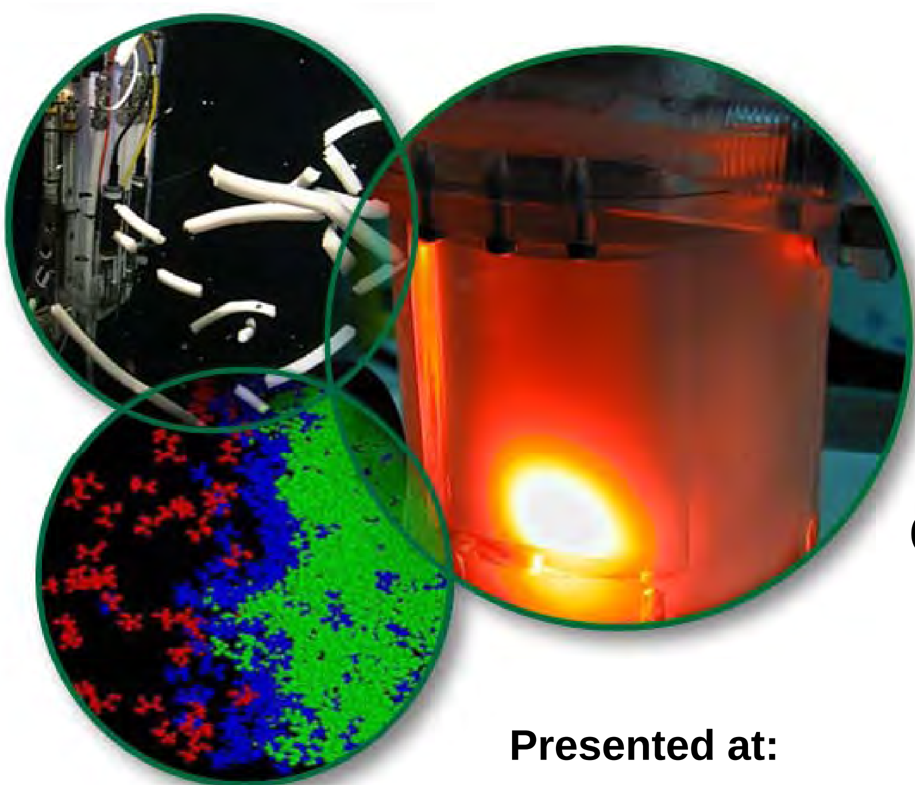
Role of Modeling and Simulation in Used Fuel Recycling



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Presented at:

Introduction to Nuclear Chemistry and Fuel Cycle Separations

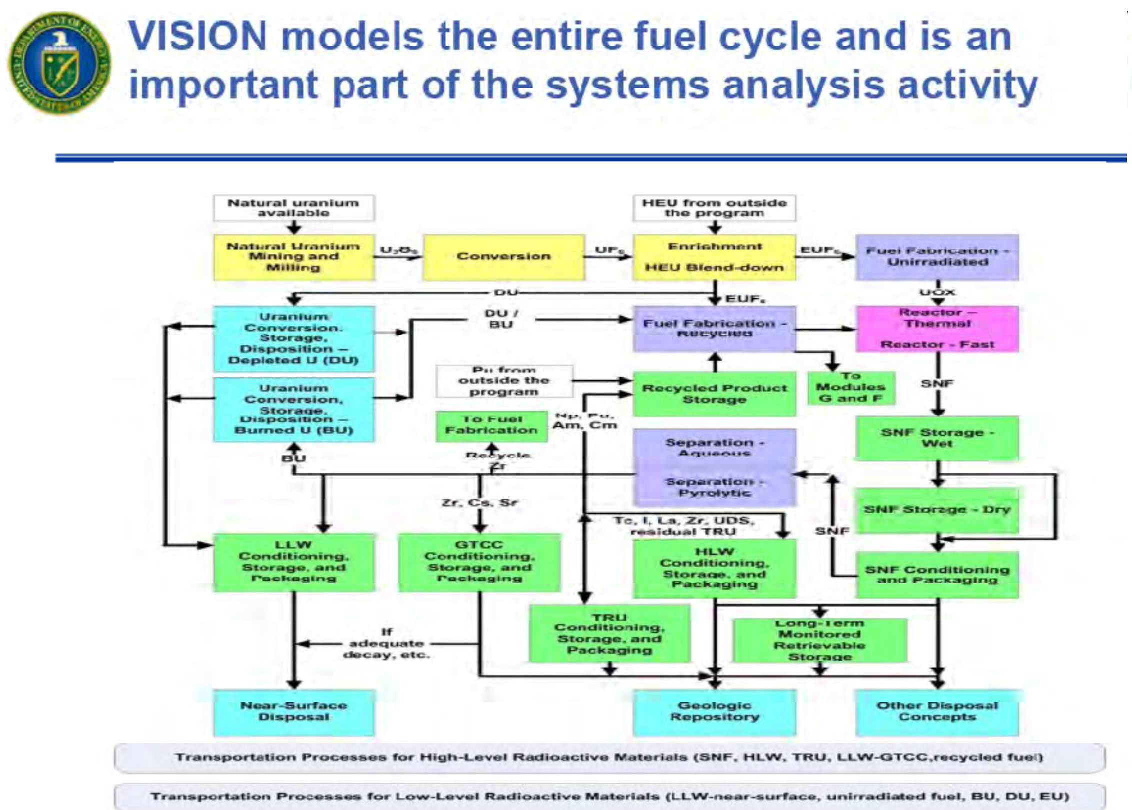
Vanderbilt University

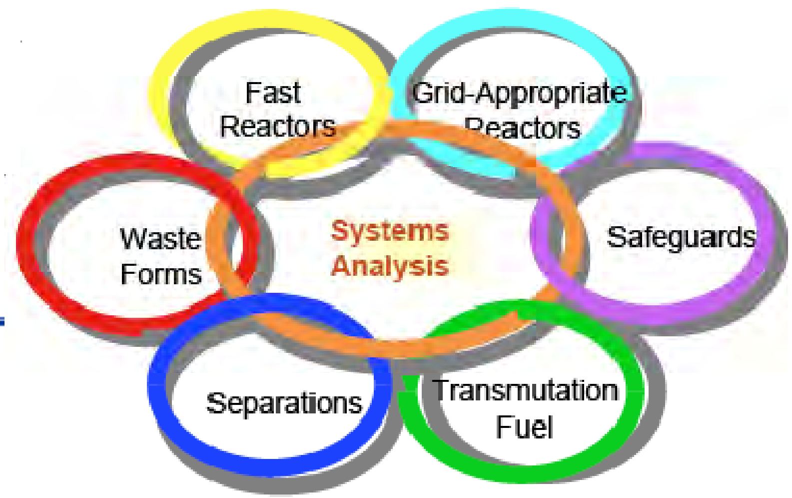
Dec. 17, 2008

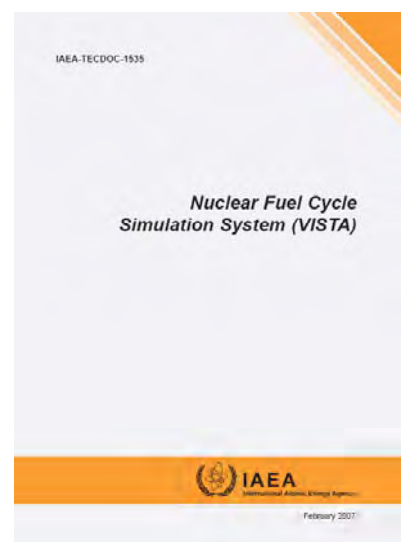
Outline

- **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**

This talk will focus on a subset of modeling and simulation of nuclear fuel cycle







IAEA-TECDOC-1535

From K. McCarthy presentation at Office of Nuclear Energy FY2009 University Program Workshop:
http://www.energetics.com/meetings/univworkshopaug08/reports.html

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

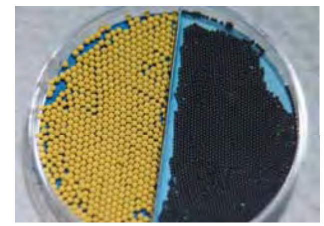
solvent extraction cycles

off-gas treatment

solidification

waste treatment

recovery systems



Fuel

Waste forms

- **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**
- **Increase 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 m… predictions of process performance…**
- **"Together modeling and simulation…**
  - **enhance understanding of know…**
  - **provide qualitative/quantitative insights and guidance for experimental work, and**
  - **produce quantitative results that replace difficult, dangerous, or expensive experiments."**

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

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

Some applications for modeling and simulation

- **Guidance for experimental development work**
- **Process design optimization and confirmation**
- **Safeguards/materials accountability studies**
- **Plant licensing**
- **Criticality safety studies**
- **Development of operational envelopes**
- **Understanding and recovery of off-normal events**
- **Process instrumentation studies**
- **Process control**
- **Operator training**

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  - Separations M&S development

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

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

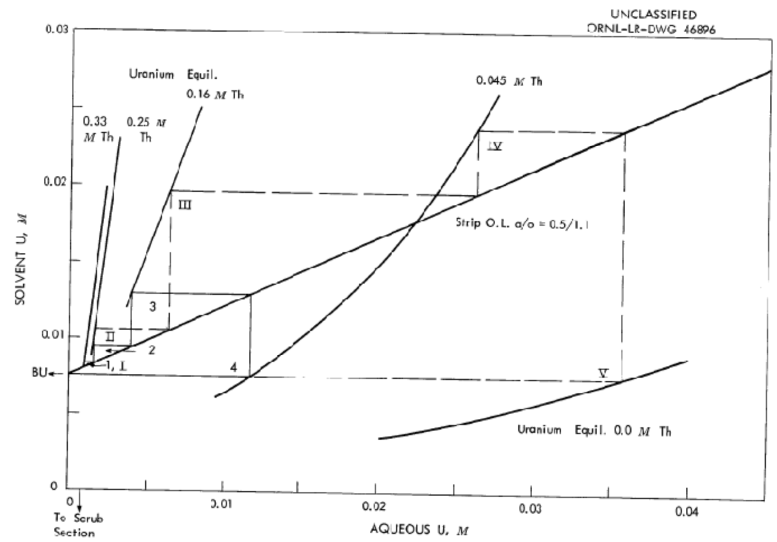


Fig. 3. Uranium diagram for strip section case for four stages shown by Arabic numerals; for five stages

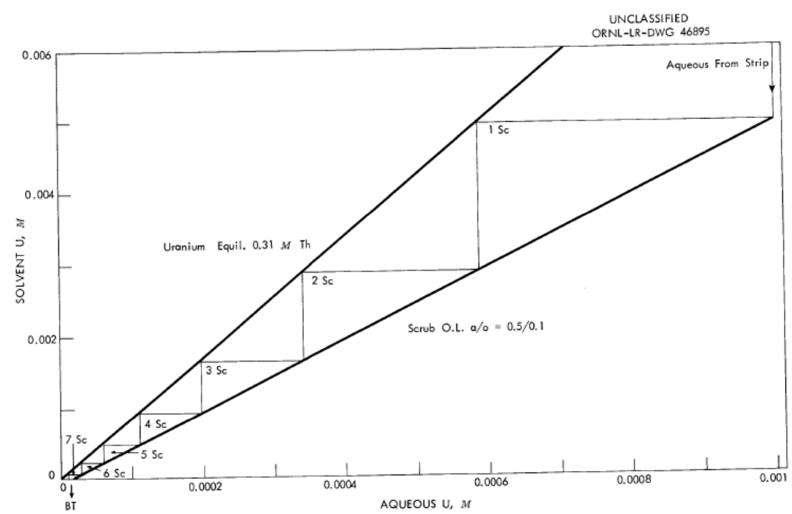
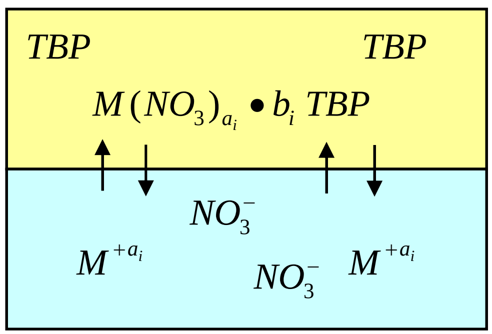


Fig. 4. Uranium diagram for scrub section (0.1% loss).

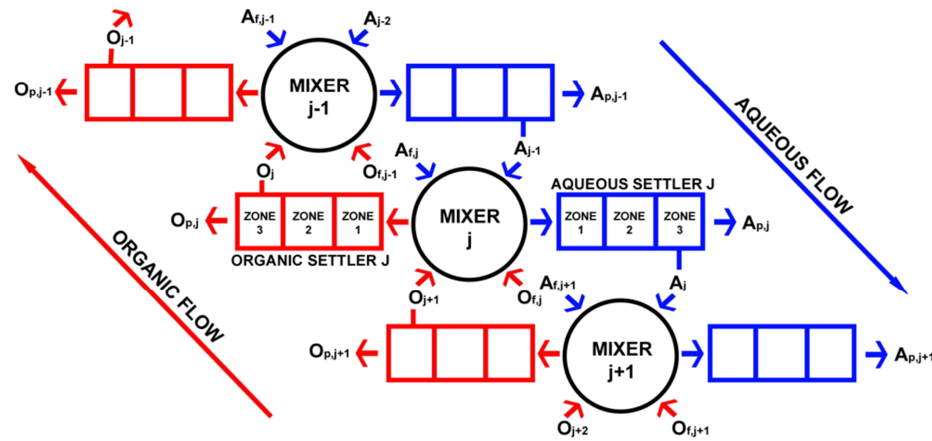
A. D. Ryon, ORNL-3045, 1961

Equations for interphase mass transfer and material balances converted to computer codes



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

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



Overview of SEPHIS model of solvent extraction stages

Existing models are based on empirical fits to experimental data

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

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

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

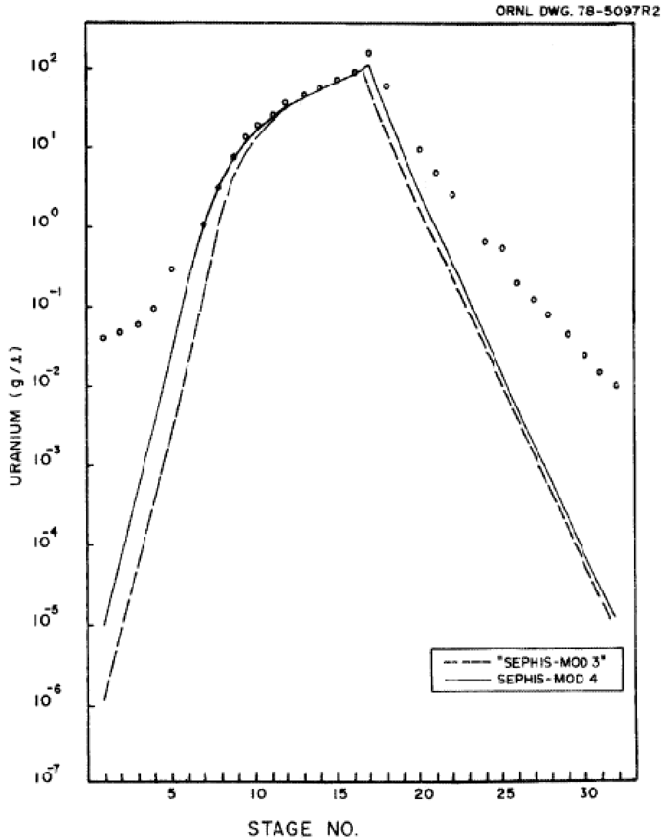
$$K_U^{'} = C_1 + C_2\ \mu + C_3\mu^2 + C_2\ \mu^3$$

