and chemistry**
    - predict what molecules will have the desired properties and can be synthesized
    - reliably predict the properties of liquids, solvation, and kinetics in solution
  - **Connecting/crossing time and length scales, with uncertainty quantification**
    - access longer times without dramatic changes in theoretical and algorithmic approaches
    - span spatial regimes; critical regime is the mesoscale (1 nm-1 μm)
      - Below 1 nm, computational chemistry; above 1 μm, continuum approaches
  - **Data management and visualization**
    - Data must be captured, managed, integrated, and mined from a wide range of sources to enable the optimal design and operation of separation processes
    - Computer resources and access
    - Export control issues

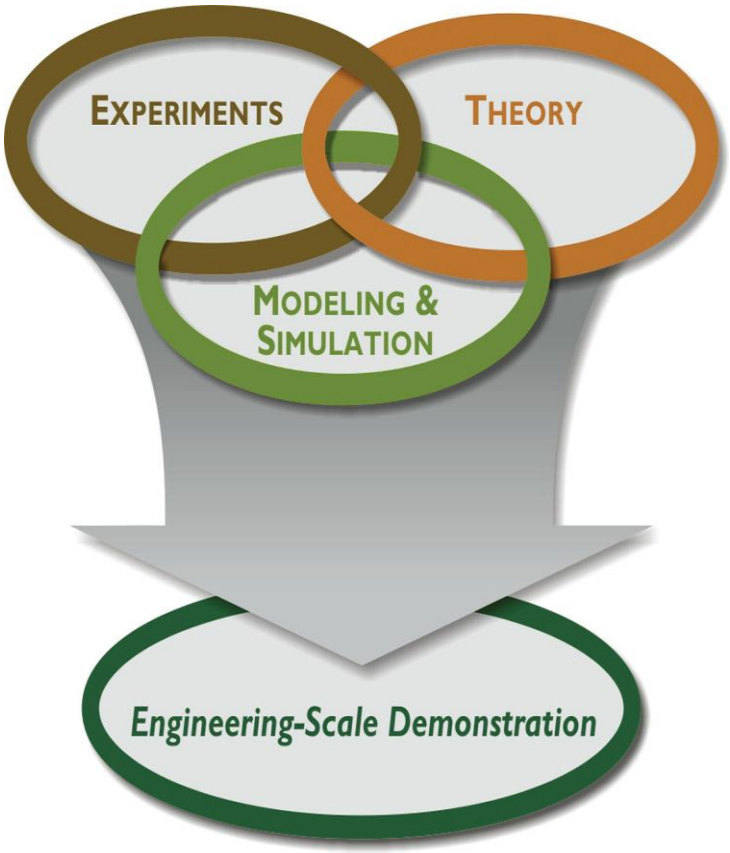


http://www-fp.mcs.anl.gov/anes/SMANES/gnep06-final.pdf



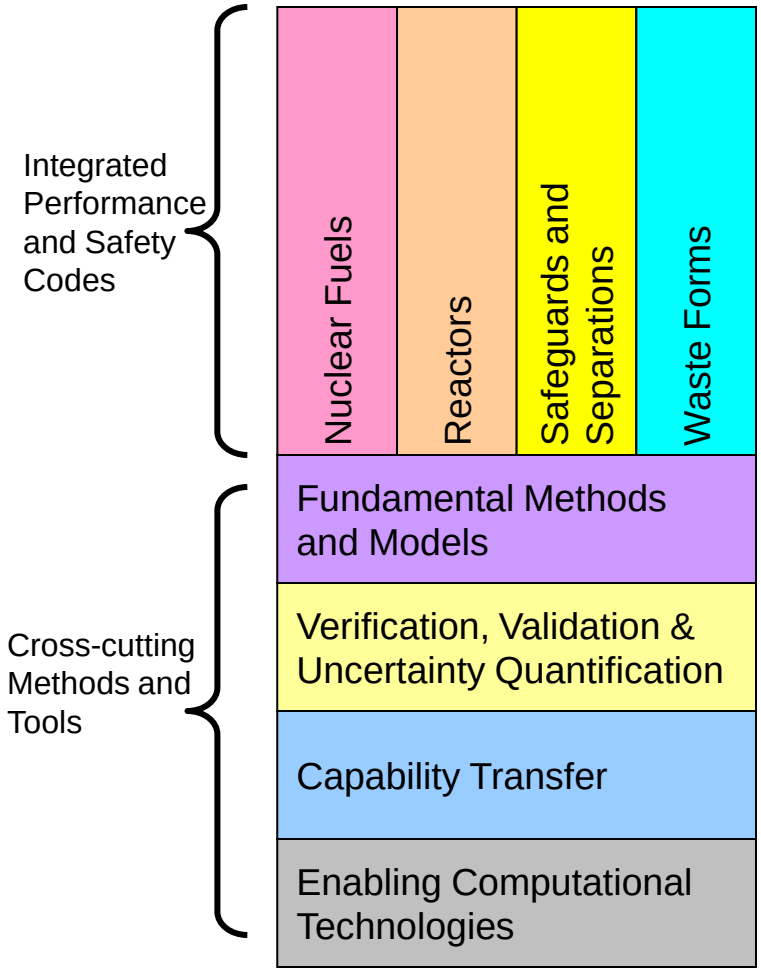
http://www.sc.doe.gov/bes/reports/abstracts.html#ANES

Advanced Modeling and Simulation has become an Essential Part of DOE-NE R&D



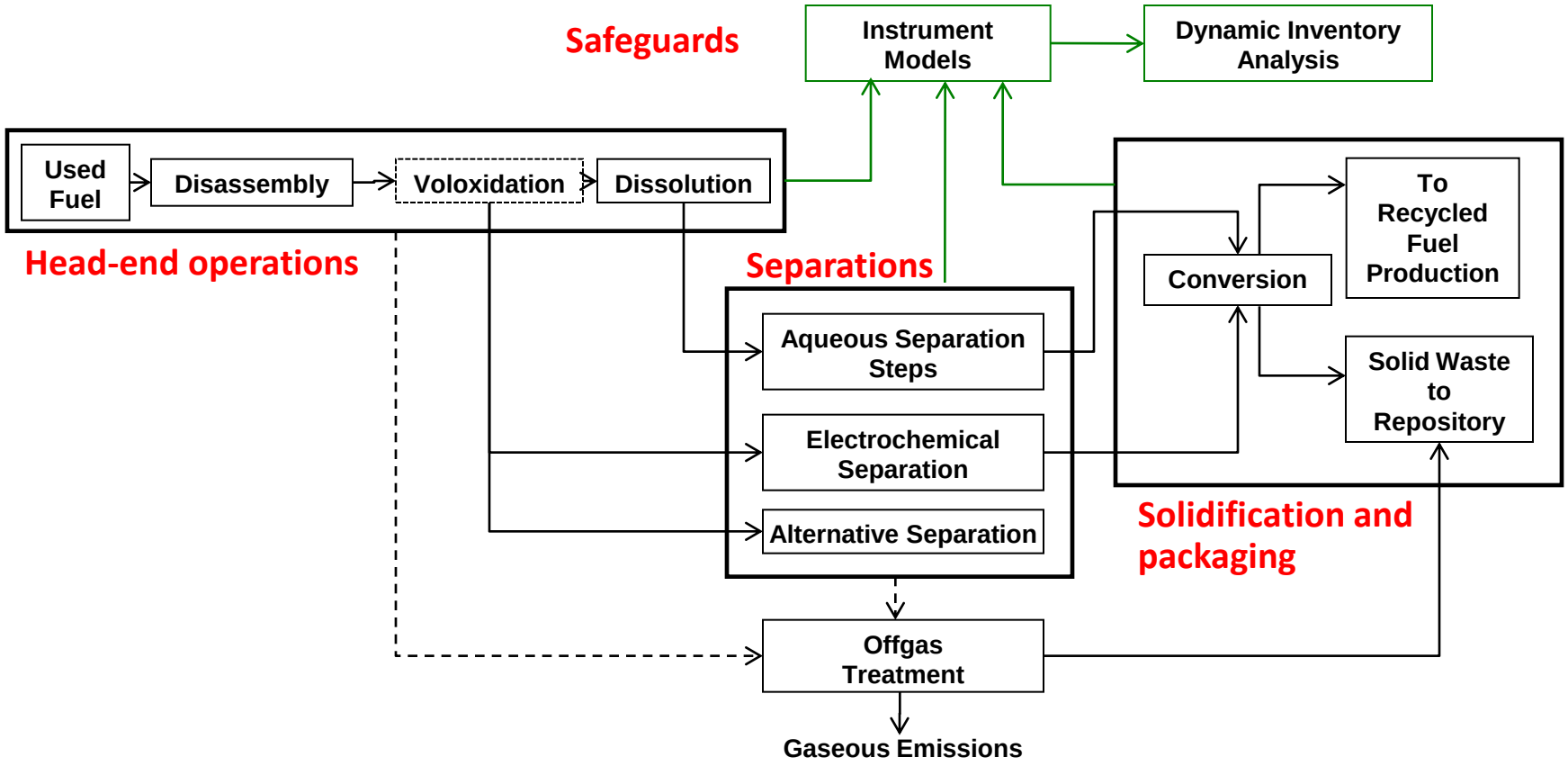
- ***R&D Objective 1*** – Develop technologies and other solutions that can improve the reliability, sustain the safety, and extend the life of current reactors.
- ***R&D Objective 2*** – Develop improvements in the affordability of new reactors to enable nuclear energy to help meet the Administration's energy security and climate change goals.
- ***R&D Objective 3*** – Develop sustainable nuclear fuel cycles.
- ***R&D Objective 4*** – Understand and minimize the risks of nuclear proliferation and terrorism.

NEAMS Program Elements



- **Integrated Performance and Safety Codes (IPSC)**
  - **Continuum level codes that will predict the performance and safety of nuclear energy systems technologies**
  - **Attributes include 3D, science based physics, high resolution, integrated systems**
  - **Using interoperability frameworks and modern software development techniques and tools**
- **Program Support Elements**
  - **Develop crosscutting (i.e. more than one IPSC) required capabilities**
    - **Fundamental Methods and Models**
    - **Verification, Validation and Uncertainty Quantification**
    - **Capability Transfer**
    - **Enabling Computational Technologies**

NEAMS Safeguards and Separations Scope



GOAL: Predictive capability for performance and safeguards aspects of reprocessing plants, to guide further research and development.