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

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

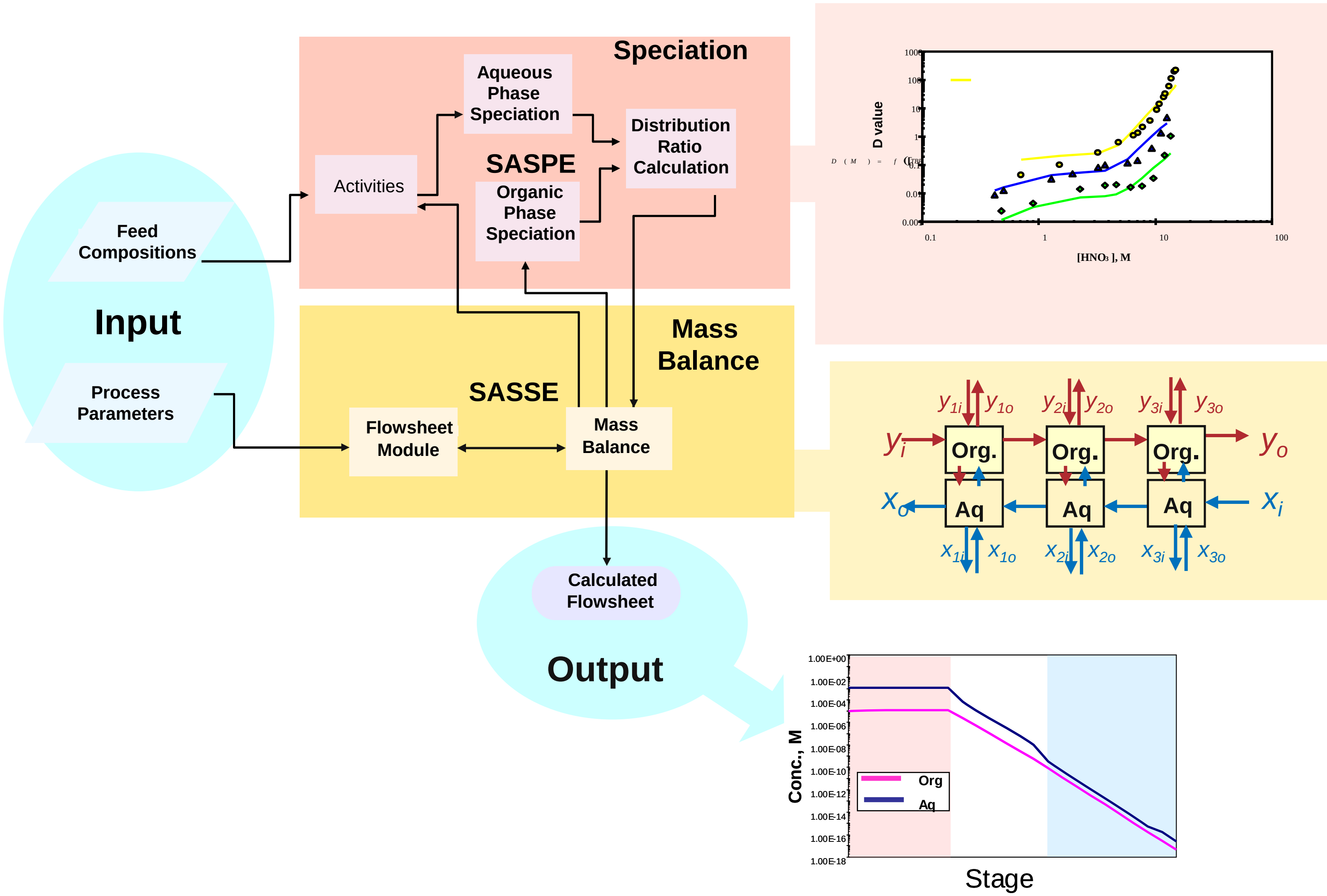
$$\mu \equiv [H^+] + 3[UO_2^{2+}] + 10[Th^{4+}]$$

Rainey and Watson, 1975



With good input data, good predictions are obtained – within conditions of fit

AMUSE Models Solvent Extraction



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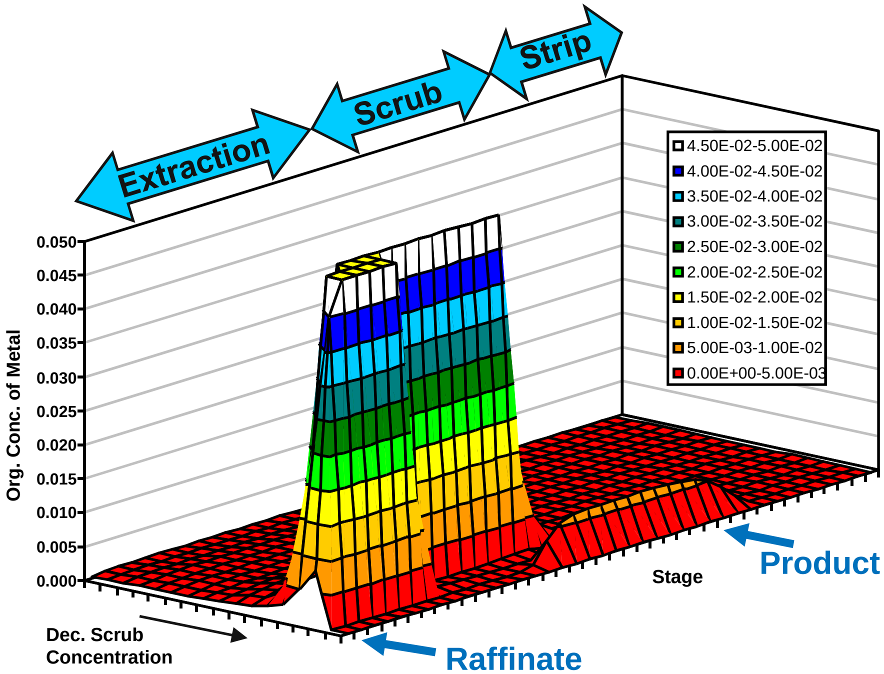
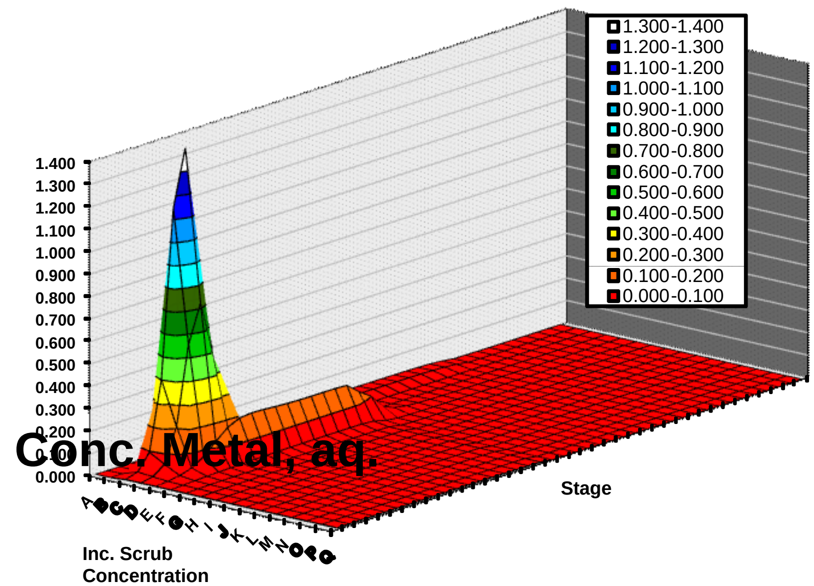
AMUSE has been used for process upset and product diversion analysis

- 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

Example: Changes in scrub stream can cause "pinching" of metals in the extraction section

- The build up, or "*pinching*" of metal in the extraction section
- Steady-state concentrations
- Results need to be verified experimentally
- ***In most cases no indication of a problem at the outlets***
- ***Small, possible indication of a problem at the product outlet***





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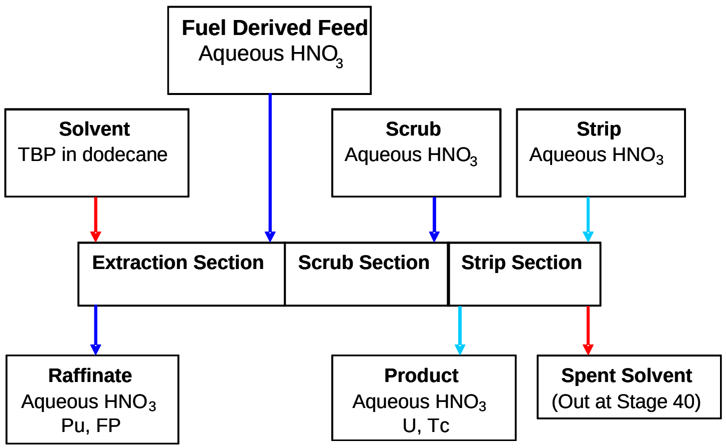
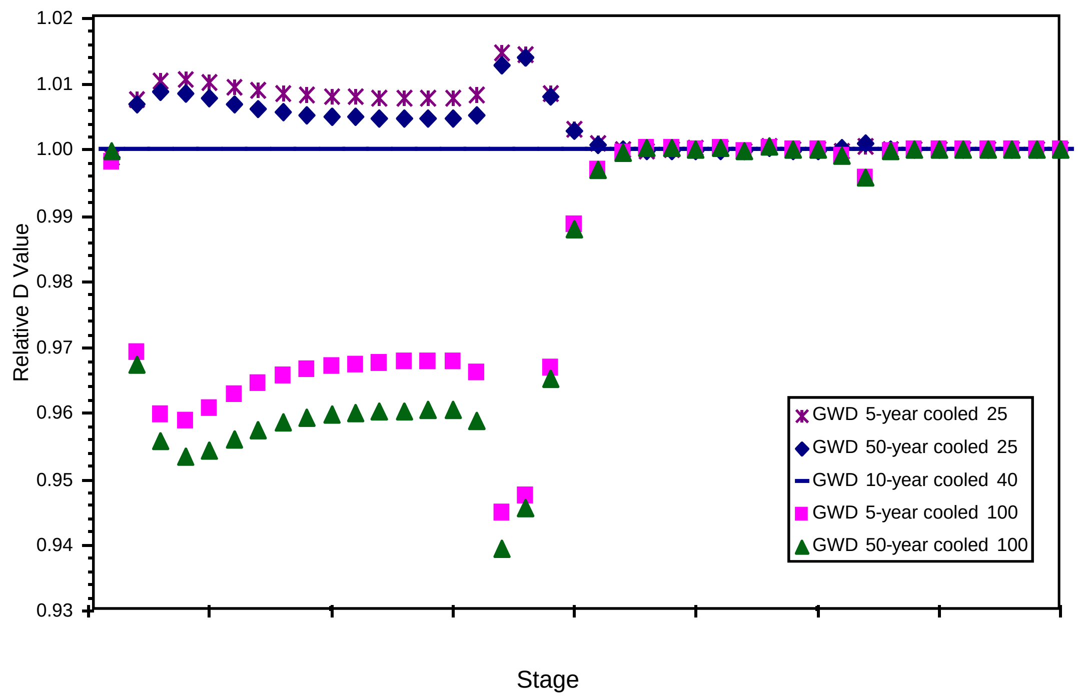
Example of the application of AMUSE to determine the effect of fuel composition on D-values

- Here the data show that the fuel composition has a minor effect on the measured D-values
  - The process proves to be robust in terms of feed variance





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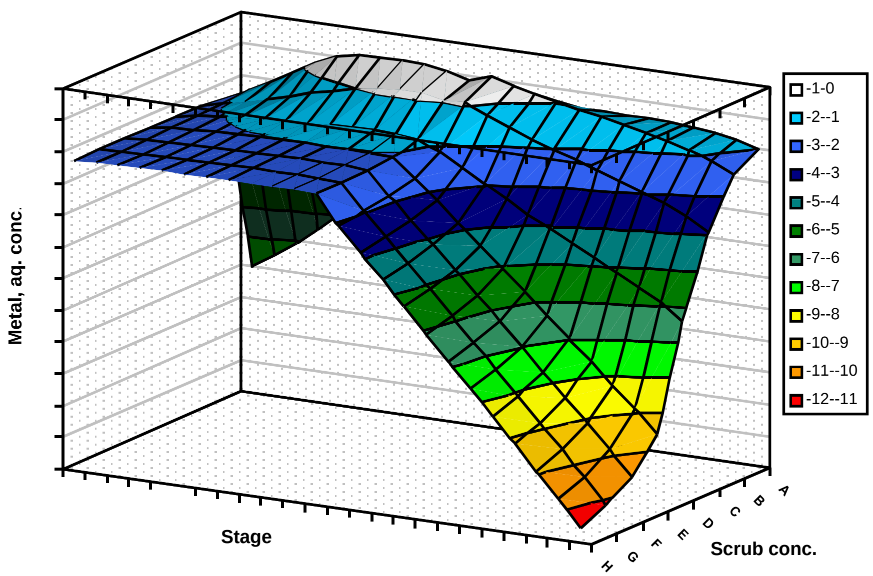
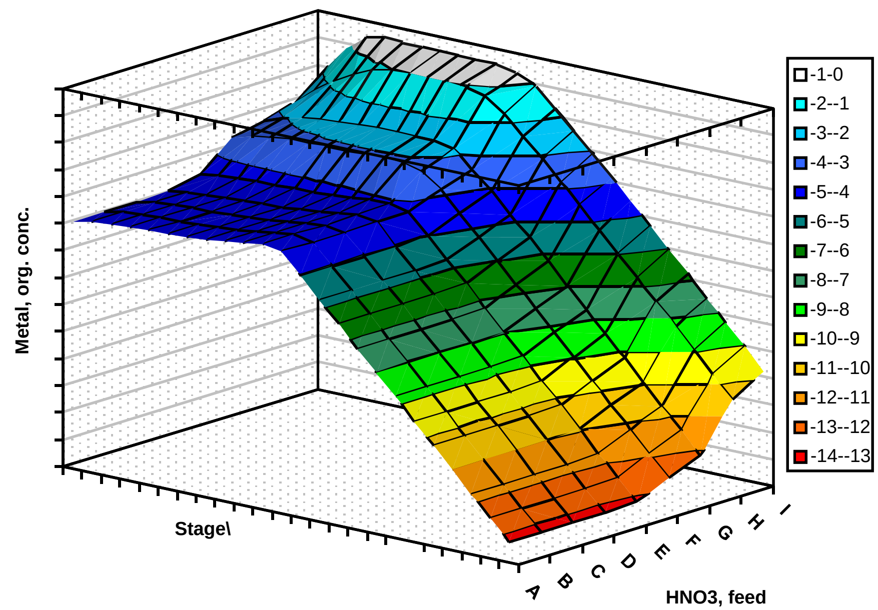
Changes in feed composition lead to changes in the concentration profiles in the aqueous and organic phases

- Automated computations valuable. For this example –
  - If the six concentrations *have no co-dependency* that results in *30* calculations
  - If the six concentrations *have a co-dependency* that results in *15,625* calculations
  - For the thirteen variables on a co-dependent basis results in *1.22 x 10^9* calculations
- Large impact from different fuel feeds





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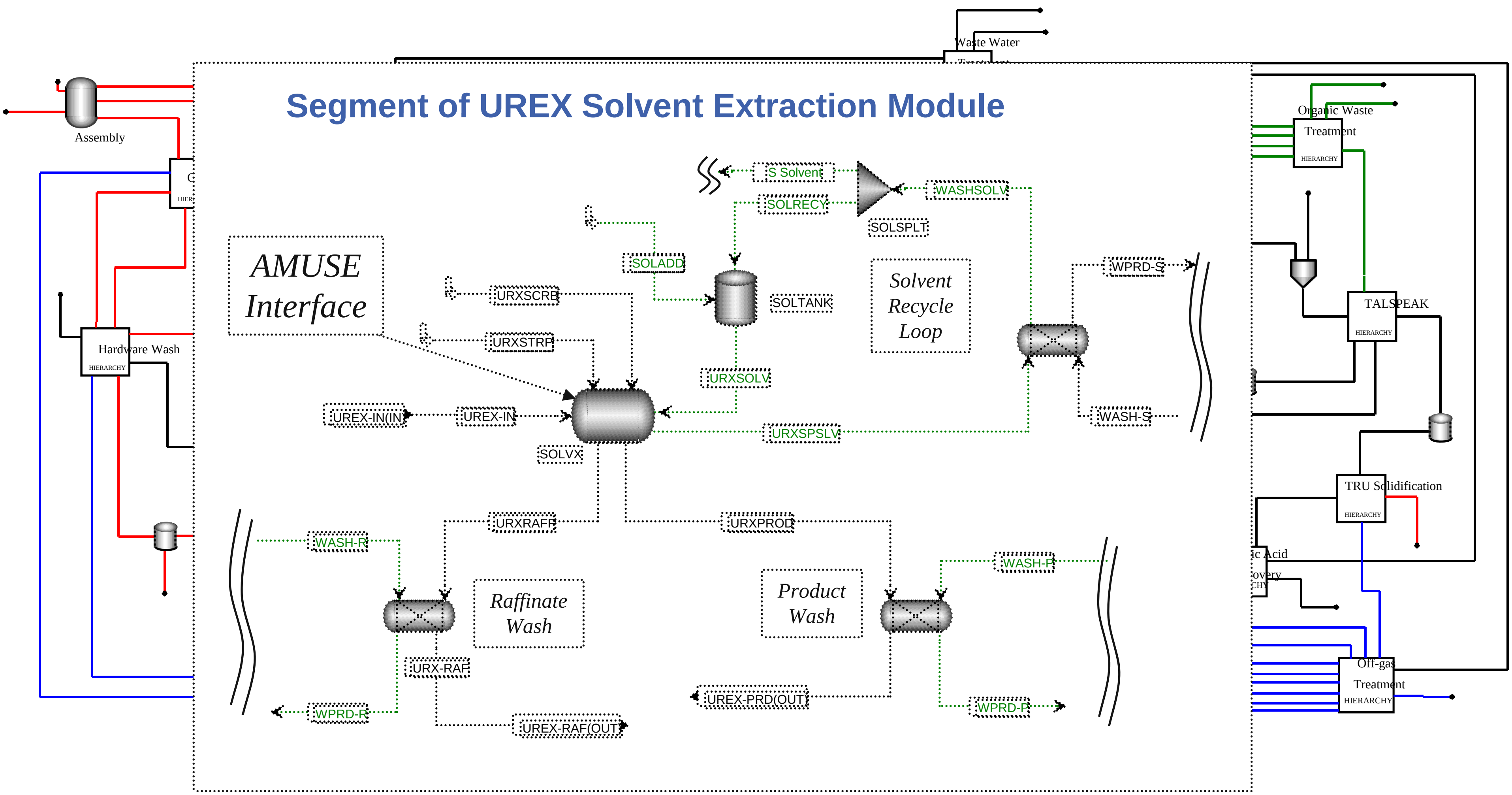
Outline

- Introduction
- Some applications to date
  - Solvent extraction
  - Plant-level modeling
    - 1980’s example
    - Current efforts
      - Separations
      - Safeguards
  - Agent design
- Key research needs
- Advancing to the future
  - NEAMS vision
  - Separations M&S development

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.**

Top Level Plant-scale Flowsheet (UREX+3a)



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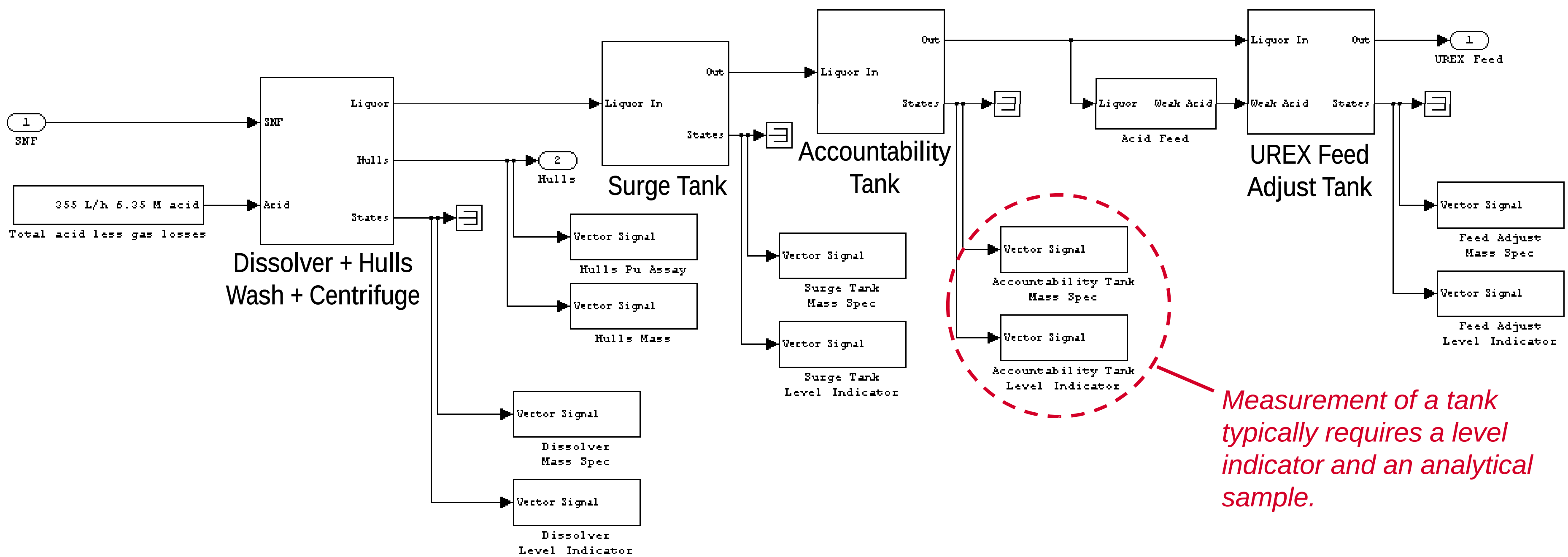
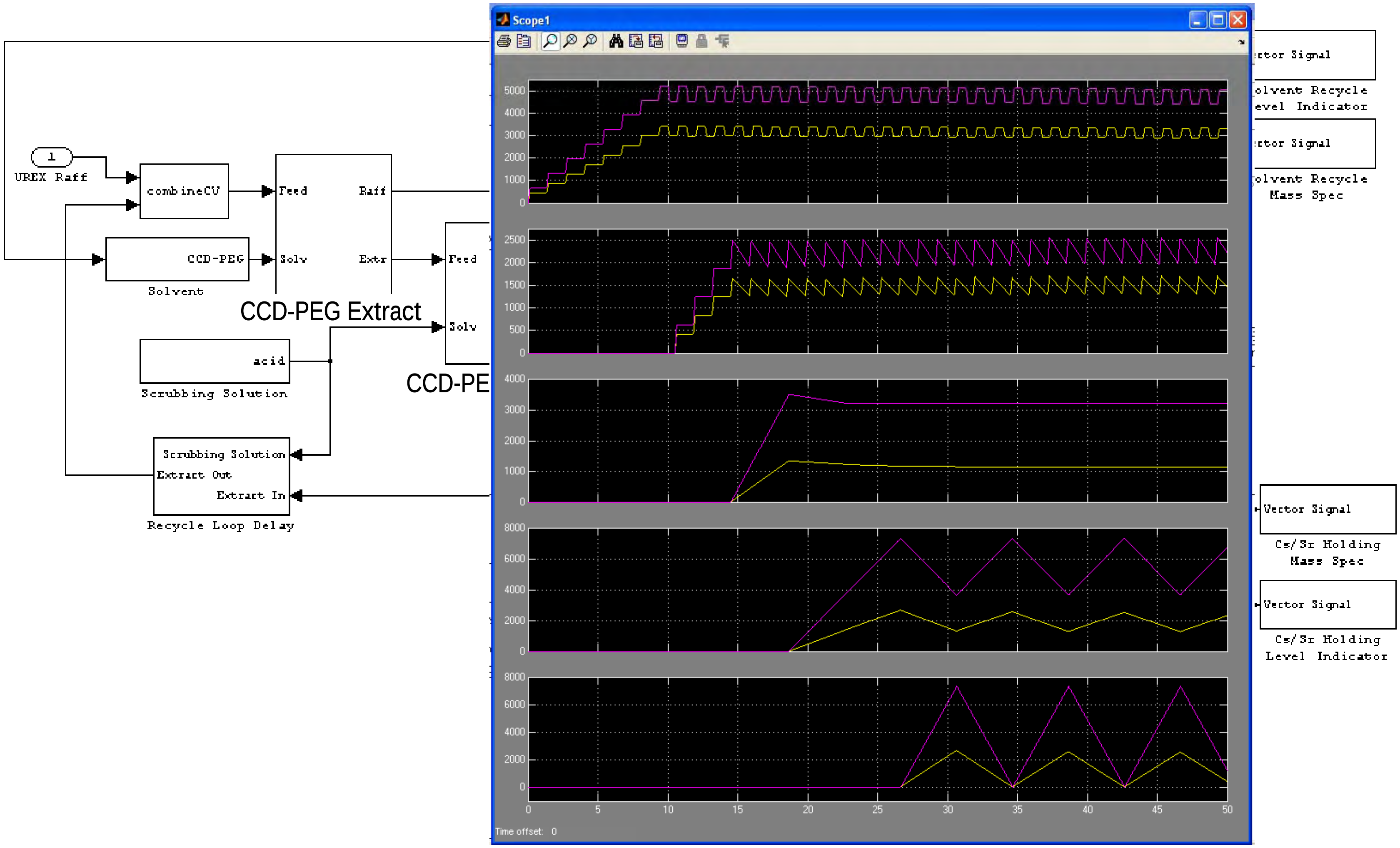
Safeguards Performance Model



- **The model uses the MatLab Simulink platform, which is used routinely in laboratories, universities, and industry.**
- **The model tracks bulk flow rates, cold chemicals, elemental concentrations, and solids**
  - Solvent extraction splits based on data generated by ANL's AMUSE spreadsheet.
- **Measurement blocks simulate a material measurement—such as a level indicator on a tank or a mass spec measurement of a sample.**

B. Cipiti and N. Ricker, SNL

Material Tracking in the Model



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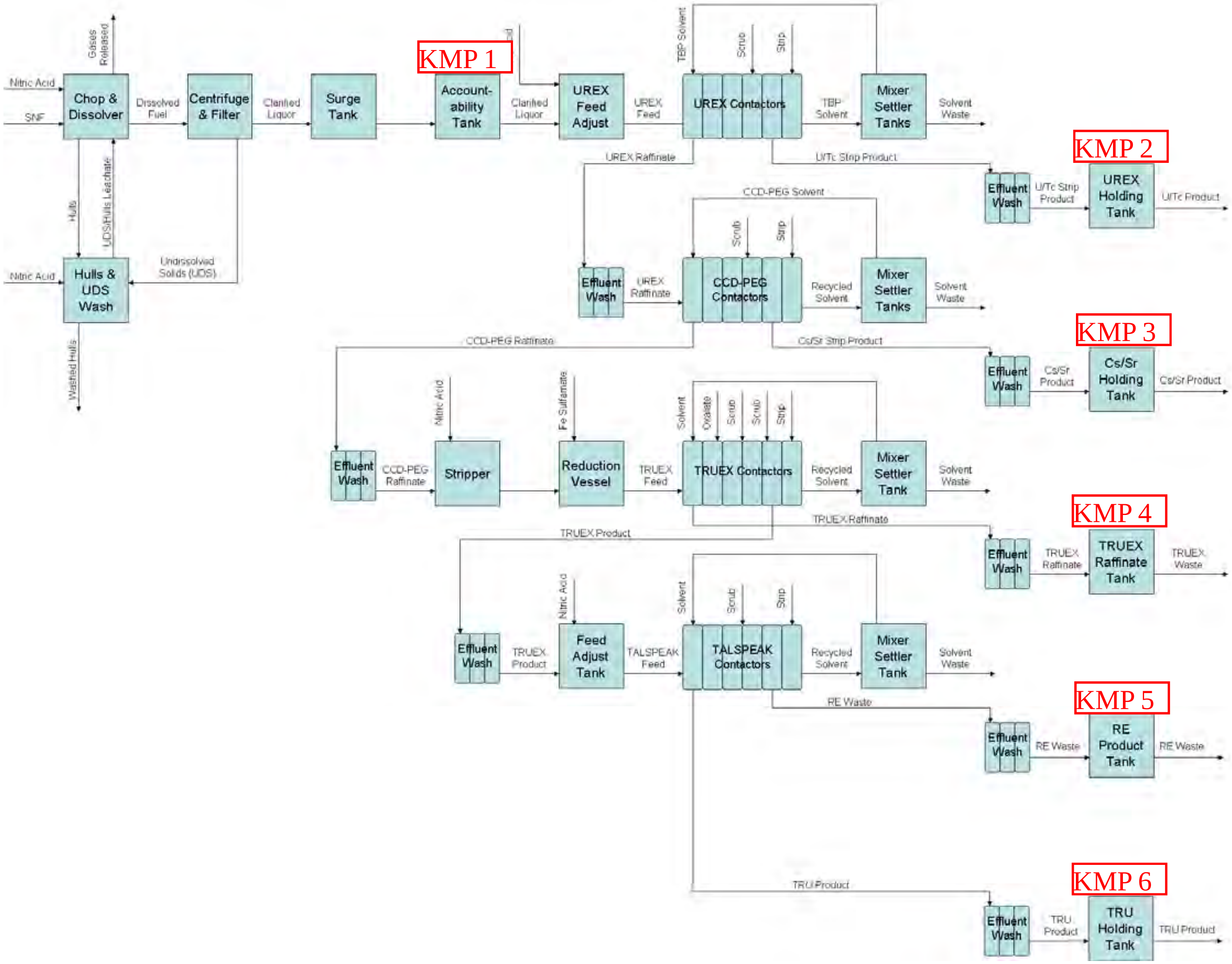
Traditional Accounting Instrumentation (Baseline)