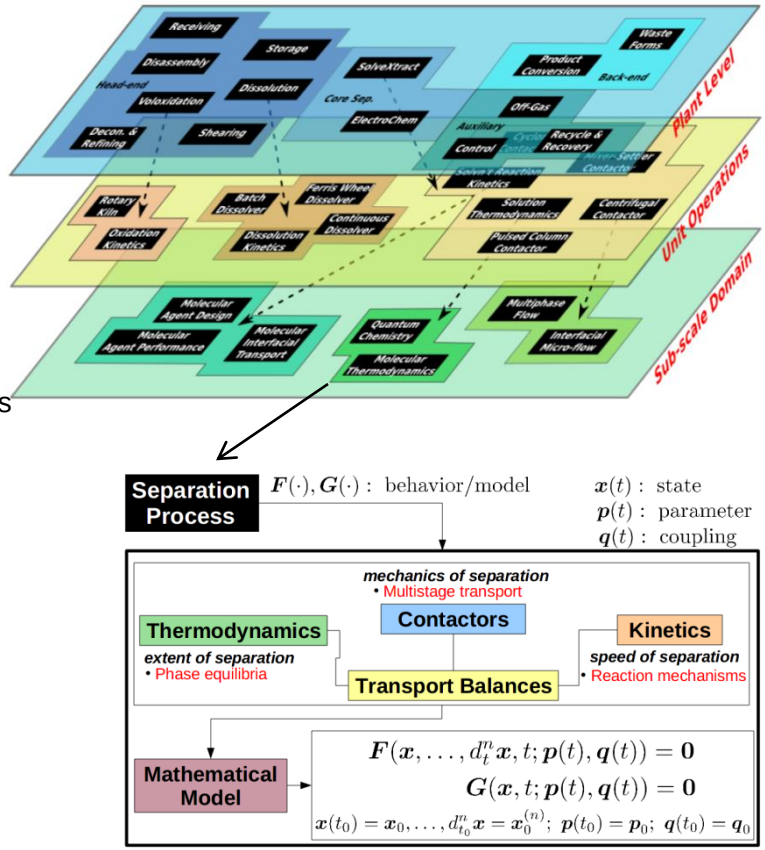
NEAMS Reprocessing Plant Simulator Toolkit

Vision

- Dynamic plant-level simulation capability encompassing entire plant and integrated safeguards
- Modules should be extensible, interoperable, and hierarchical to ensure continued usability
- Structured as a three-tiered collection of modules to aid in development and implementation
- Toolkit is open-source, but will enable use of controlled modules

Scientific Needs and Features

- Plant-level modeling and simulation of major sub-systems
- Dynamically coupled plant-level physicochemical modules.
- Integrated instrument models and inventory analysis modules.
- Loosely coupled unit operation modules as higher fidelity models
- Support stand-alone first-principles simulation capability
- Support analysis and design of alternative reprocessing technology
- Support safeguards by design

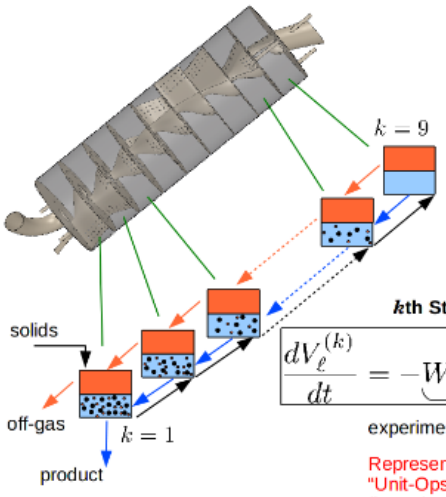


Software Needs and Features

- Complex plant simulations through dynamic integration of user plug-in software modules
- Detailed visualization of real-time, dynamic simulation data and analysis
- Job launch capability on multiple computational platforms
- Distributed computing capabilities
- Support verification, validation, and uncertainty quantification
- Documentation and materials that facilitate usage of the toolkit

Plant-level models are under development for main unit operations. Example: Dissolver

Contactor



Continuous Process
- Countercurrent (intermittent solid flow)
- Rotary dissolver

Prototype
- Rotary dissolver
- DOE Fuel Reprocessing Program 70-80's
- 0.5 ton/day HM full-scale ORNL

***k*th Stage "Liquid Volume Balance"**

$$\frac{dV_\ell^{(k)}}{dt} = -\underbrace{W(V_\ell^{(k)})}_{\text{experimentally measured (ORNL-TM-9019)}} + F^{k+1} \quad k = 1, \ldots N_s$$

Represents a connection to the reprocessing toolkit "Unit-Ops Tier" which will compute this function from first-principles continuum mechanics.

Kinetics

Speciation

$$\mathrm{UO_{2(s)}} + 2.7\,\mathrm{HNO_3} \xrightarrow{[\mathrm{HNO_3}] \le 8\,\mathrm{M}} \mathrm{UO_2(NO_3)_2} + 0.7\,\mathrm{NO_{(g)}} + 1.3\,\mathrm{H_2O_{(aq)}}$$

$$\mathrm{UO_{2(s)}} + 4\,\mathrm{HNO_3} \xrightarrow{[\mathrm{HNO_3}] > 8\,\mathrm{M}} \mathrm{UO_2(NO_3)_2} + 2\,\mathrm{NO_{2(g)}} + 2\,\mathrm{H_2O_{(aq)}}$$

$$\mathrm{PuO_{2(s)}} + 4\,\mathrm{HNO_3} \longrightarrow \mathrm{Pu(NO_3)_4} + 2\,\mathrm{H_2O_{(aq)}}$$

$$\mathrm{FPO_{1.18(s)}} + 2.36\,\mathrm{HNO_3} \longrightarrow \mathrm{FP(NO_3)_{2.36}} + 1.18\,\mathrm{H_2O_{(aq)}}$$

$$\dot{m}_s := K_s^{(k)}\,[\mathrm{HNO_3}^{(k)}]^m\, f\, A_s \quad \text{(empirical rate law)}$$

$$K_s^{(k)} := \left(0.48\exp\left(-0.091\rho_s'\right)\right)^{w_{\mathrm{UO_2}}} \left(5\exp\left(-0.27\rho_s'\right)\right)^{(1-w_{\mathrm{UO_2}})}$$

Mass & Energy Balance

Mass balance for each specie in the liquid phase of each stage:

$\rho_{\mathrm{UO_2(NO_3)_2}}$ $\rho_{\mathrm{Pu(NO_3)_4}}$ $\rho_{\mathrm{HNO_3}}$ $\rho_{\mathrm{FP(NO_3)_{2.36}}}$ $\rho_{\mathrm{H_2O}}$

$$d_t\left(\rho_i^{(k)}\right) V_\ell^{(k)} + \rho_i^{(k)}\, d_t\left(V_\ell^{(k)}\right) = -F^{(k)}\,\rho_i^{(k)} + S_{\ell,i}^{(k)}$$

*i*th species, *k*th stage

Mass balance for each specie in the solid phase of each stage:

$n_{\mathrm{FPO_{1.18}}}$ $n_{\mathrm{PuO_2}}$ $n_{\mathrm{UO_2}}$

$$\rho_s\, d_t\left(V_s^{(k)}\right) = -\dot{m}_s^{(k)}\left(V_s^{(k)}\right) + S_s^{(k)}$$

*i*th species, *k*th stage

$$\dot{n}_i = \frac{\dot{m}_s^{(k)}\left(V_s^{(k)}\right) m_i}{M_i}$$

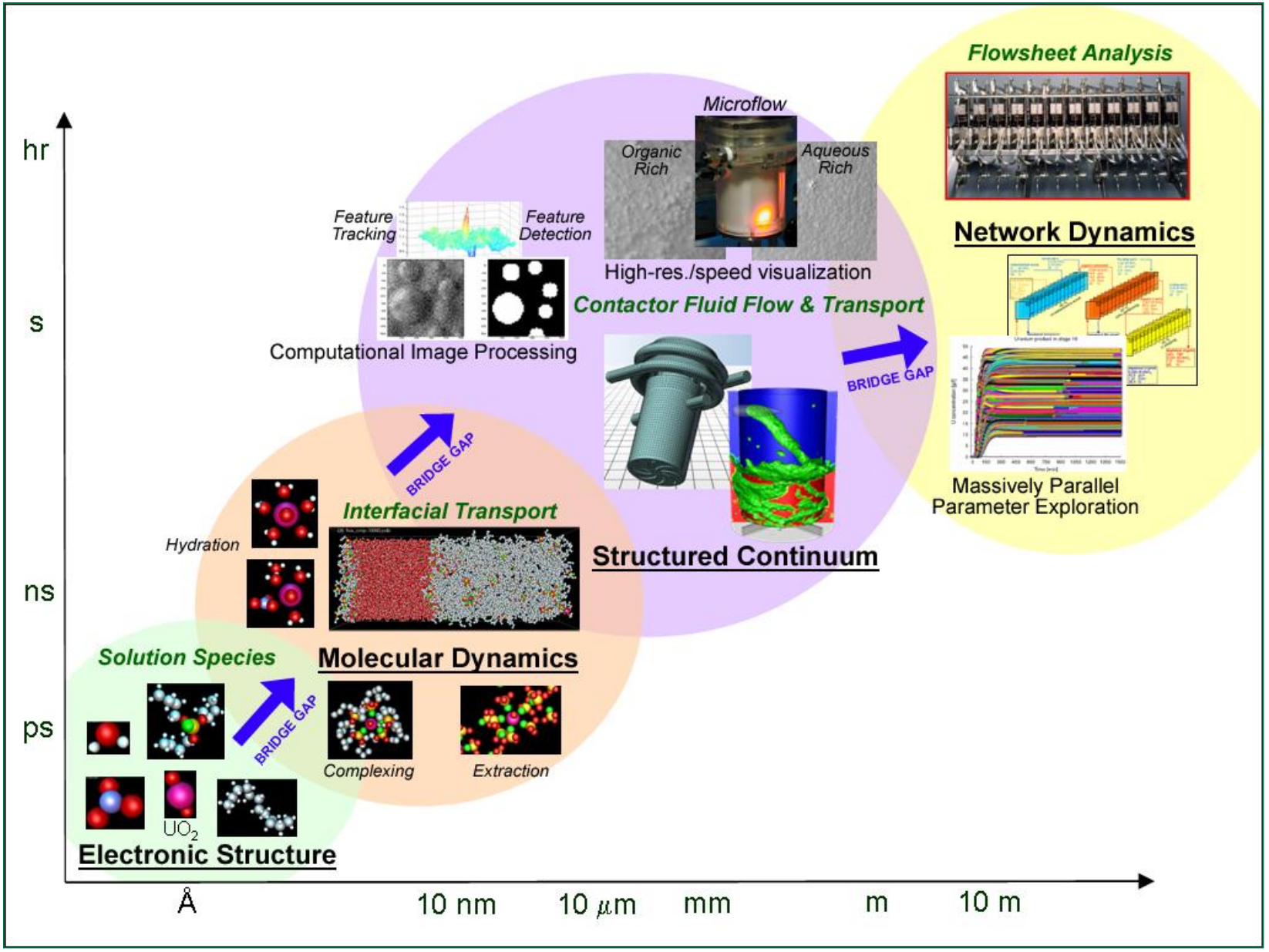
Thermodynamics

Non-ideal liquid solution

$$\rho_\ell^{(k)} = R(T, P, \rho_{\mathrm{H_2O}}^{(k)}, \rho_{\mathrm{HNO_3}}^{(k)}, \rho_{\mathrm{UO_2(NO_3)_2}}^{(k)})$$

OAK RIDGE

Modern M&S for Solvent Extraction



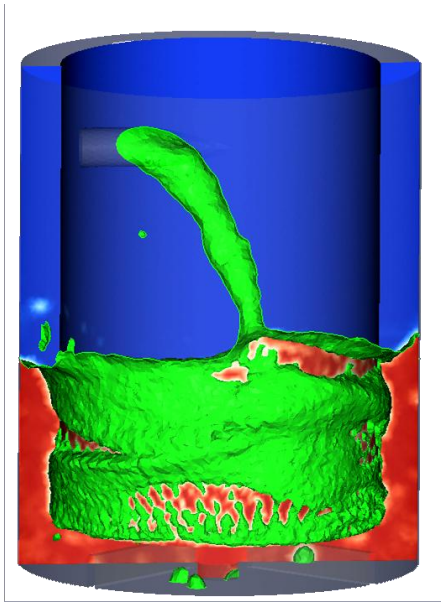
Centrifugal Contactor Simulations Using Open-Source CFD

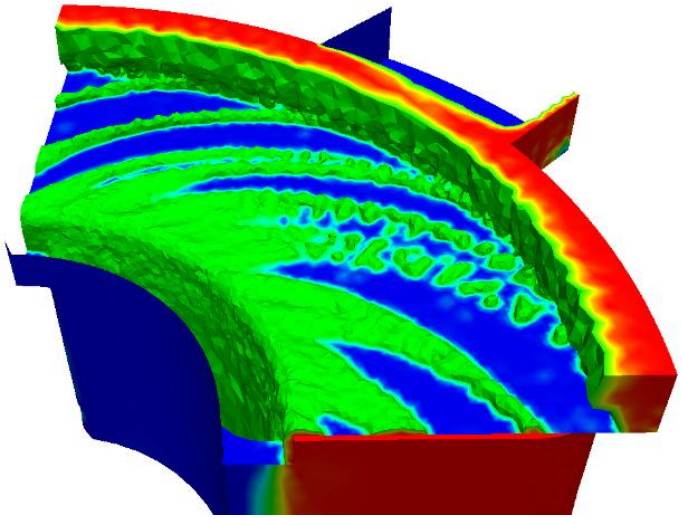
Goal – Provide a pathway for:

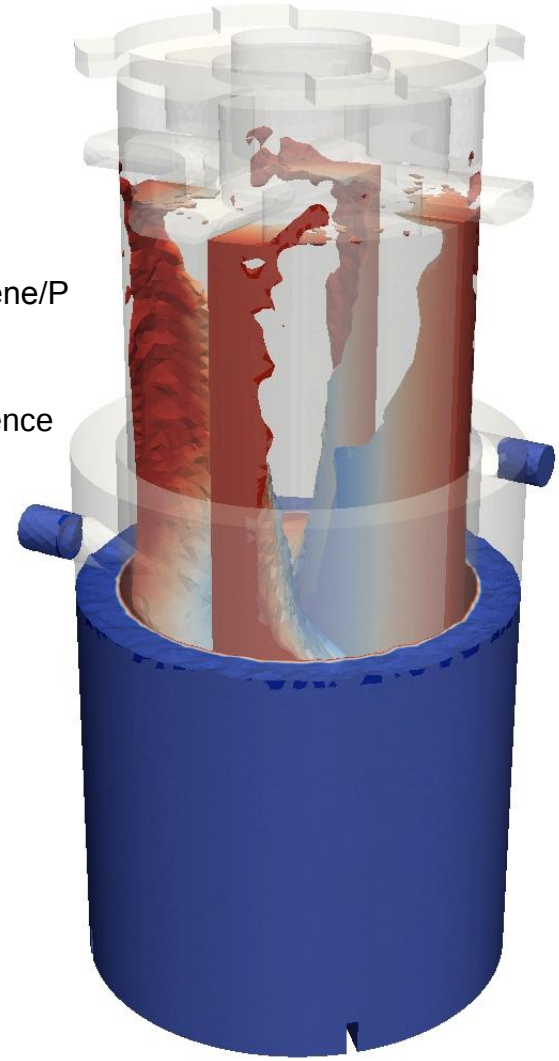
- **Predicting stage efficiency for given conditions**
- **Developing lower fidelity models for plant-level unit operations models**

FY10 Results

- **Finite Element-based (unstructured) Lattice Boltzmann Method (FELBM)**
  - Testing of modifications to code's solver and BC implementation
  - Verified excellent parallel scaling performance up to 2048 cores on Argonne's BlueGene/P
- **OpenFOAM**
  - Demonstration of limits to approach for three phase liquid-liquid-air simulation
  - Coupled mixing/separation zone contactor models – exploring BC and mesh dependence

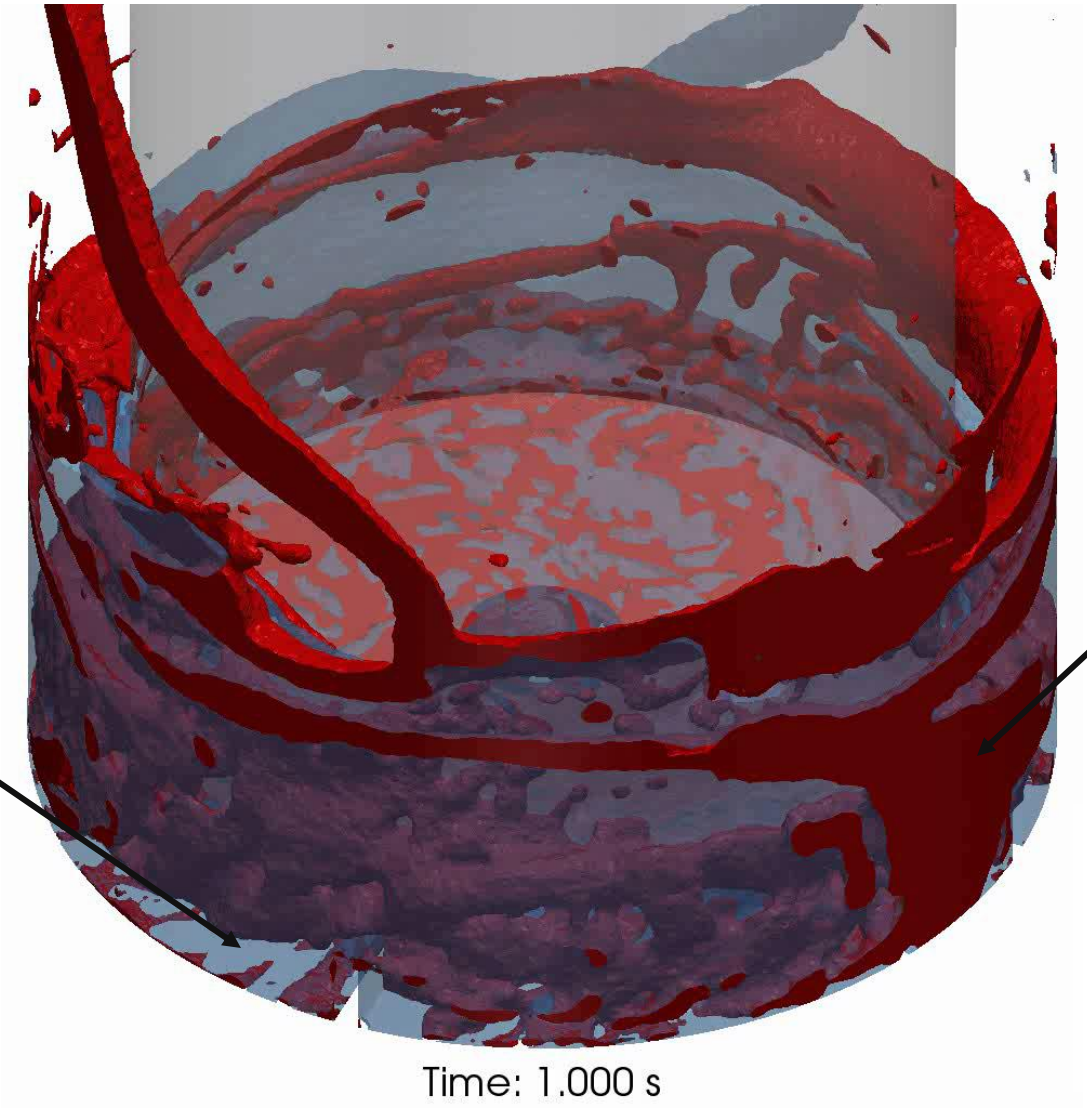






K. E. Wardle, ANL

Animation of Liquid-Liquid Mixing



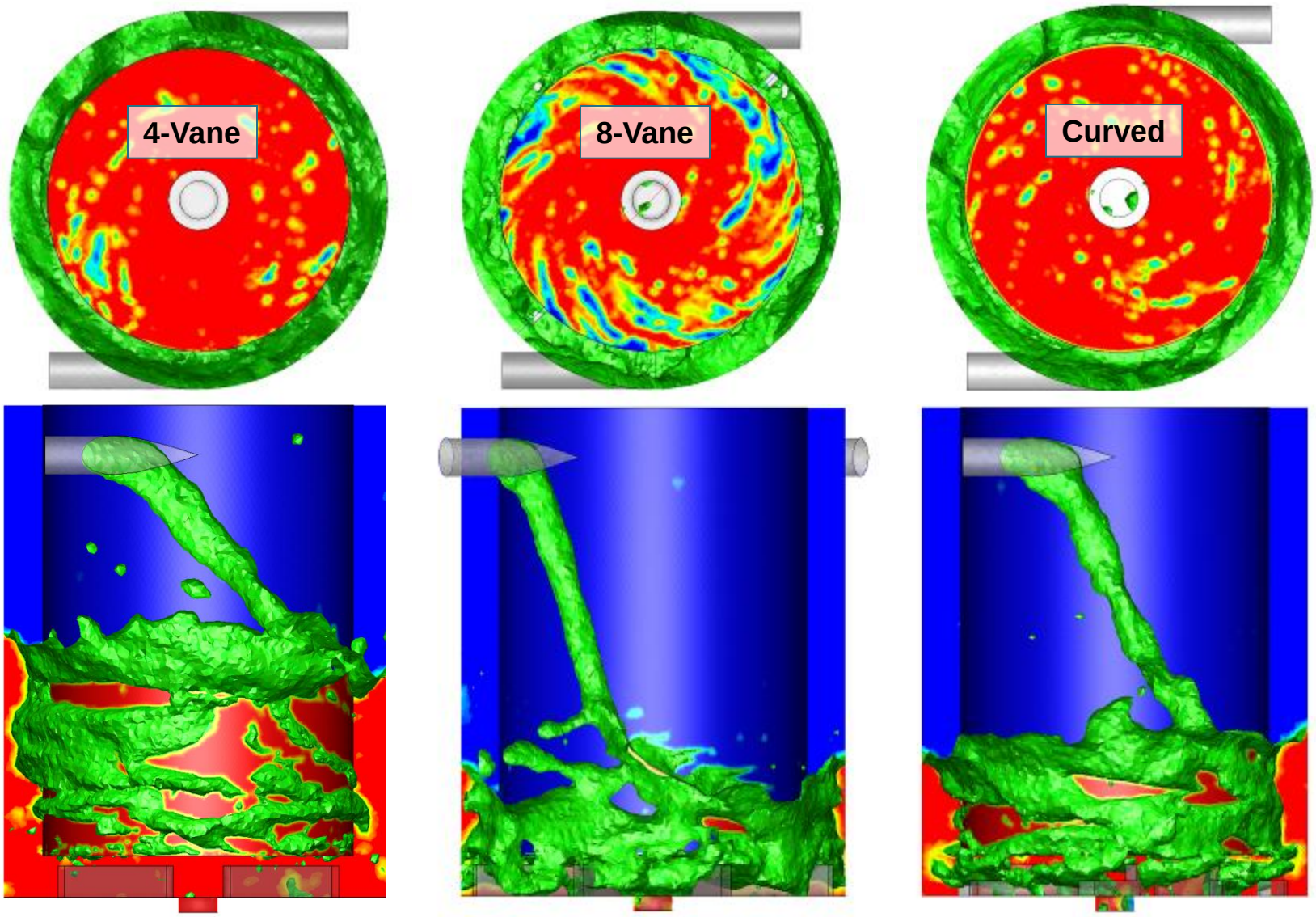
water is transparent blue

oil is red

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 ↓

Comparison of effect of vane geometry on mixing



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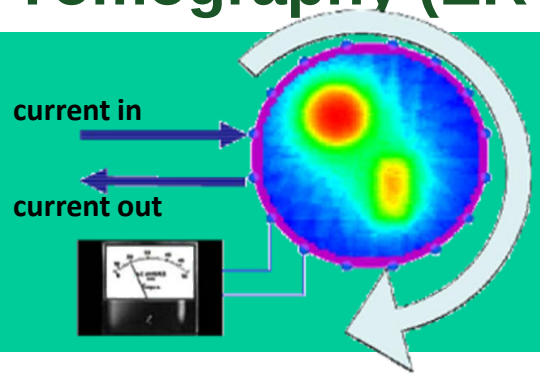
Interface with Experimental Work

Contactor CFD Validation Using Electrical Resistance Tomography (ERT)



Contactor CFD Validation Facility

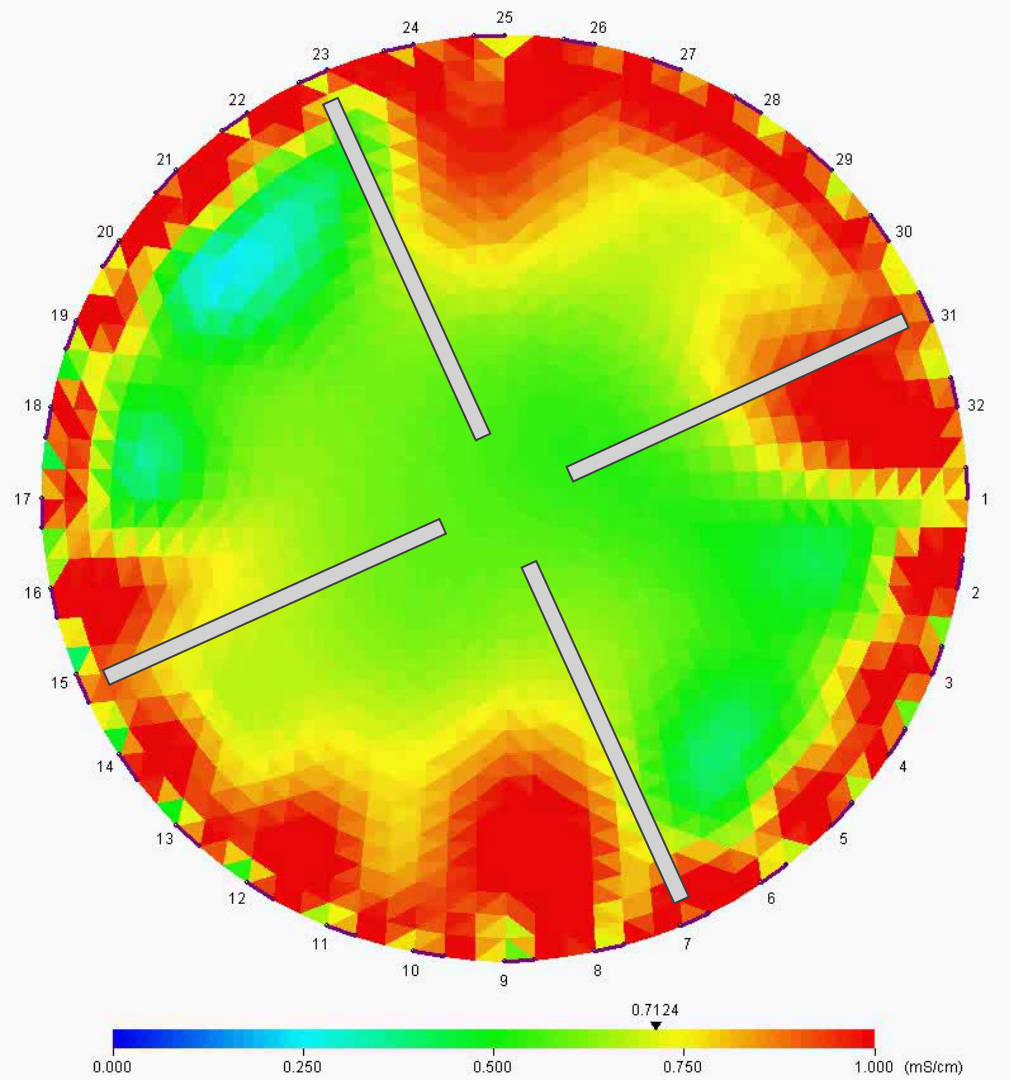
Engineering-scale contactor (CINC V-5)

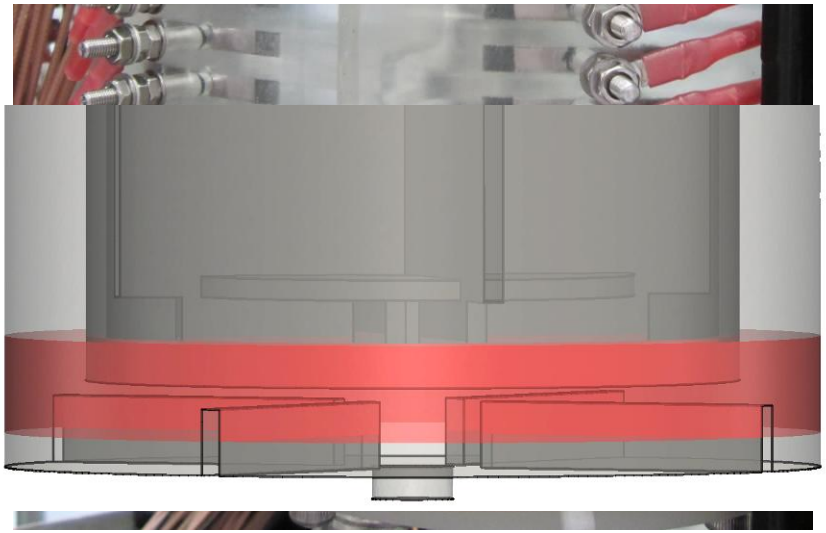
Multiphase measurements using ERT

Detailed operational diagnostics

K. E. Wardle, ANL

Circular 32-Electrode Array Tomography Data: 4-Vane



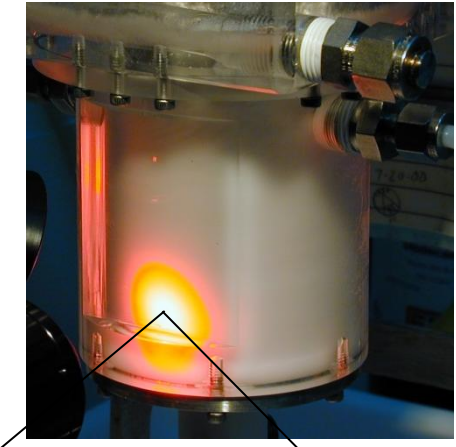


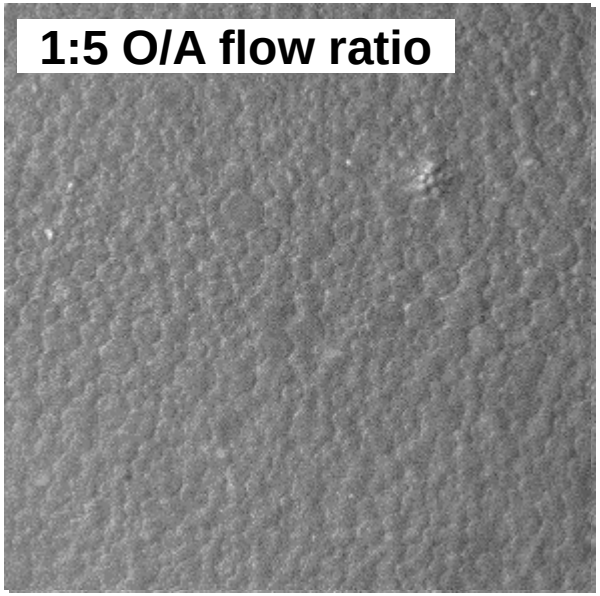
- Acquired data is a temporal and spatial average
  - Temporal: ~0.75 s (overall rate of ~1.4 Hz)
  - Spatial:
    - Out of plane: electrode size, 7.6mm x 7.6mm
    - In plane: ITS quotes 5% of vessel diameter (5% of 6" = 0.3" = 7.6mm)
- Approximate vane location is shown
  - Measurements are relative 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

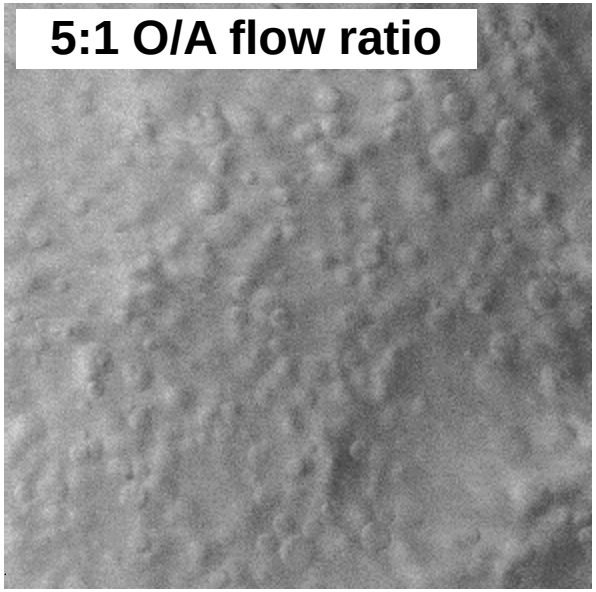
Wang, M. *Meas. Sci. Technol. 13:101* (2002).

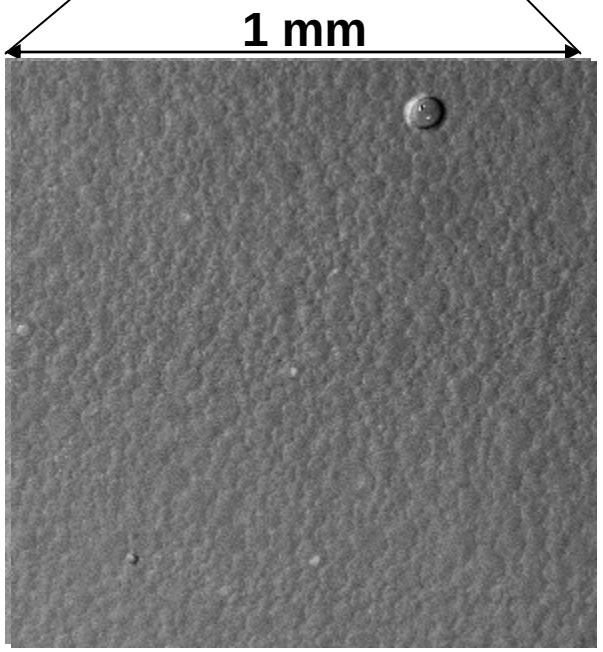
Flow Regime Visualization

- **State-of-the-art high-speed digital video imaging, solid-state light, and optics provide needed insight**
- ***Sub-millimeter flow regime never seen before***
- ***Reveals significant time and length scales under realistic system and operating conditions***









• **Elapsed time:** 37 ms

• **Elapsed time:** 18.5 ms

Spatial resolution: ~7 μm

Organic-rich flow regimes possess greater air entrainment

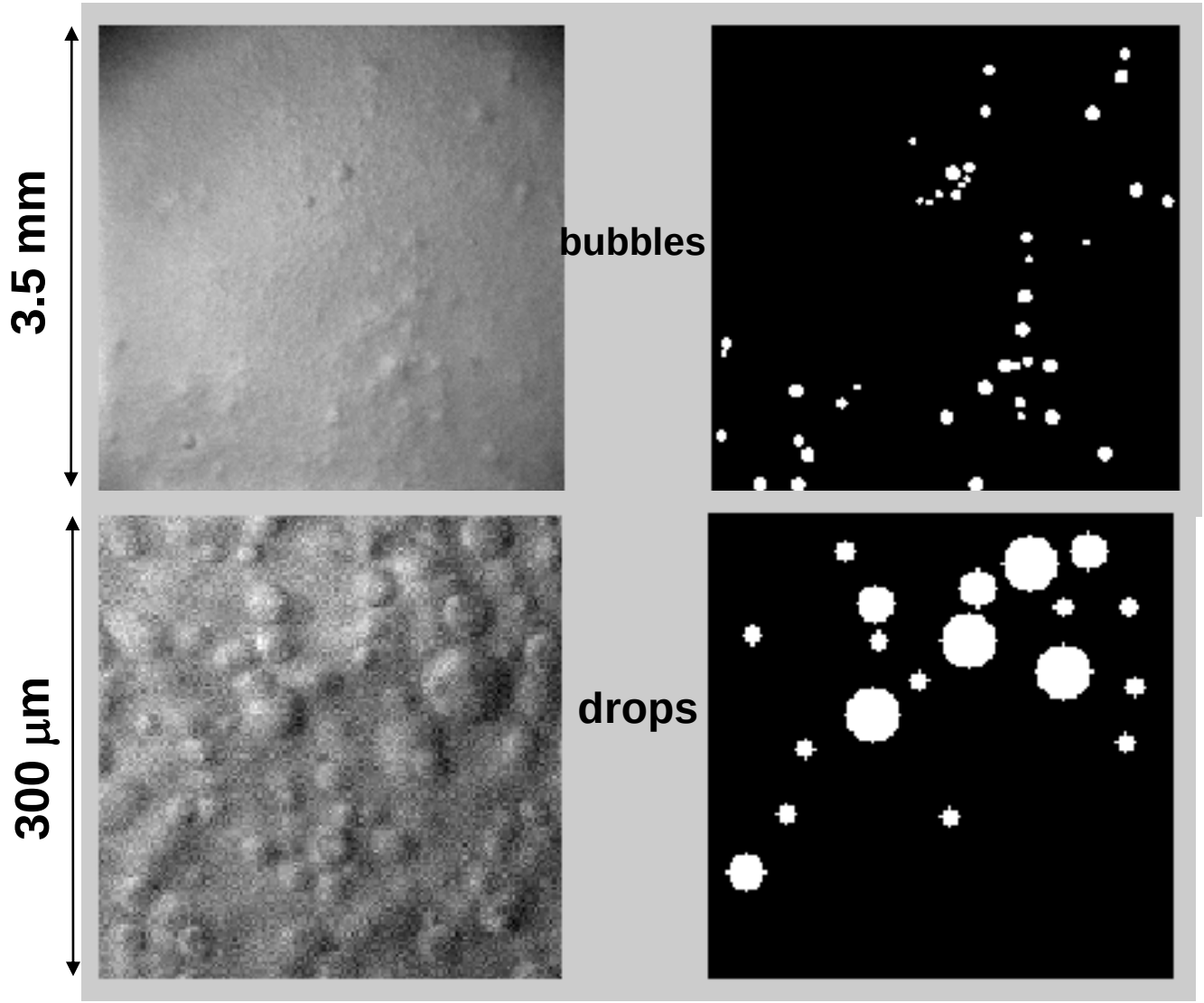
seeing is believing . . .