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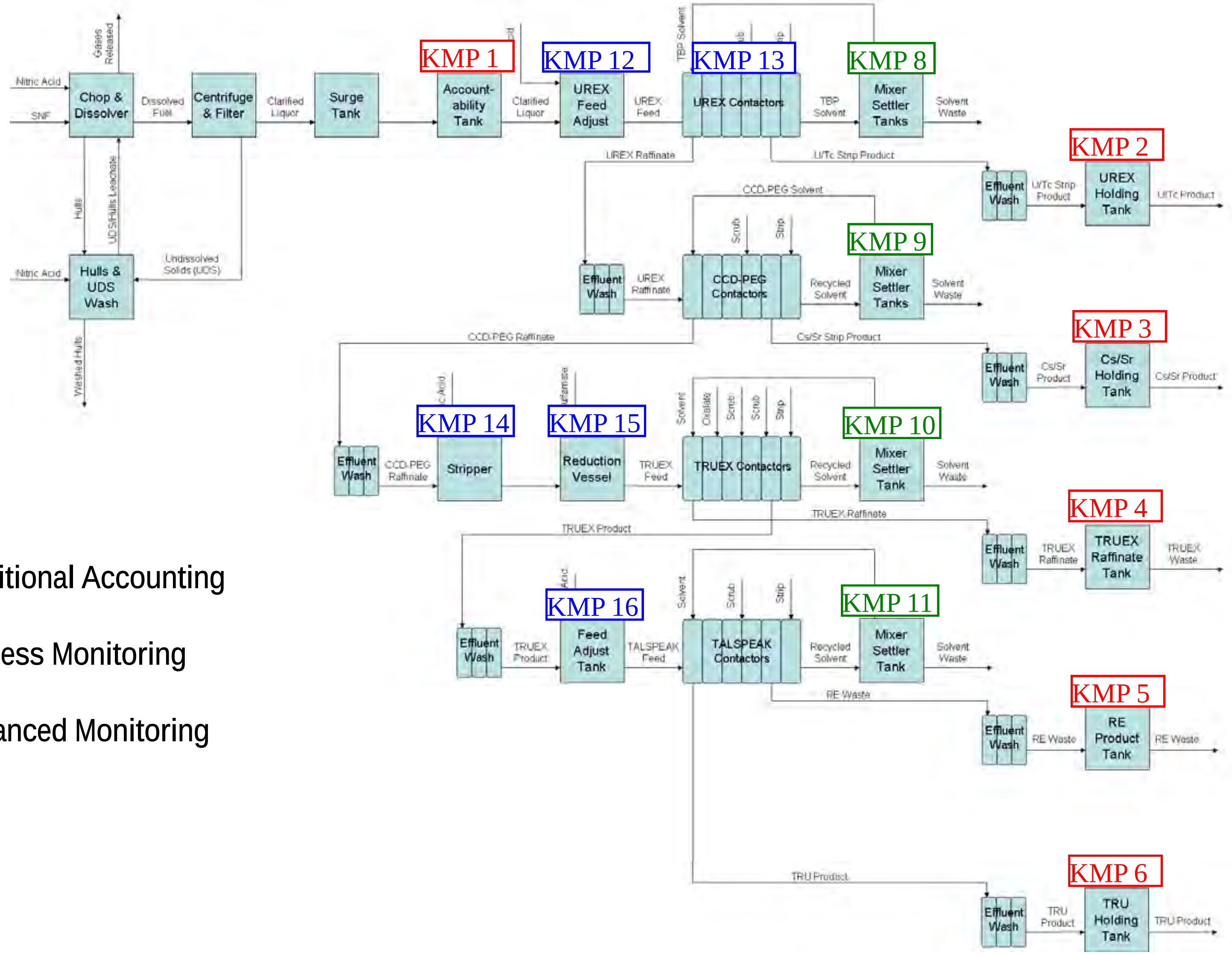
Additional Accounting Instrumentation (Advanced)



Red	Traditional Accounting
Green	Process Monitoring
Blue	Advanced Monitoring

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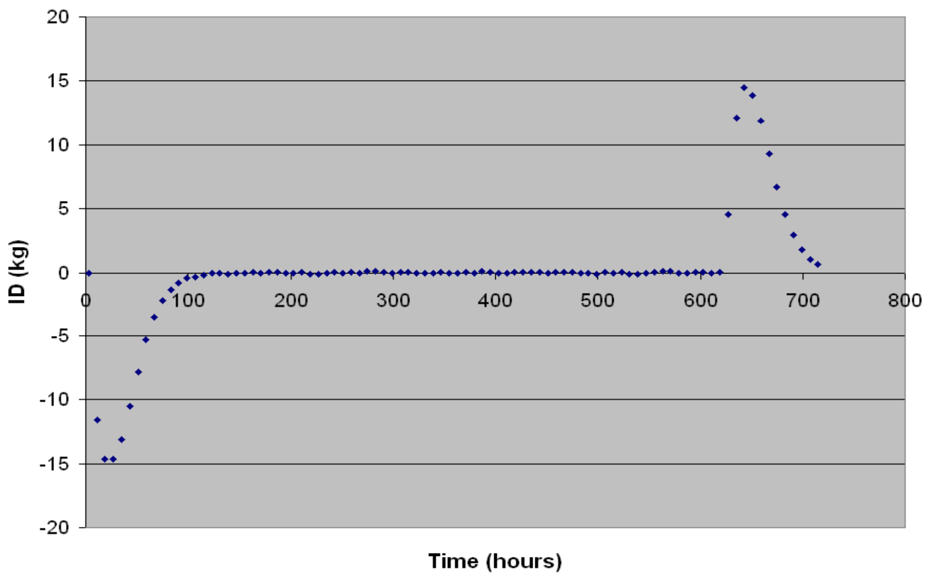
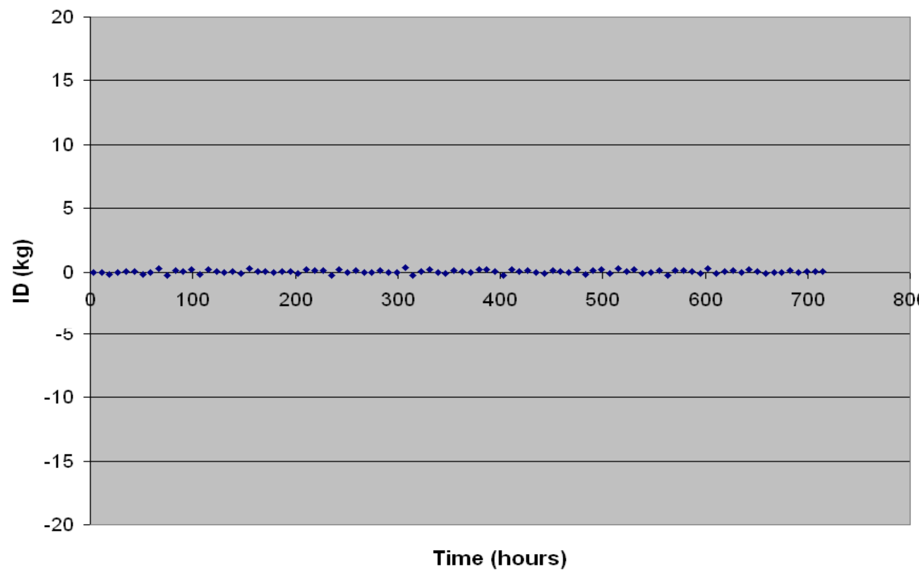
Pu Inventory Difference

(Baseline)



(Advanced)



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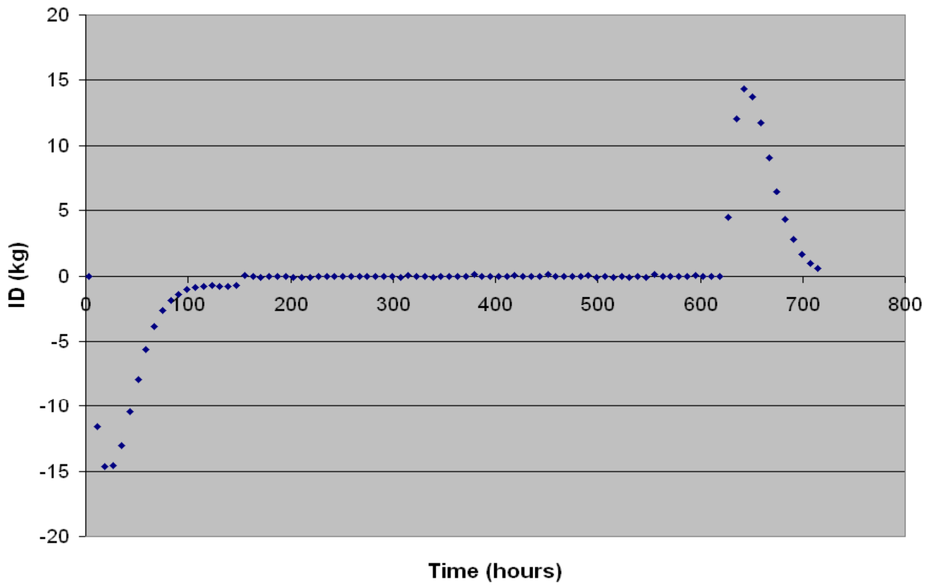
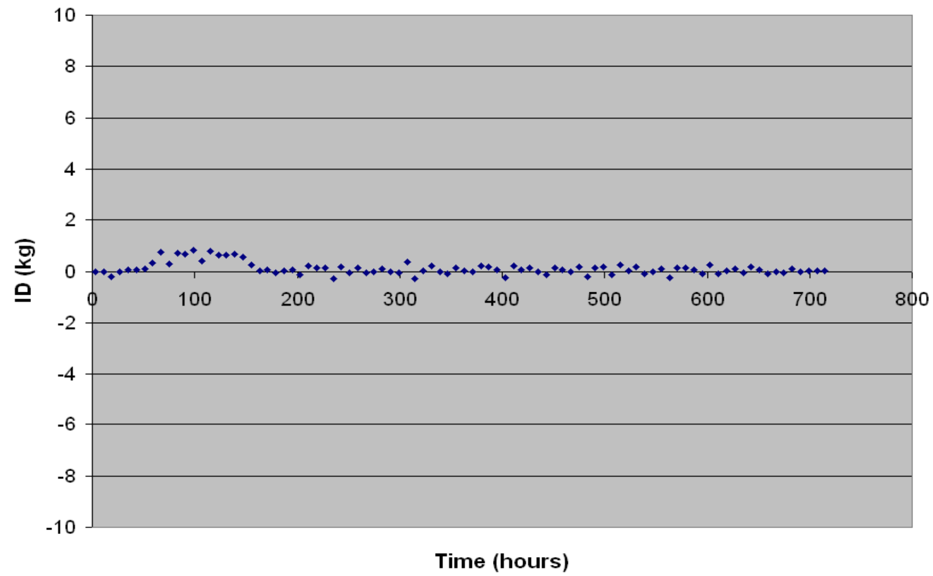
Diversion Scenario

(Baseline)



(Advanced)



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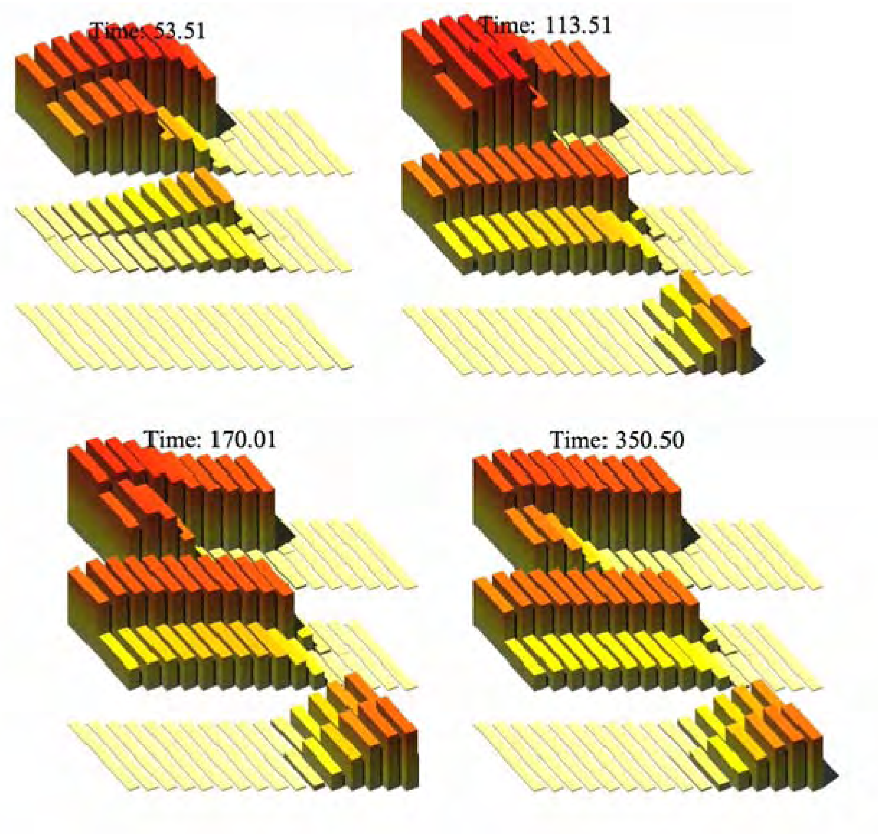
Current state of separations process modeling

- **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.