- ***These videos provide more than insight for modeling . . .***

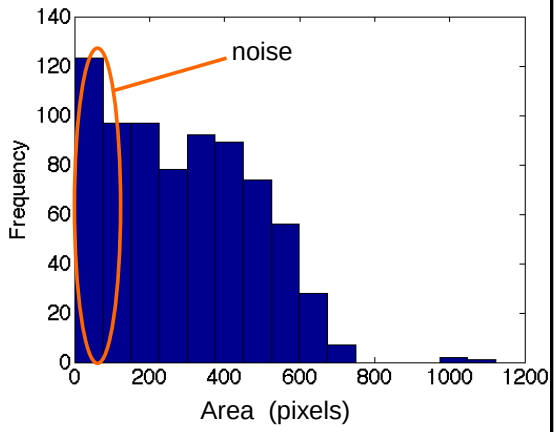
V. de Almeida, ORNL

Computer-Aided Image Analysis

- Large data sets are obtained (8 GB for 1-s elapsed time)
- Can utilize powerful tools of computer image analysis (machine vision)
- Computing intensive – need to inspect every pixel and its vicinity



Generate data useful for model development



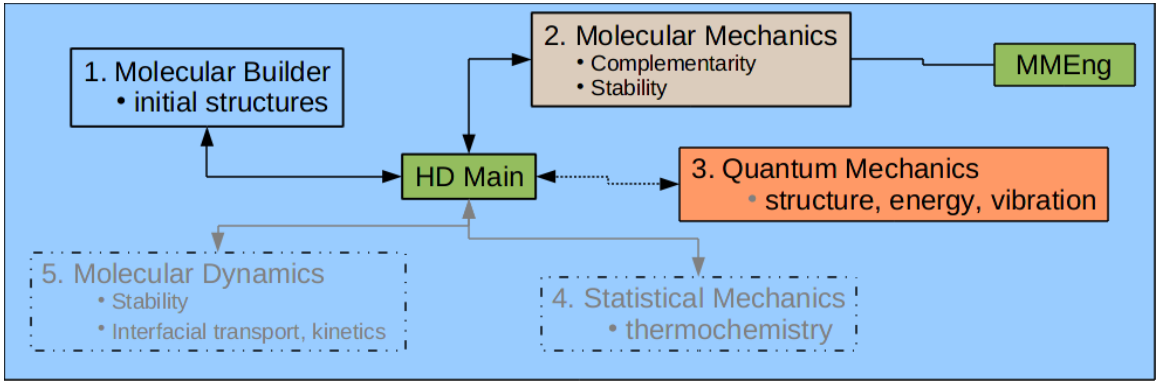
- Drop and bubble size distribution
- Velocity tracking
- Calibration of phase mixture turbulent momentum balance

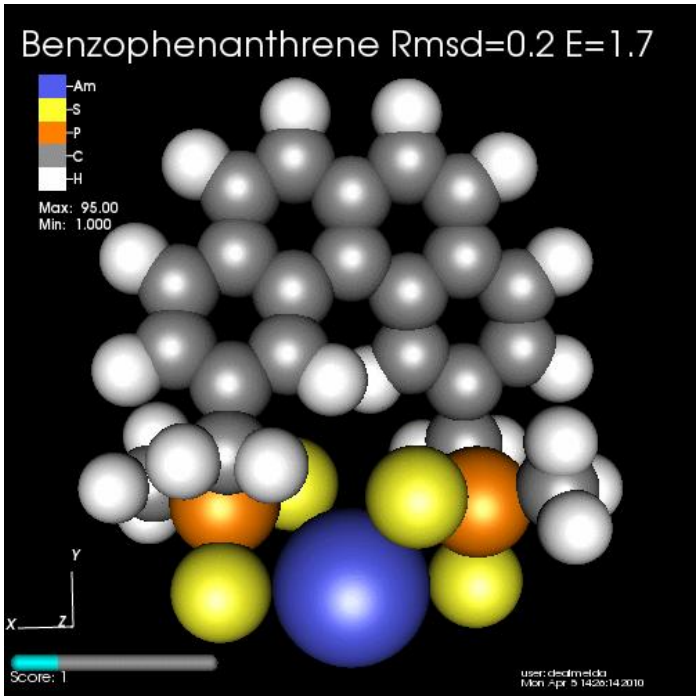
V. de Almeida, ORNL

Solvent Extraction Agent Design

HostDesigner code parallelized for minor actinides solvent extraction agent design

- **Previous simulation capability:** limited MM analysis on 10 to 20 ligands (~days wall-clock time)
- **Current capability:** MM conformer search on > 1000 ligands in ~1.5 hours wall-clock time





Current focus:

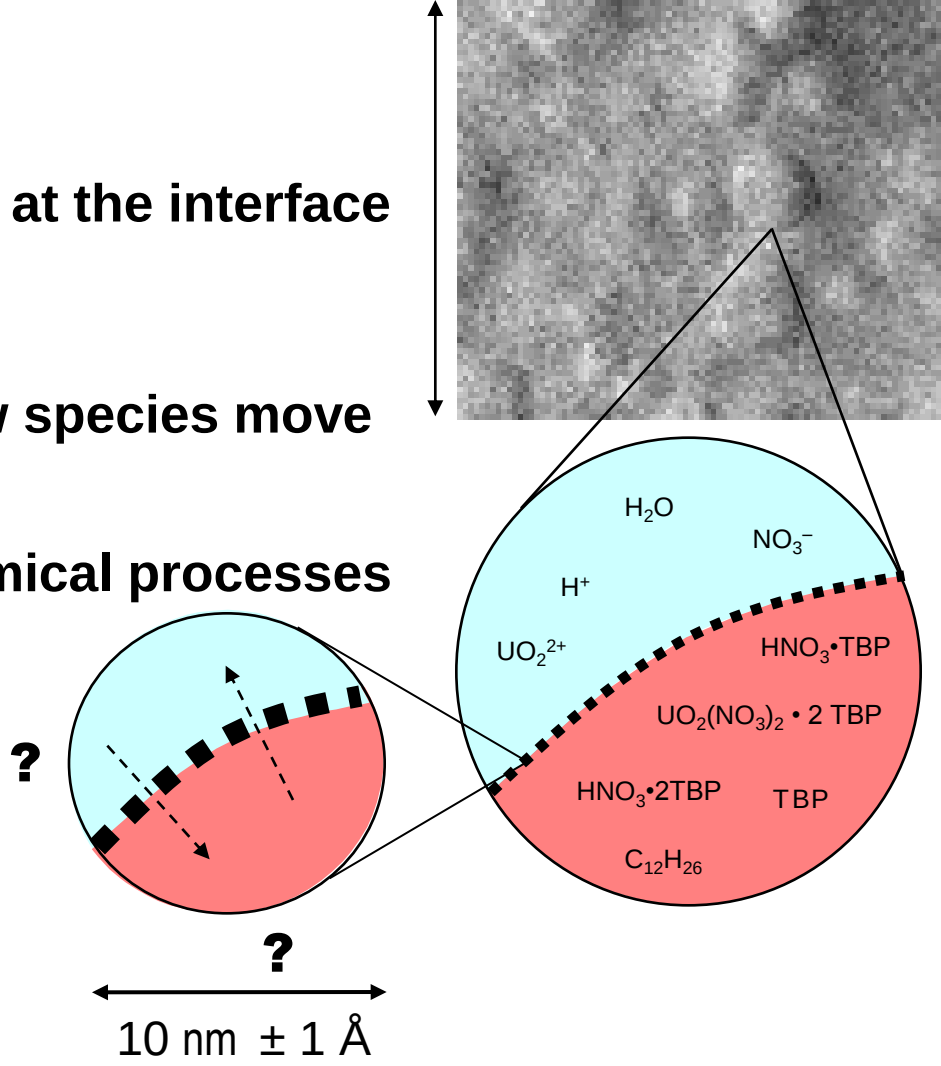
- Improving functionality by adding quantum mechanics based scoring of candidates
- Improving computing throughput by embedding a quantum mechanics library in HostDesigner

Chemical Transport

- Important chemical reactions occur at the interface

Challenges

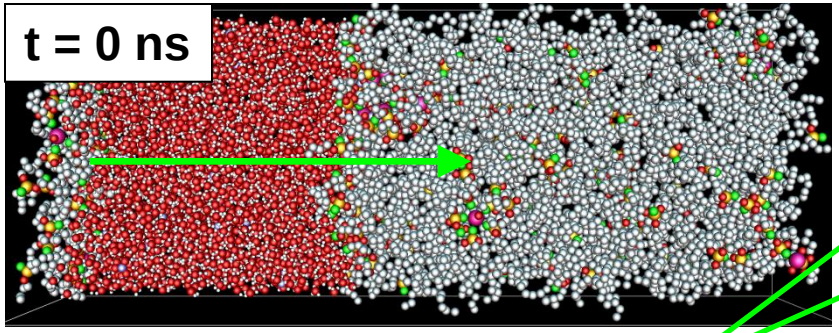
- Lack of basic understanding of how species move across interfacial "region"
- Strongly coupled physical and chemical processes

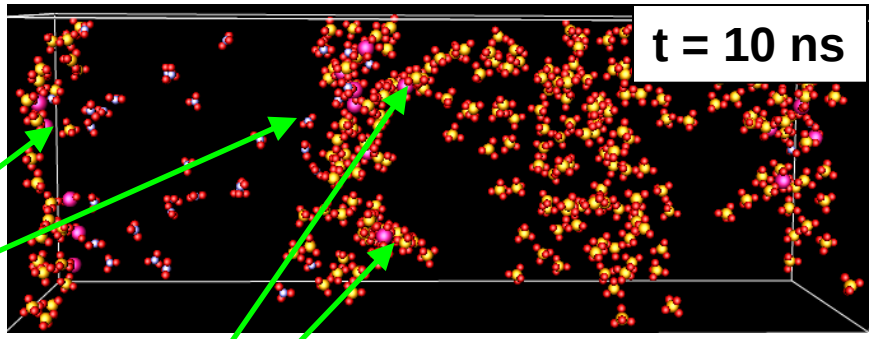


An approach to understand solvent extraction

- Molecular dynamics simulation
- Calibration from experimental data
- Insight from molecular quantum chemistry calculations when experimental data are not available

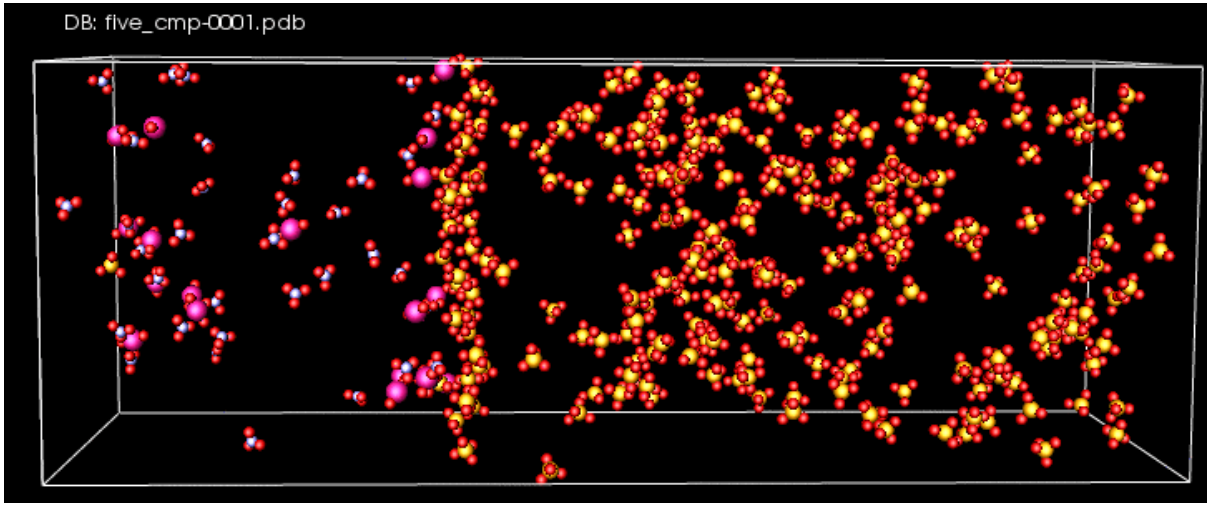
Interfacial Transport "Visualization" by Molecular Dynamics Simulation

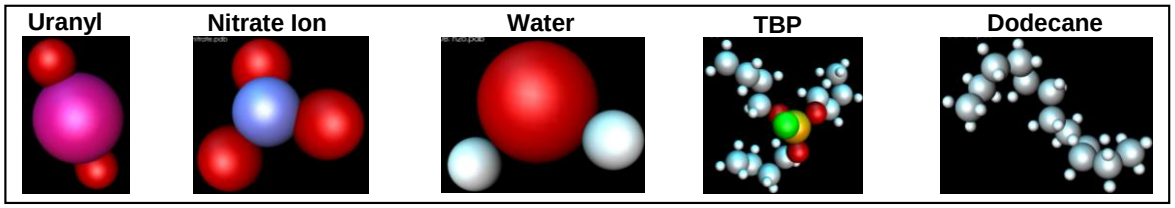




- All uranyl adsorbed on interface
- Some nitrate ion also adsorbed

- Onset of extraction of UO_2^{2+} , NO_3^- , H_2O
- Species have crossed the TBP surfactant layer
- H_2O and organic hidden; TBP butyl tails hidden





Phys. Chem. Chem. Phys., 2010, ***12,*** *15406–15409*
Solv. Extr. Ion Exch., 2010, ***28,*** *1–18*
J. Phys. Chem. B 2009, ***113***, *9852–9862*

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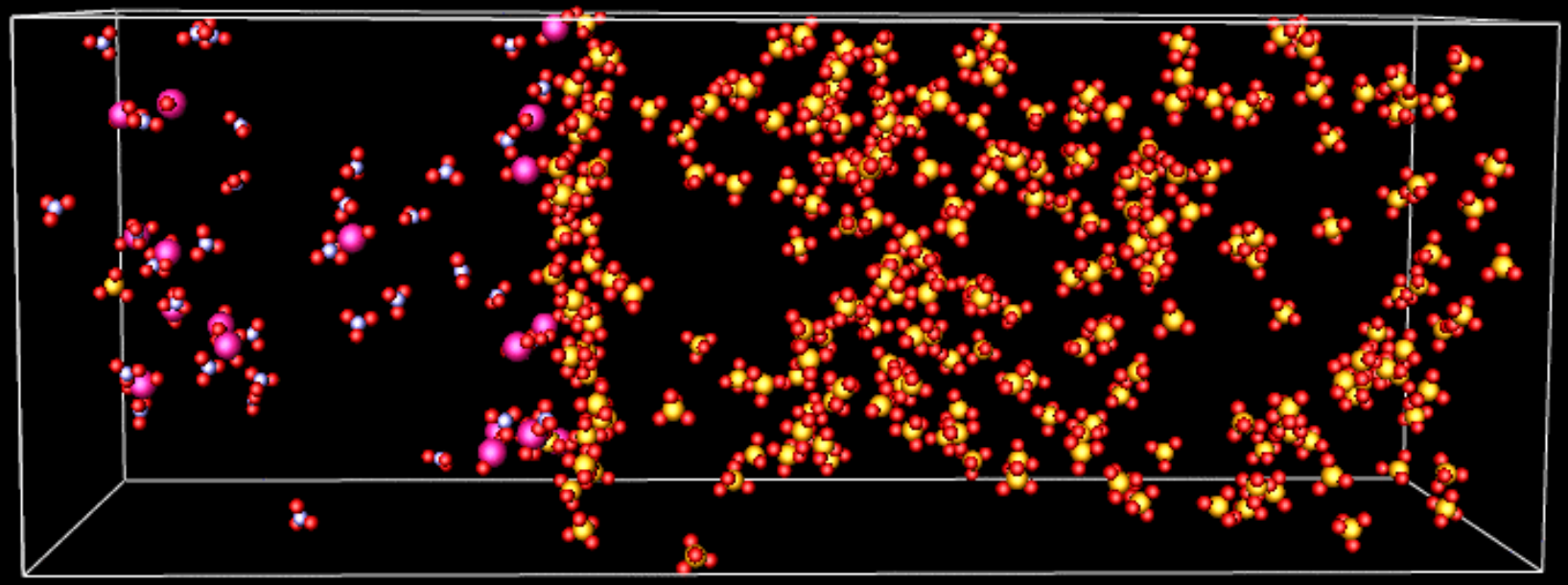
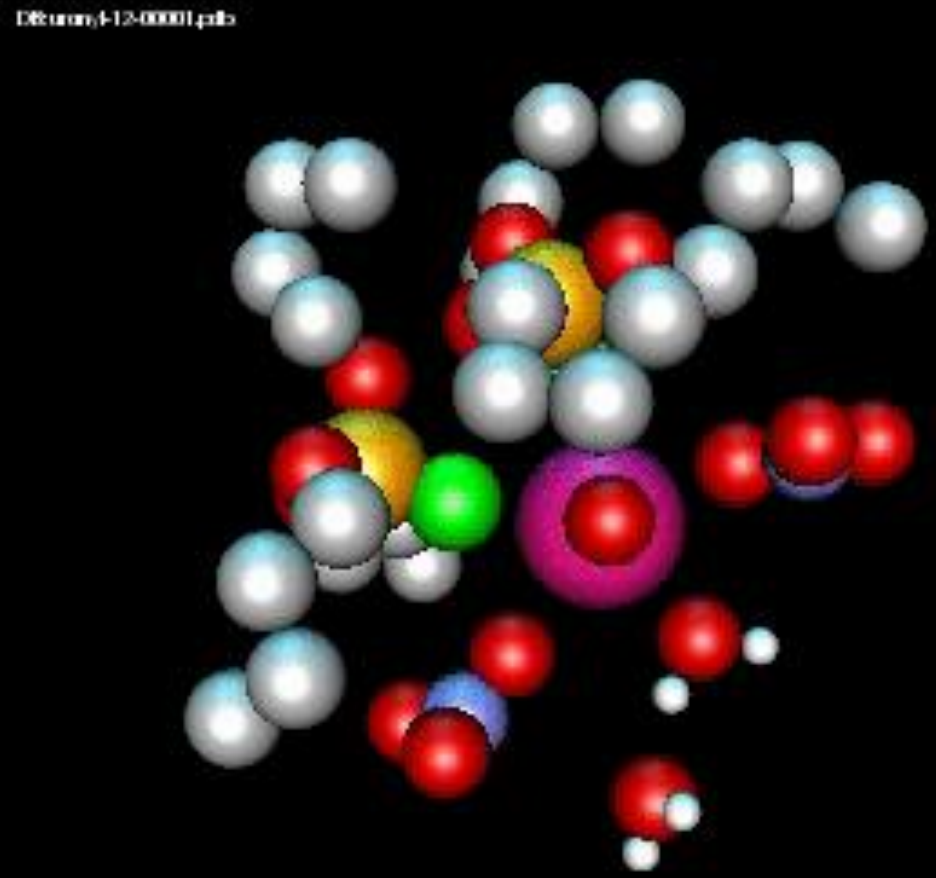
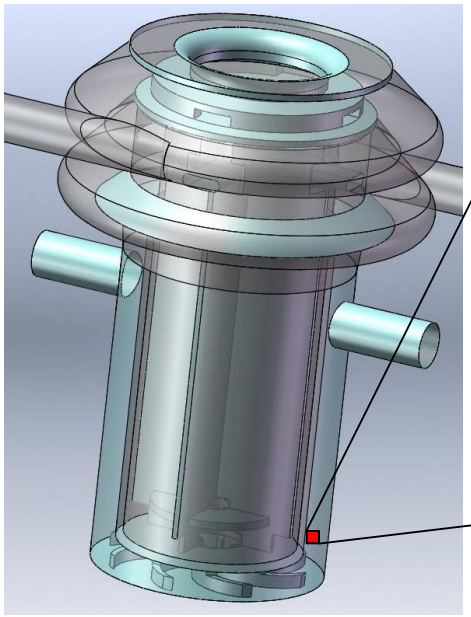
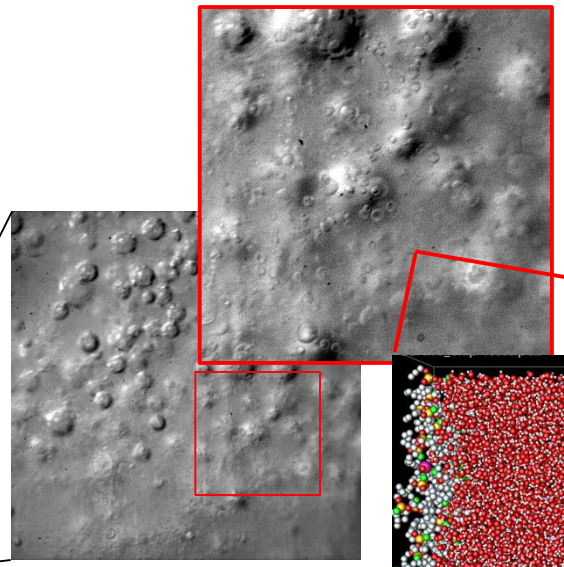
DB: five_cmp-0001.pdb



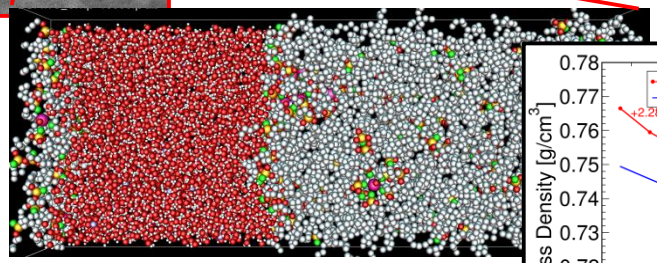


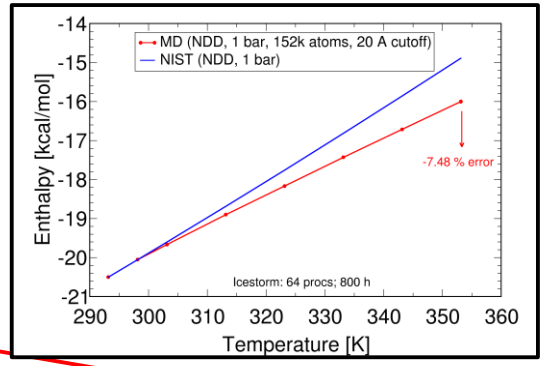
Quantifying Water Extraction by TBP/Dodecane via MD