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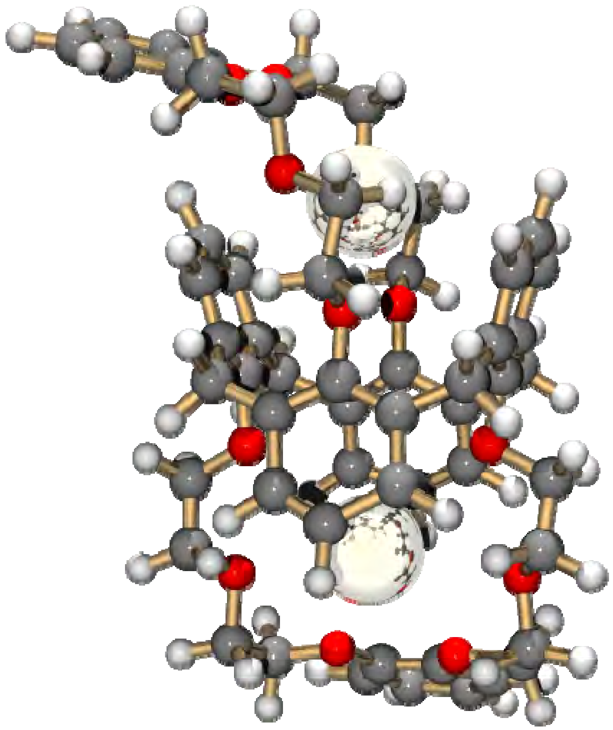
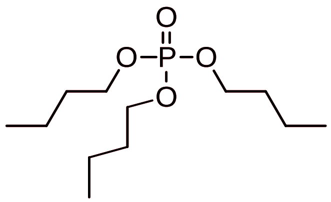
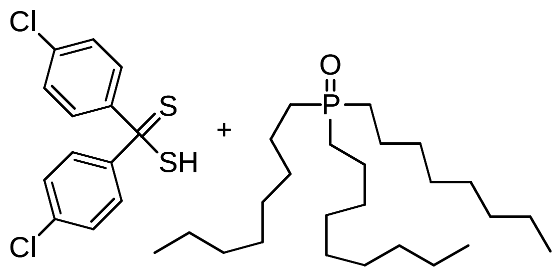


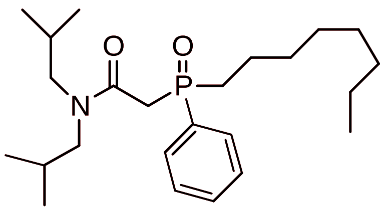
Sequestering agents are the basis for separations



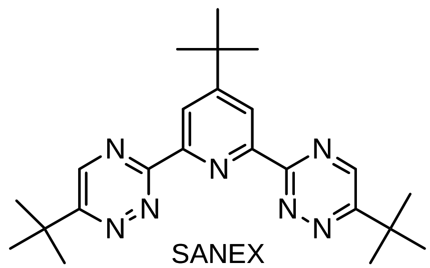
PUREX
(HANFORD, 1950s)



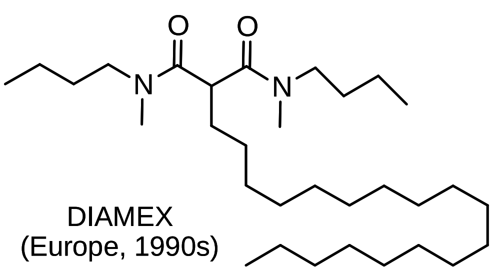
SANEX
(Europe, 1990s)



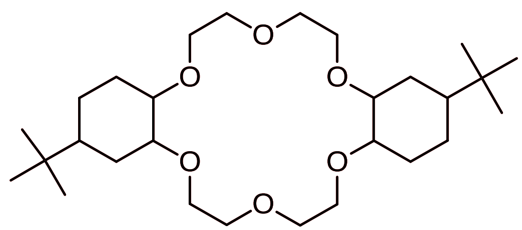
TRUEX
(ANL, 1980s)



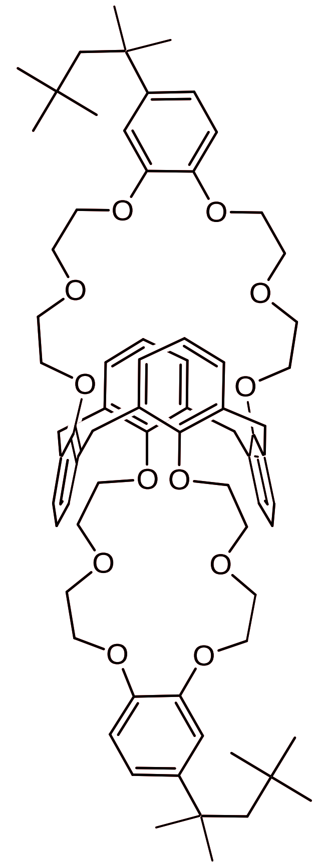
SANEX
(Europe, 2000s)



DIAMEX
(Europe, 1990s)



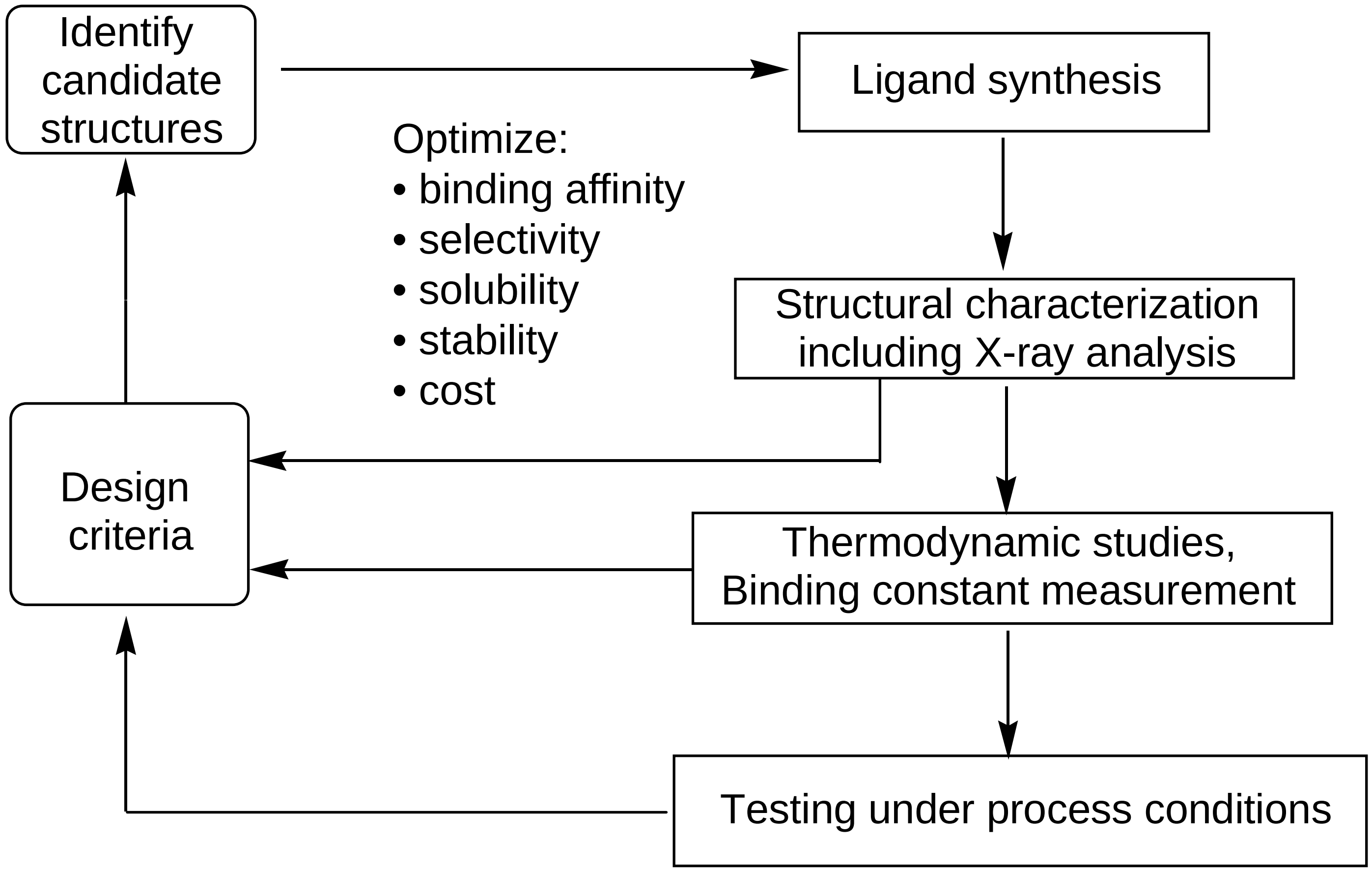
SREX
(ANL, 1990s)



CSEX
(ORNL,1990s)

B.Hay, ORNL

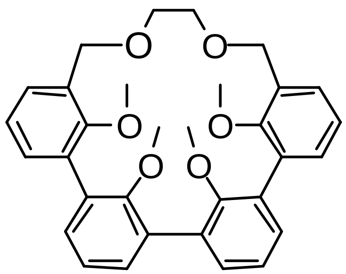
Experimental development is slow and expensive



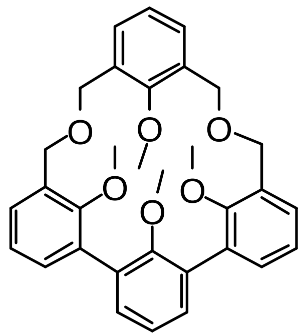
B.Hay, ORNL

Influence of ligand architecture

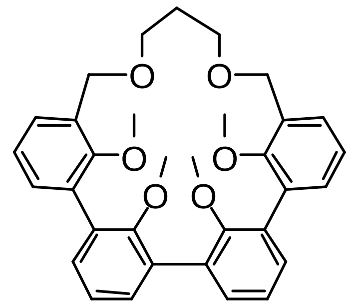
Large effects on binding affinity:



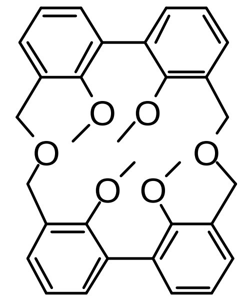
10^{10}



10^{6}

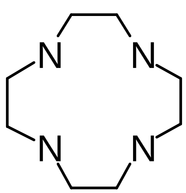


10^{5}

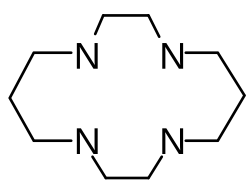


10^{3}

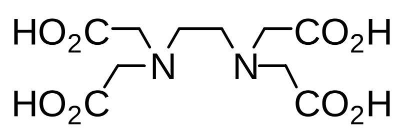
and significant impacts on selectivity:



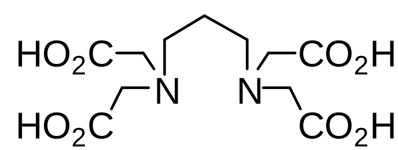
$Hg^{2+}/Cu^{2+} = 5$



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



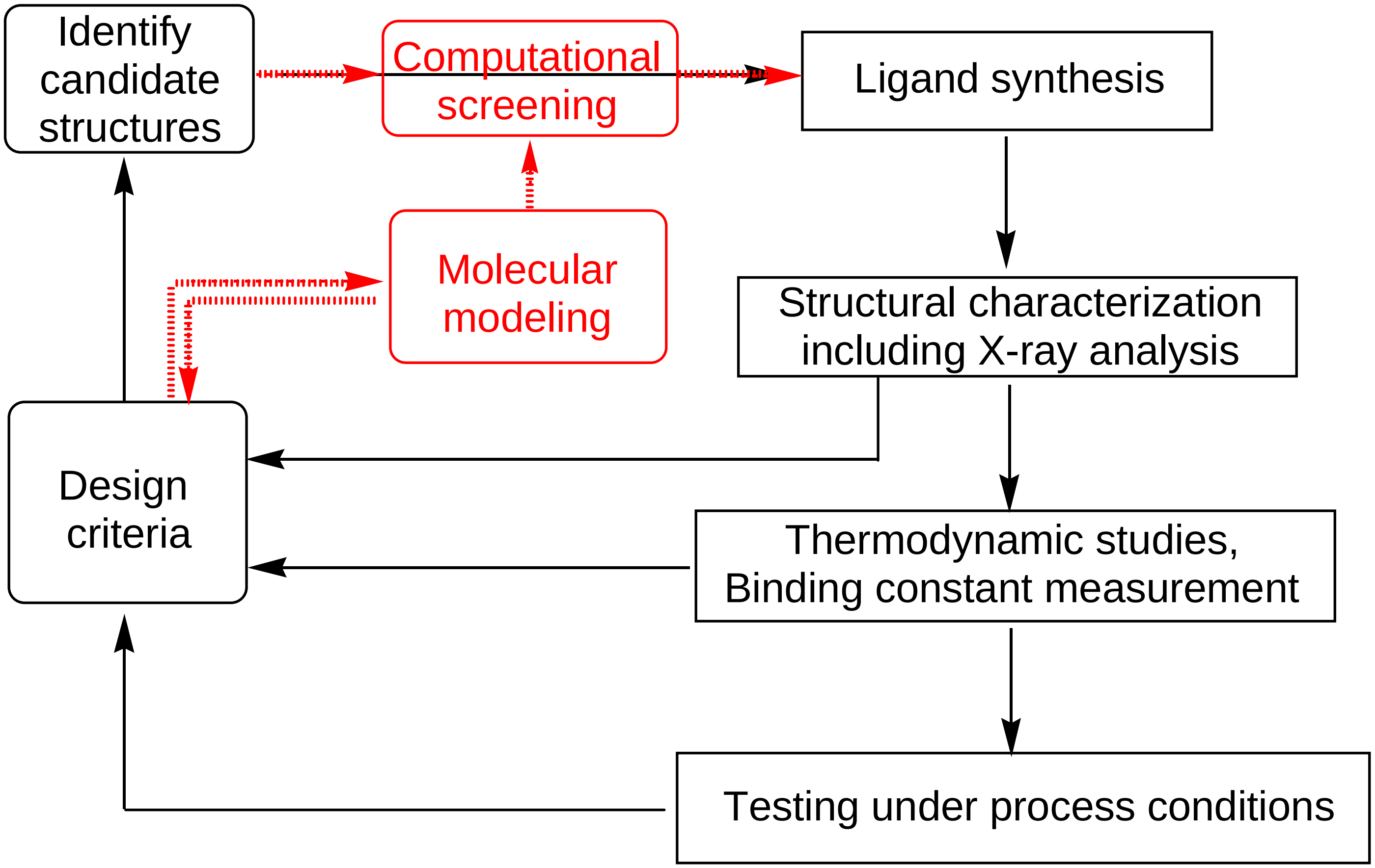
$Eu^{3+}/Al^{3+} = 13$



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

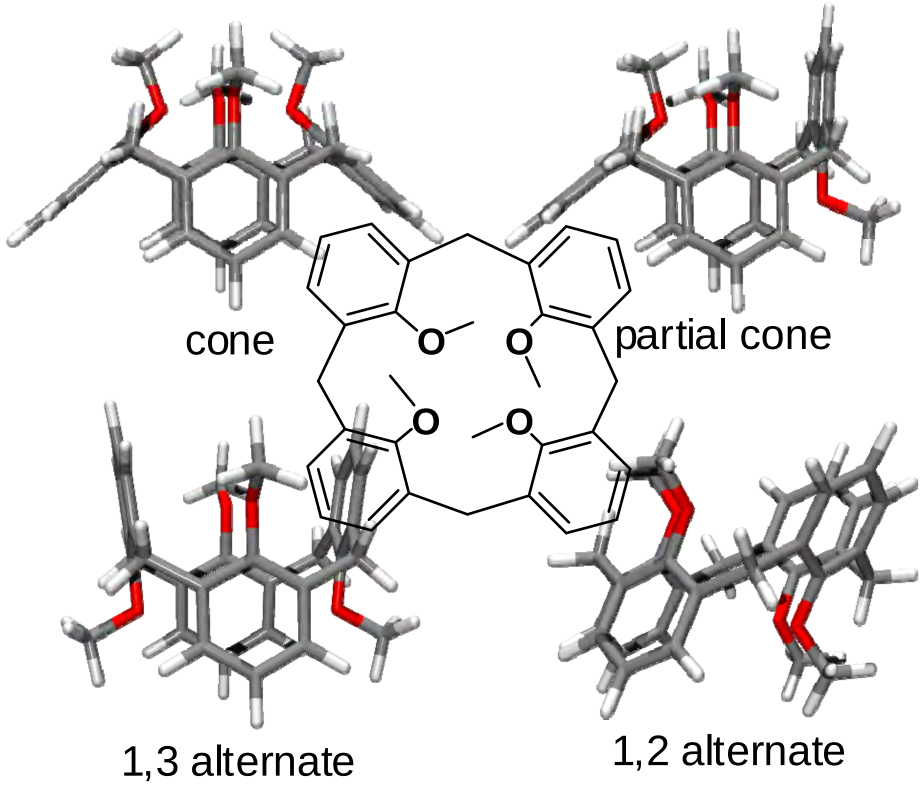
B.Hay, ORNL

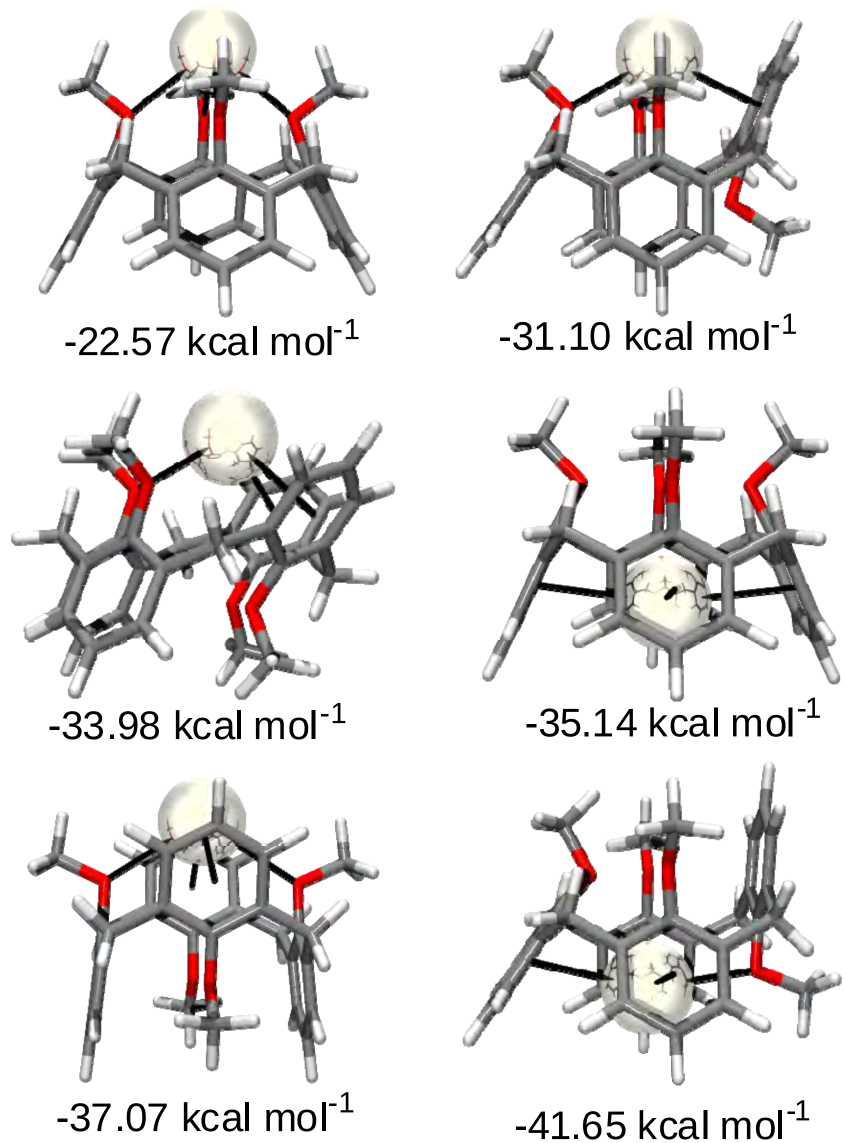
Computer-aided ligand development



B.Hay, ORNL

Electronic structure (quantum mechanics) models



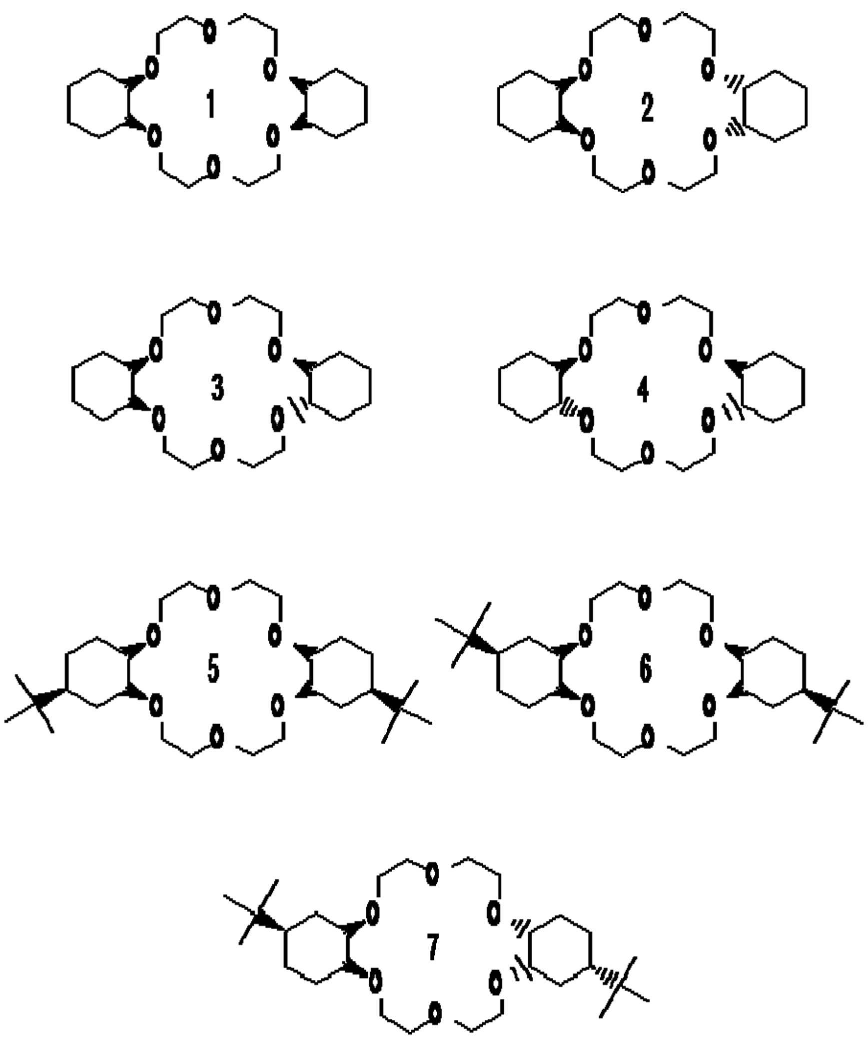


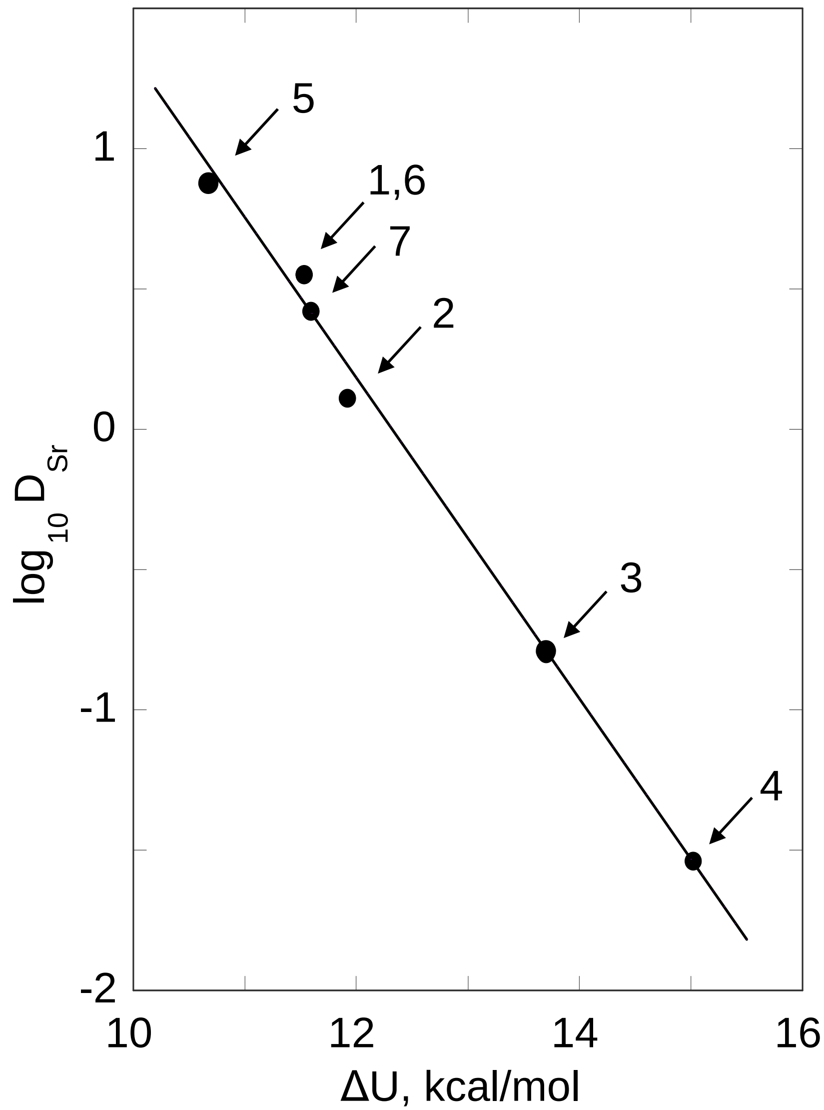
Geometry optimized B3LYP/6-31+G*
Single point energies MP2/aug-cc-pVDZ

50,000 cpu/hr on EMSL MPP1
(6 cpu/yr for 10 structures)