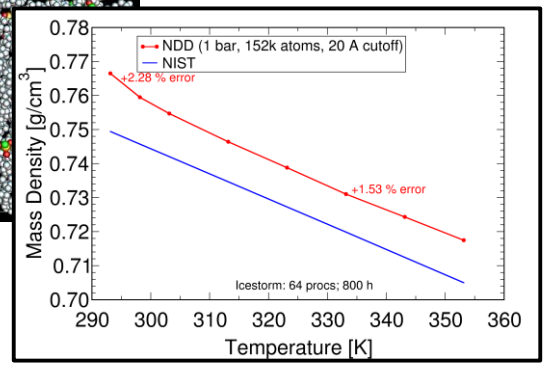




Water-
TBP-NDD



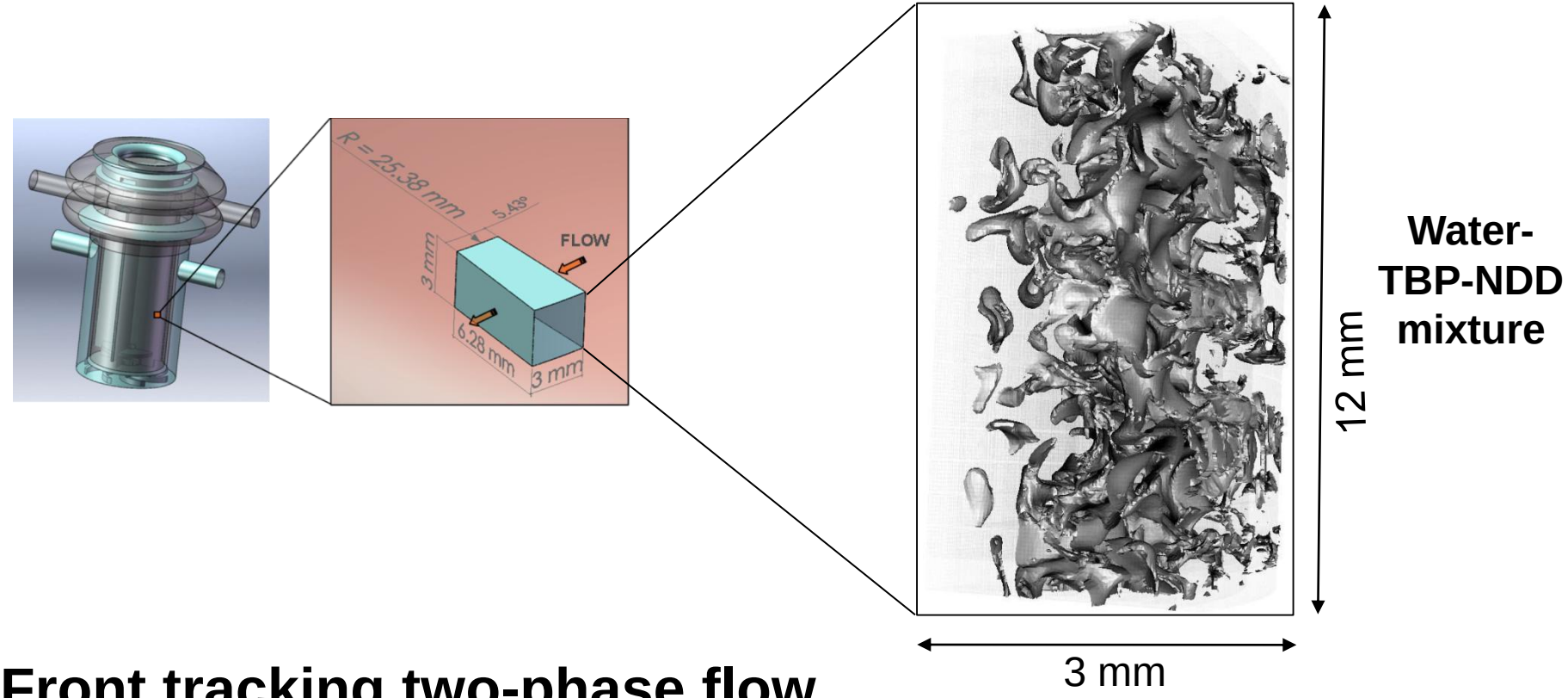




- **Molecular dynamics of aqueous/organic interfacial transport of water**
  - **Modeling TBP (QM parameterized)**
  - **Testing various FF: AMBER, CHARMM, GROMOS, OPLS**
  - **Large scale simulation 1 M atoms (ORNL/INL machines)**
  - **Prediction of thermodynamic (density/enthalpy) and transport properties**
  - **Extraction simulations in progress**

NEUP: UTK (B. Khomami) / ORNL (V.F.de Almeida)

Sharp Interface Tracking in Rotating Microflows of Solvent Extraction



- **Front tracking two-phase flow**
  - **Development of incompressible flow, high-order accuracy interface tracking**
  - **Simulation on New York Blue Gene (1024 cores)**
  - **Porting code to INL machines**
  - **Further development on correcting interface impermeability**

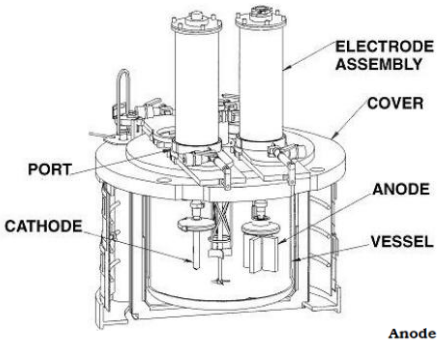
NEUP: SUNY-SB (Glimm) / ORNL(V. F. de Almeida)

E-chem modeling

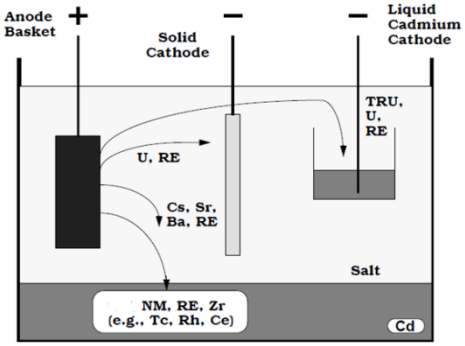
- **Goal: Predictive capability of electrorefiner performance**

- **Phenomena in an electro-refiner include:**

  Solid electro-dissolution, Electrohydrodynamics, Electro-deposition composition and electrode morphology, Thermodynamics, Electro-chemical reaction



Mark-IV

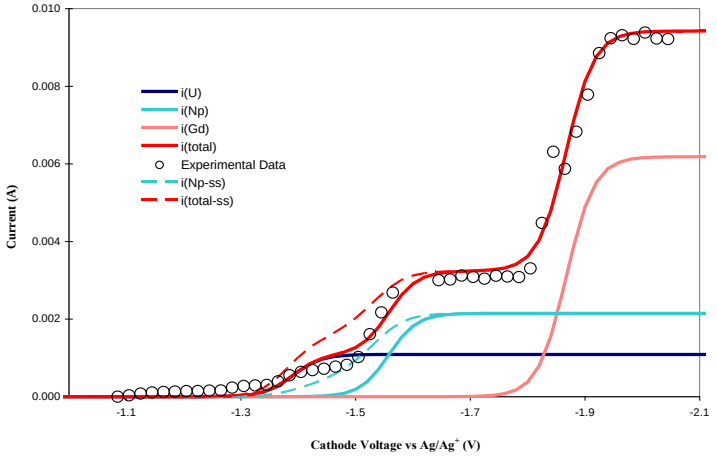


Recent Progress: Initial model developed. Results for co-deposition of metals at cathodes are in agreement with experimental studies

•Uses current available data for activity and diffusion coefficients, apparent standard electro-potential; assumes the fuel is an ideal solid solution

•Considers surface area changes due to dissolution and deposition

•Calculates behaviors of co-dissolution at the solid anode and co-deposition at the solid cathode of Zr-U-Pu alloys.



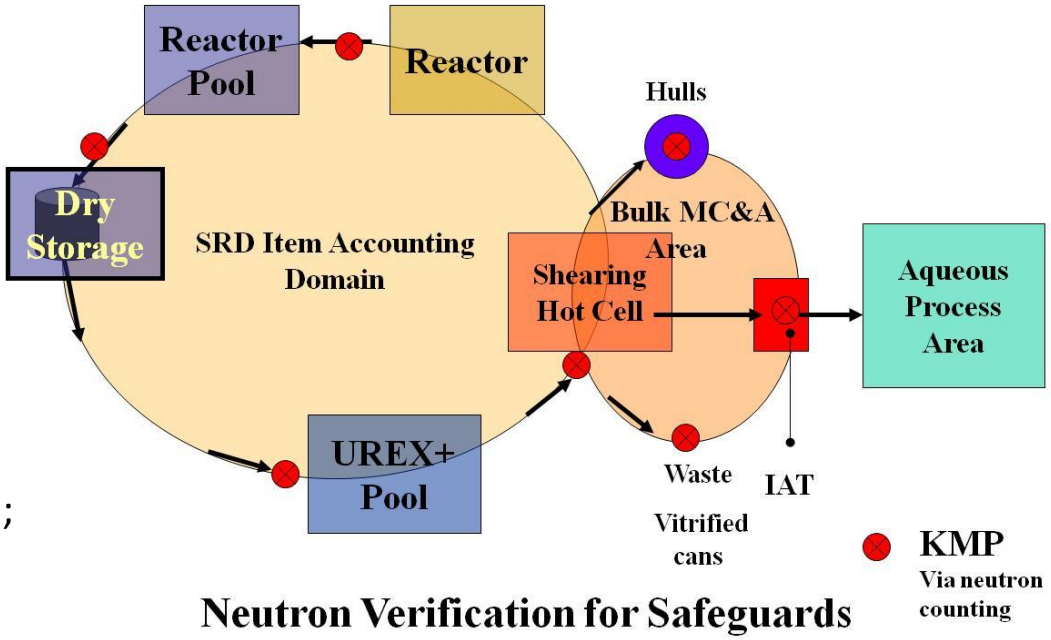
FY15 Target:

Model that incorporates electrochemical kinetics, phase morphology, and property data.

J. Zhang (LANL) & J. Willet (ANL)

Example of Safeguards Modeling: Neutron Balance Approach for Head-end Safeguards

- Concept: Correlate number of neutrons escaping fuel bundle to number escaping Input Accountability Tank (IAT).
- Used nuclear fuel emits spontaneous and (α,n) neutrons primarily from ^{244}Cm.
- The ratio of Cm/Pu can be determined from burnup to yield Pu mass in both places.
- The number of neutrons emitted/gram from the used fuel in an assembly should be the same as in an Input Accountability Tank (IAT); only these two locations in the plant are currently analyzed.