B.Hay, ORNL

Experimental validation

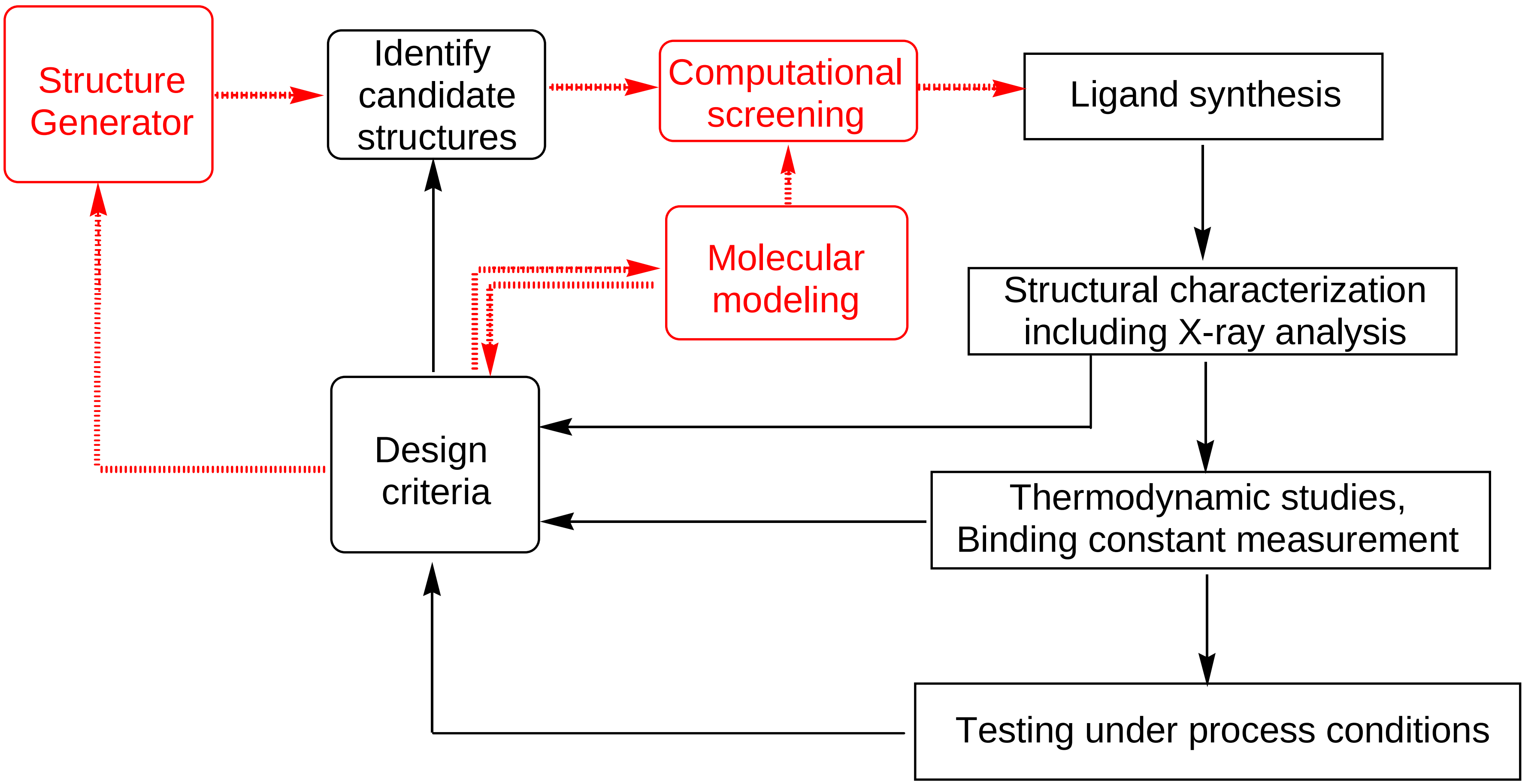




Extraction of Sr^{2+} from 1M HNO_3 using 0.1 M ligand in n-octanol, 25 °C

B.Hay, ORNL

Computer-aided ligand design



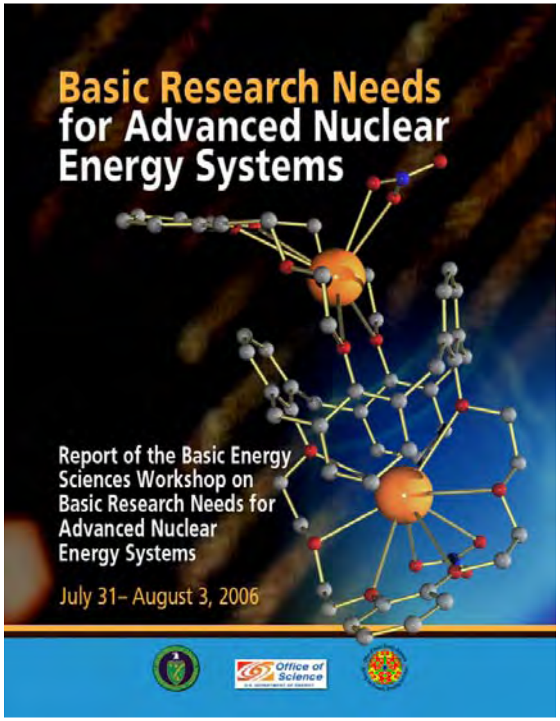
B.Hay, ORNL

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

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

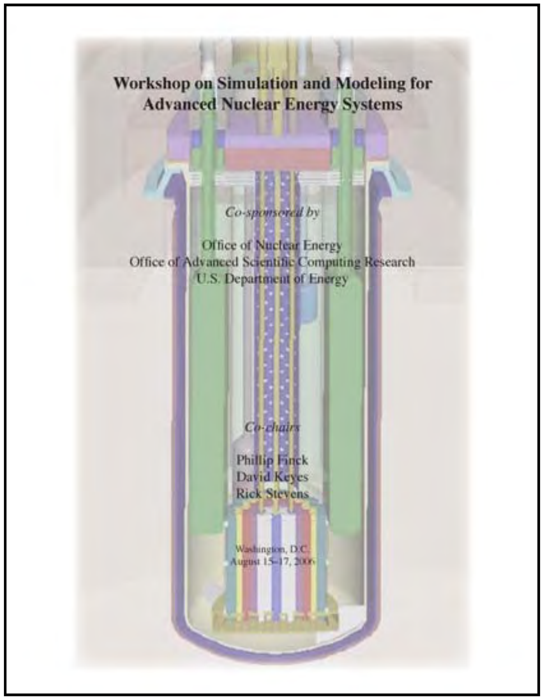
- **Scientific Grand Challenges**
  - ***Resolving the f-electron challenge to master the chemistry and physics of actinides and actinide-bearing materials.***
  - ***Developing a first-principles, multiscale description of material properties in complex materials under extreme conditions.***
  - ***Understanding and designing new molecular systems to gain unprecedented control of chemical selectivity during processing.***
- **Priority Research Directions**
  - ***Physics and chemistry of actinide-bearing materials and the f-electron challenge.***
  - ***Microstructure and property stability under extreme conditions.***
  - ***Mastering actinide and fission product chemistry under all chemical conditions.***
  - ***Exploiting organization to achieve selectivity at multiple length scales.***
  - ***Adaptive material-environment interfaces for extreme chemical conditions.***
  - ***Fundamental effects of radiation and radiolysis in chemical processes.***
  - ***Predictive multiscale modeling of materials and chemical phenomena in multi-component systems under extreme conditions***
- **Crosscutting Research Themes**
  - ***Tailored nanostructures for radiation-resistant functional and structural materials.***
  - ***Solution and solid-state chemistry of 4f and 5f electron systems.***
  - ***Physics and chemistry at interfaces and in confined environments.***
  - ***Physical and chemical complexity in multi-component systems.***



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

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

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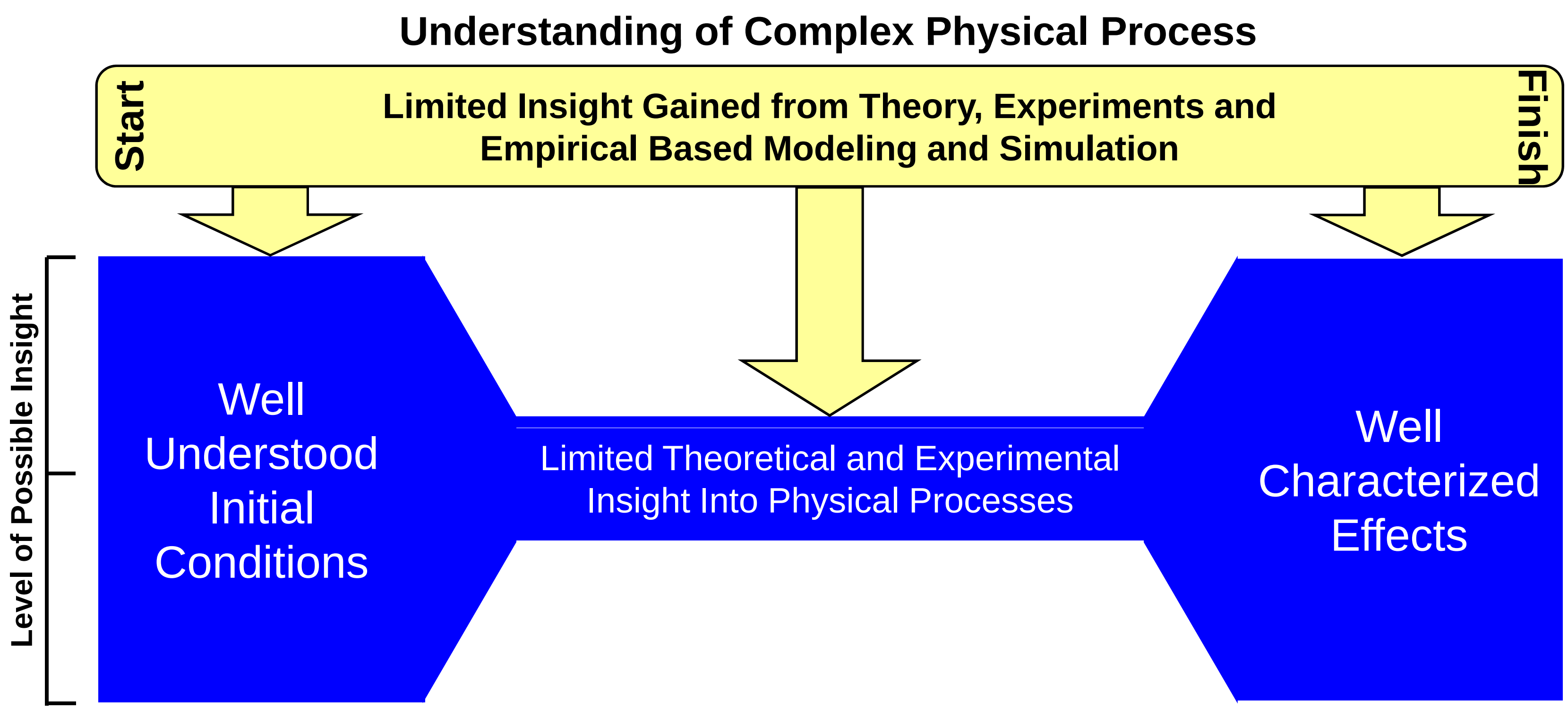
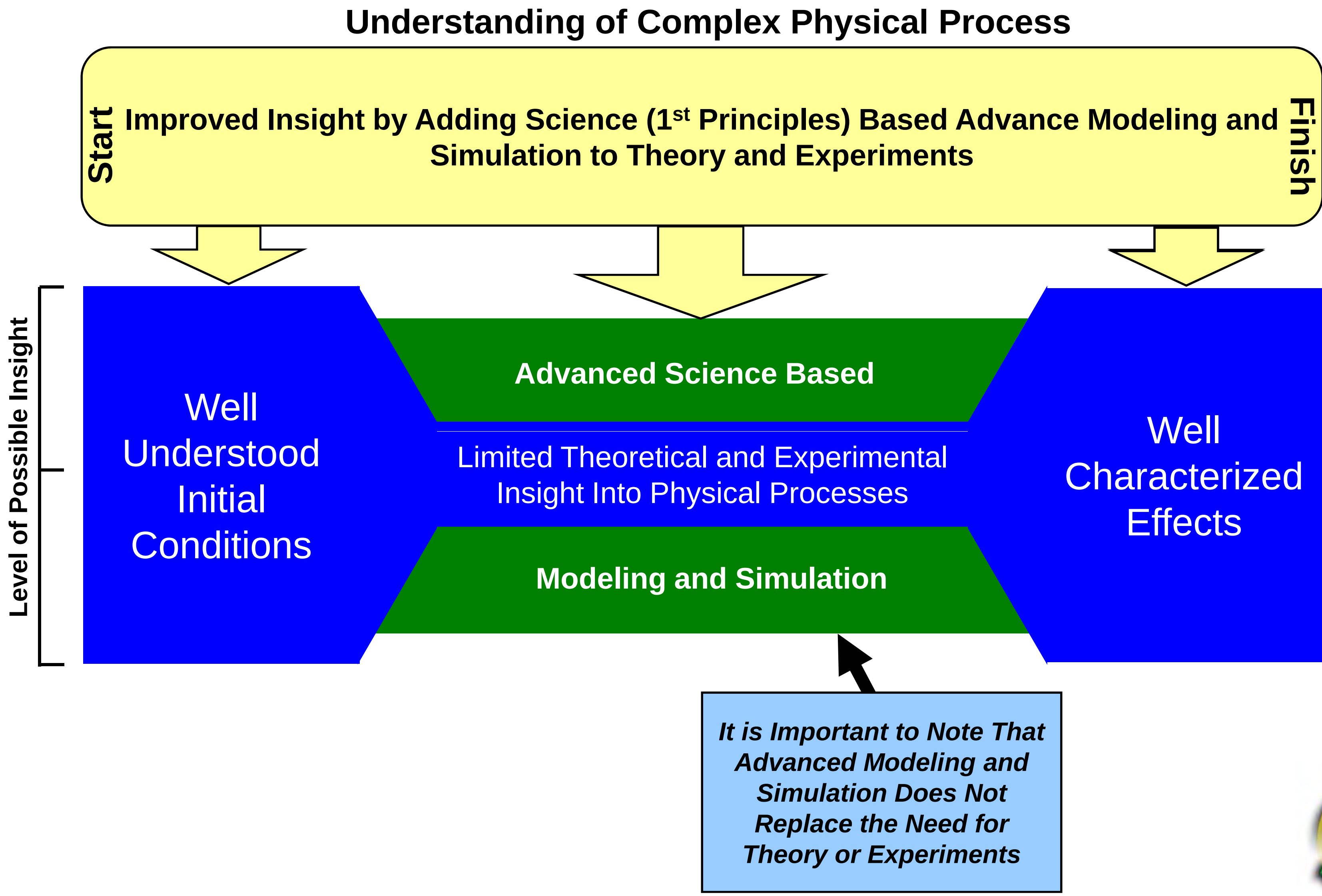
Improving Our Vision into Complex Physical Processes



A. Larzelere, DOE-NE

Improving Our Vision into Complex Physical Processes

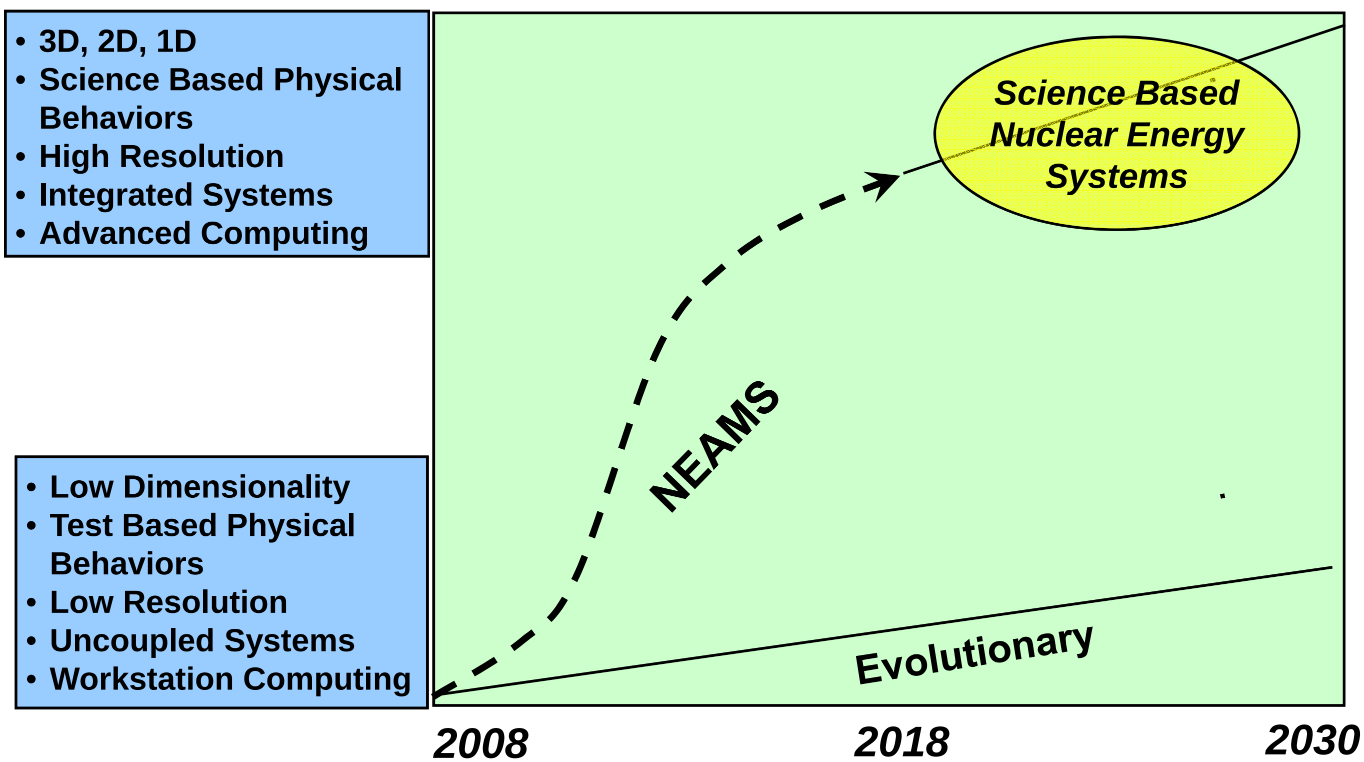


A. Larzelere, DOE-NE

Stepping Up to the New Level of Understanding!