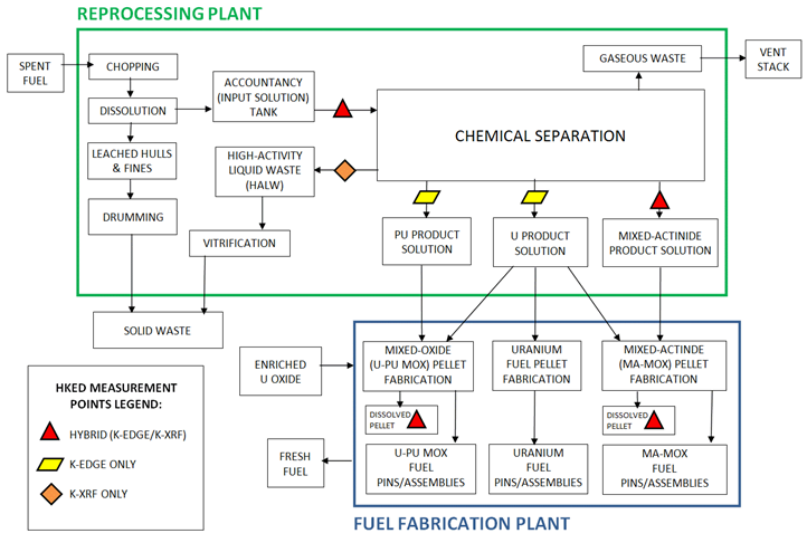


Methodology:

- Isotopic composition estimates of fuel assemblies calculated using Monte Carlo burnup
- Determine neutron source terms and use MCNP for transport and multiplication calculations

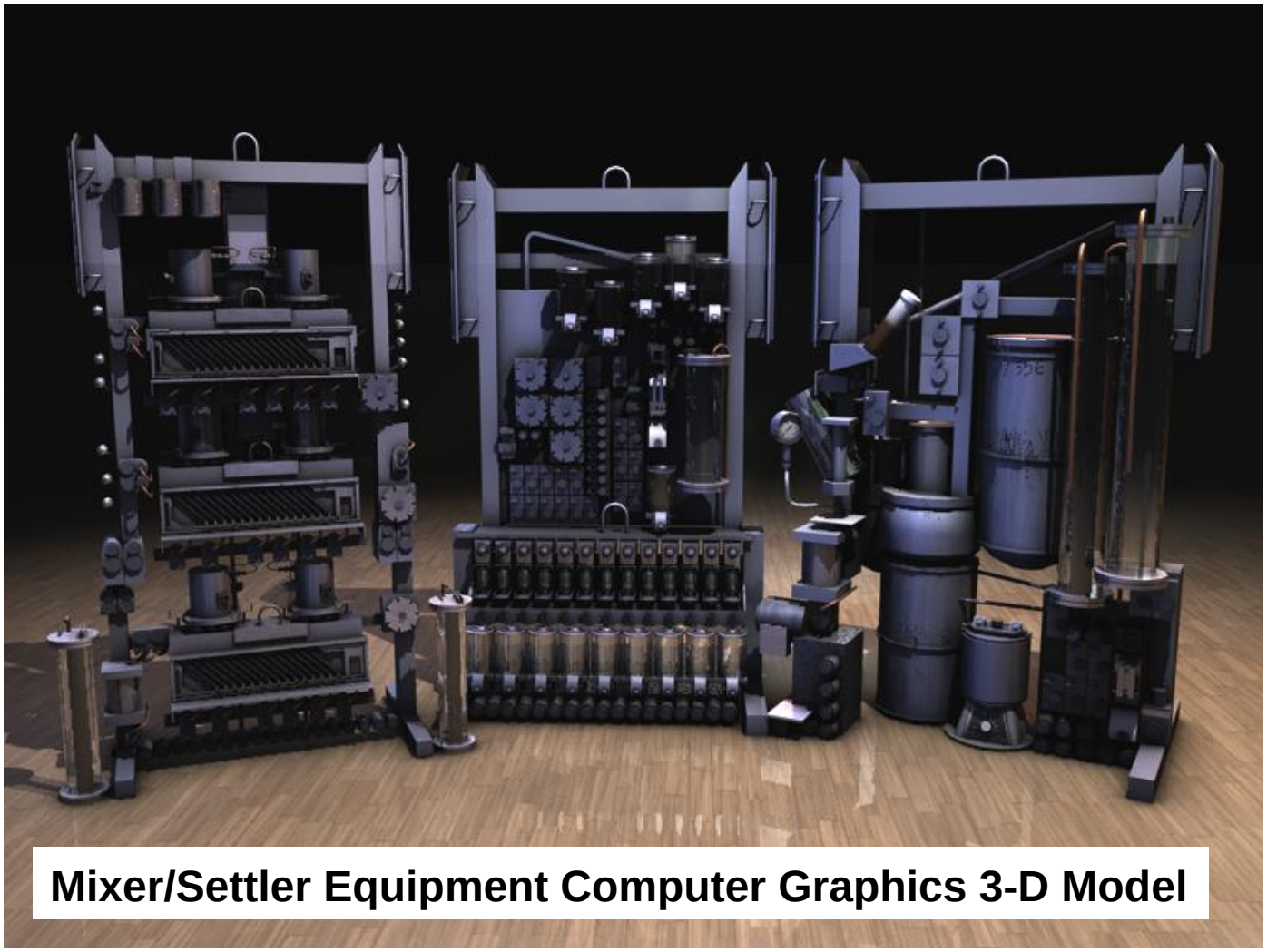
Example of Instrumentation Modeling: Hybrid K-Edge Modeling

- Hybrid K-Edge method uses two simultaneous x-ray measurement techniques to determine the actinide content of a liquid sample
- **GOAL of the Modeling Activity: Simulate the act of measuring a liquid specimen with a hybrid densitometer**
  - Develop a safeguards module for Hybrid K-Edge/X-ray Fluorescence Densitometer (HKED) simulation
  - The module will read user-defined input parameters (including simulated concentrations of thorium, uranium, neptunium, plutonium, americium, and curium) into the plant-level code and produce the desired spectra.



M. Collins, LANL

Photorealistic and Physics-Realistic Interactive Models for Test, Evaluation and Analysis



Mixer/Settler Equipment Computer Graphics 3-D Model

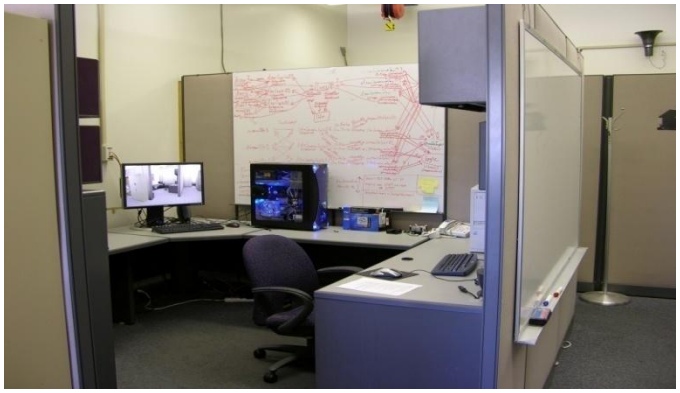
- Model built and textured from scratch in 1.5 work days by the Los Alamos National Laboratory VISIBLE development team, using only photos of the original equipment.
- Each part of the modeled equipment can be manipulated and custom programmed for behavior.

K. Michel, LANL

Real-world vs. Virtual World



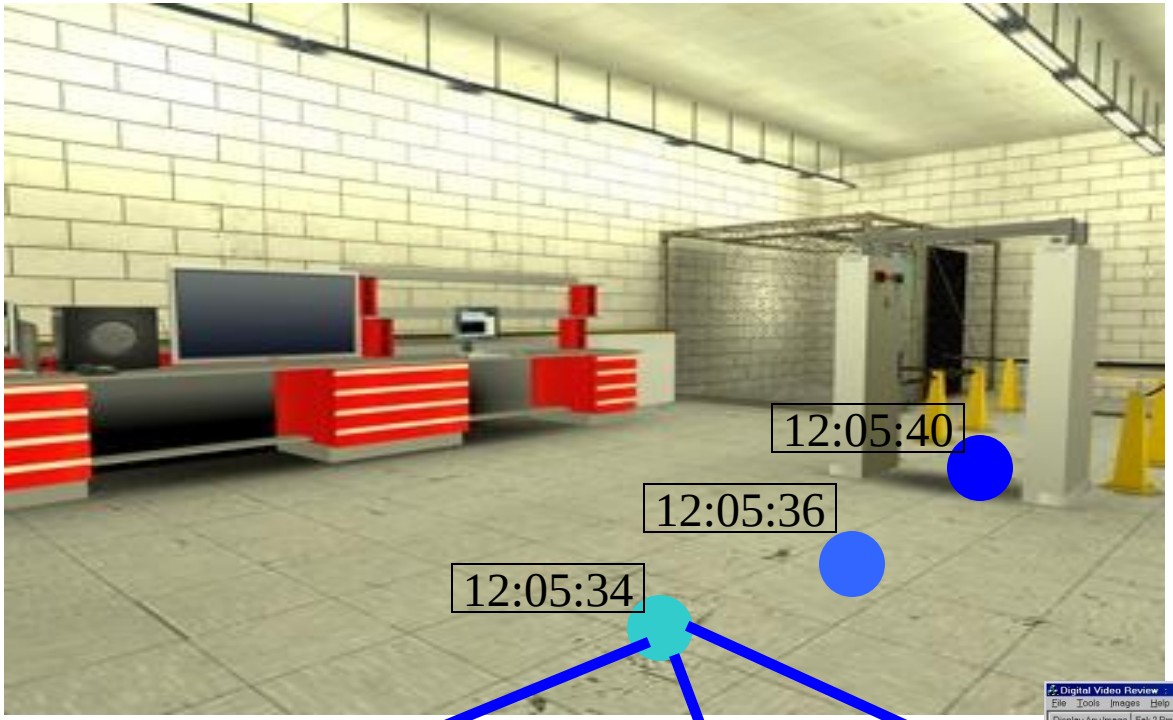


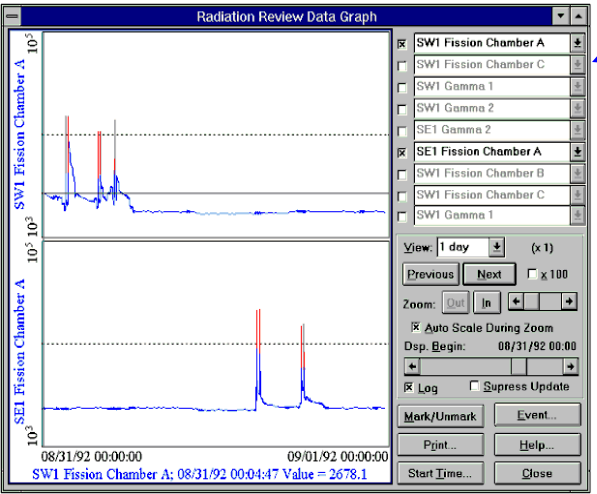


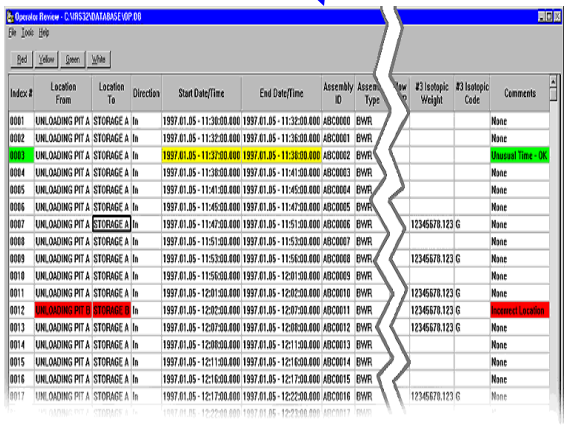

- A virtual model can have as much, or as little detail as needed.

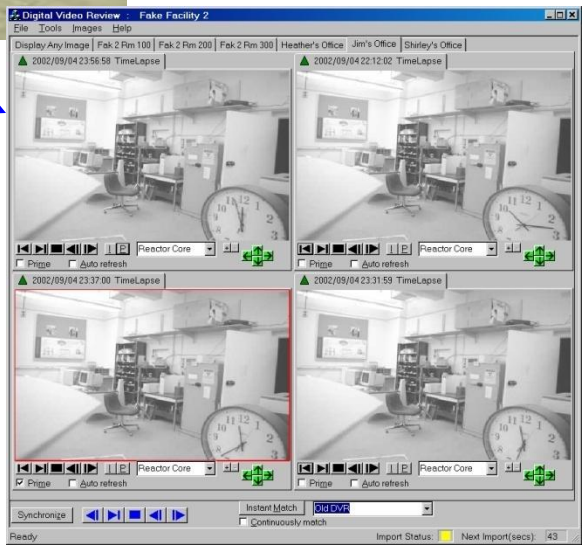
K. Michel, LANL

Future Safeguards Data Review Interface: Safeguards Data Shown in Context for Evaluation and Analysis of Events









Summary

- **Modeling and simulation have provided useful input to the development of fuel cycle separations over the past several decades.**
- **With significant scientific advancements and vast increases in computational power, modeling and simulation can play an increasing role in solving the complex challenges to be overcome in developing advanced nuclear energy systems.**

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