NEAMS Vision

To rapidly create, and deploy next generation, verified and validated nuclear energy modeling and simulation capabilities for the design, implementation, and operation future nuclear energy systems to improve the U.S. energy security future.



A. Larzelere, DOE-NE

Nuclear Energy Advanced Modeling and Simulation (NEAMS)

FY-10 Proposed Program Overview

Nuclear Fuels
Reactor Core & Safety
Separations and Safeguards
Waste Forms and Near Field Repositories

Strategies

- **Integrated Performance & Safety Codes (IPSC)** – High resolution, 3D, integrated systems codes to predict performance
- **Fundamental Methods and Models (FMM)** – Lower length scale performance understanding
- **Verification, Validation & Uncertainty Quantification (VU)** – Understanding the "believability" of simulation results
- **Capability Transfer (CT)** – Moving modeling and simulation tools out of the research environment
- **Enabling Computational Technologies (ECT)** – Computer science resources needed to make the vision a reality

Major Milestones

- **Year 1**
  - Create product requirement documents for integrated codes
  - Initiate robust interaction with NRC on V&V and UQ
  - Establish overall plans and processes for FMM, CT and ECT el
- **Year 3**
  - Deliver initial versions of integrated codes and modeling and simulation interoperability framework
- **Year 5**
  - Deliver integrated codes with proper V&V and UQ pedigrees
- **Year 7**
  - Deliver codes with empirical "knobs" removed
- **Year 10**
  - Deliver predictive, science based modeling and simulation capabilities for new nuclear energy systems

Approach

- Built on a **robust experimental program** for model development and V&V
- **Appropriate flexibility** so that the simulation tools are applicable to a variety of nuclear energy system options and fuel cycles
- **Continuously deliver** improved modeling and simulation capabilities relevant to existing and future nuclear systems (in the near, mid, and long term)

A. Larzelere, DOE-NE

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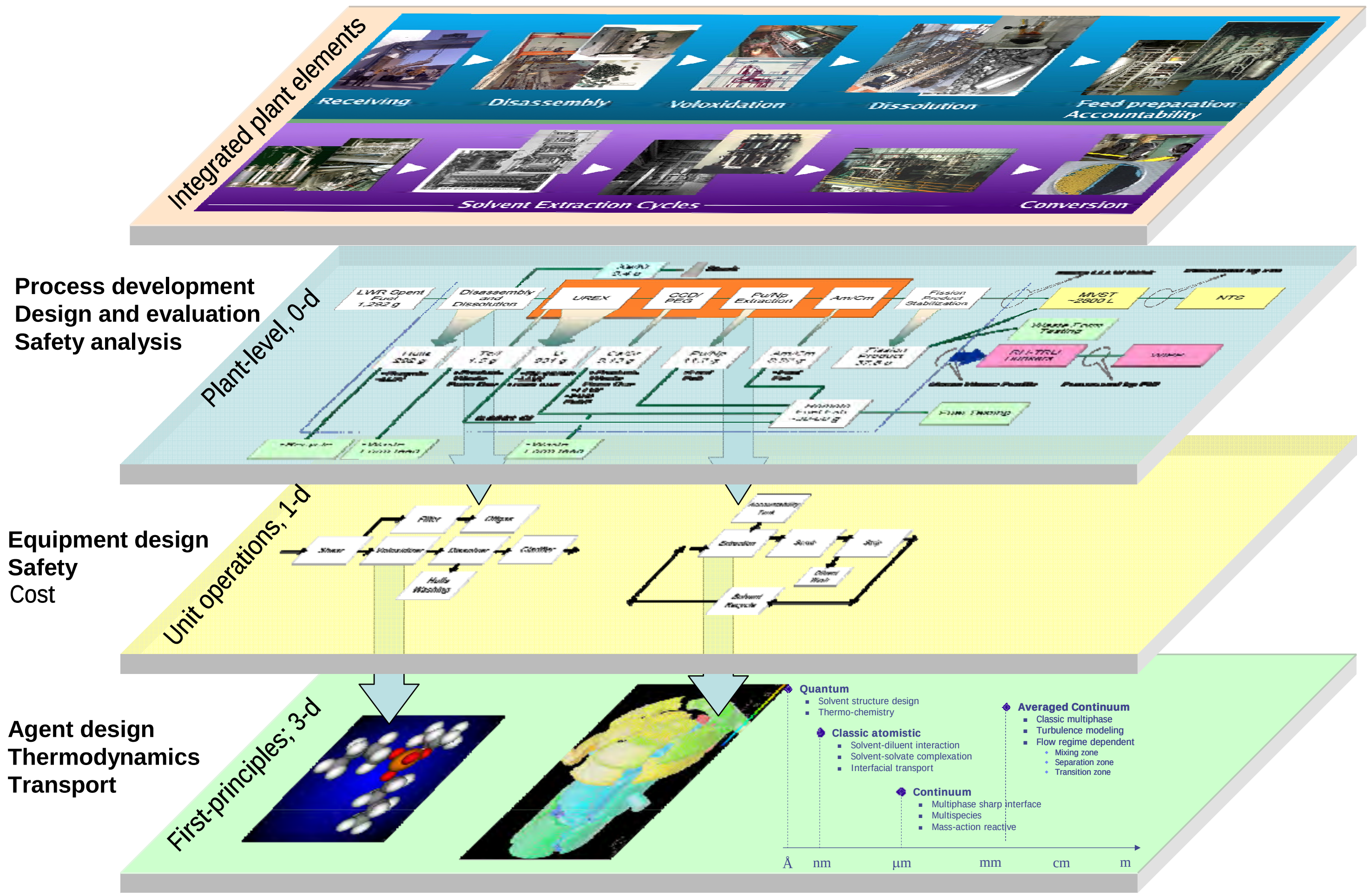
    - Solvent extraction
      - Continuum
      - Molecular-level
    - Visualization with interactive models

Separations M&S development

A primary goal is the development of an integrated plant model that allows dynamic simulations of the operation of separations plants of various configurations and operating conditions. Subscale models to provide required fidelity in chemical and physical processes.



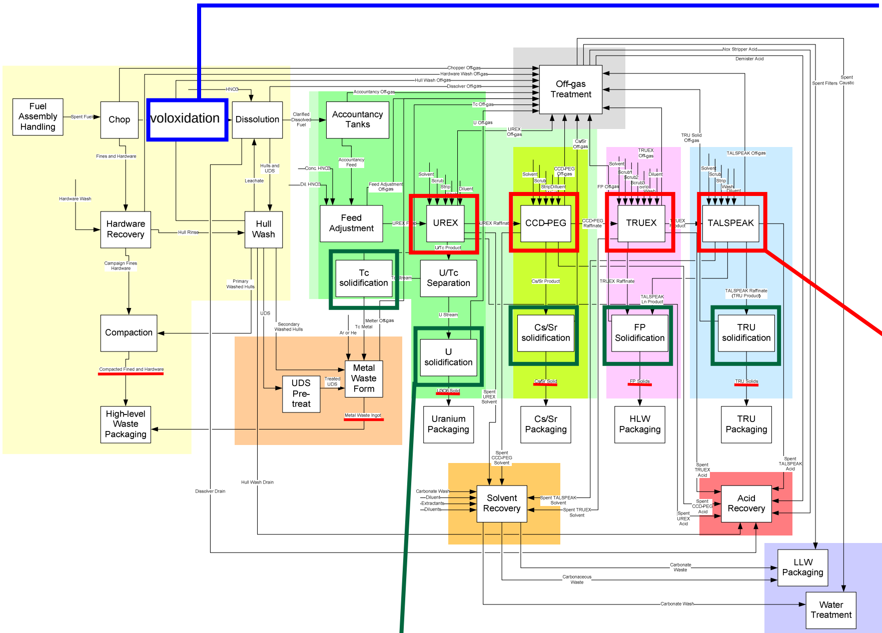
Needs

Integrated, transient plant simulator
Modern, expandable architecture
Bridging to detailed models

Improved models of multicomponent, multiphase unit operations
- Solvent extraction contactors, dissolvers, etc.
- Electrochemical separators
- Voloxidizers, calciners, etc.

Detailed models
- Thermodynamic and physical properties
- Chemistry fundamentals
- Transport in multiphase, reactive flows

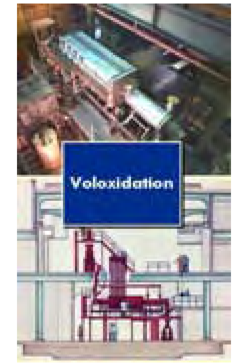
Some Priority Unit Operations



Voloxidation –treatment of chopped oxide fuel with oxygen or ozone at high temperature to drive off tritium and other volatile fission products.

Technical issues – uncertainty in design/scale-up of process and operating conditions to ensure sufficient FP volatilization from a variety of fuels; validate opportunity to simplify flow sheet.

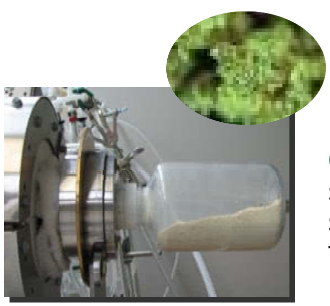
M&S issues: Many common to **fuel performance**; fuel chemistry and reactions, grain structure evolution, fission-product transport, etc.



Solvent extraction – contacting of solutions containing dissolved fuel components with immiscible solutions containing selective separating agents.

Technical issues: uncertainty in design of process and operating conditions to ensure scale-up

M&S issues: multicomponent, multiphase, reactive transport; performance affected by molecular-level processes, including interfacial phenomena, degradation of separating agents by radiolysis and hydrolysis, etc.



Calcination – high-temperature conversion of solutions containing separated species into solids suitable for **fuel and waste form** fabrication.

Technical issues – design and scale-up of process for production of solids with desired particle size, density, homogeneity, etc.

M&S issues –multiphase (solid/liquid/gas) flow, heat transfer, nucleation and growth of solids

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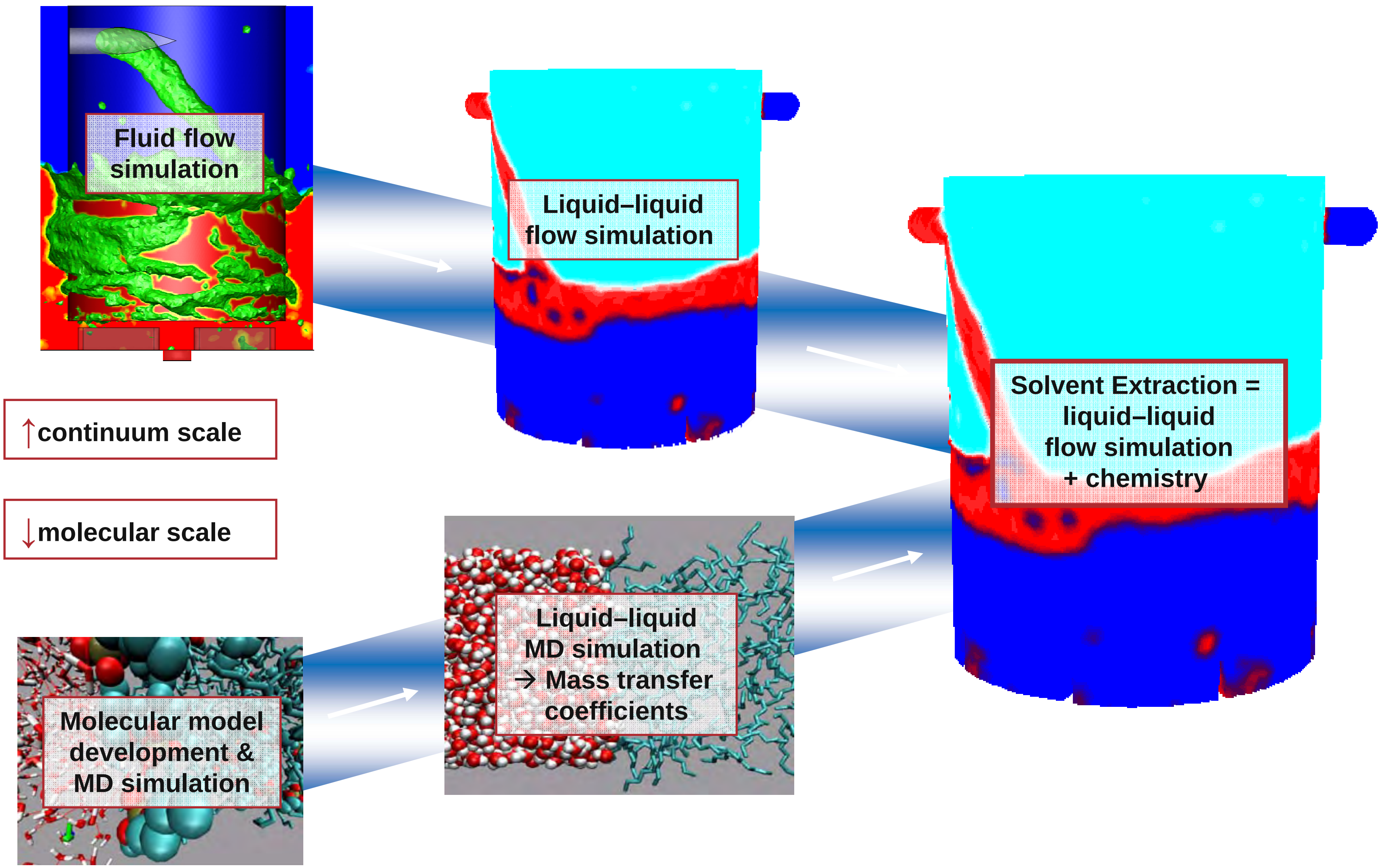
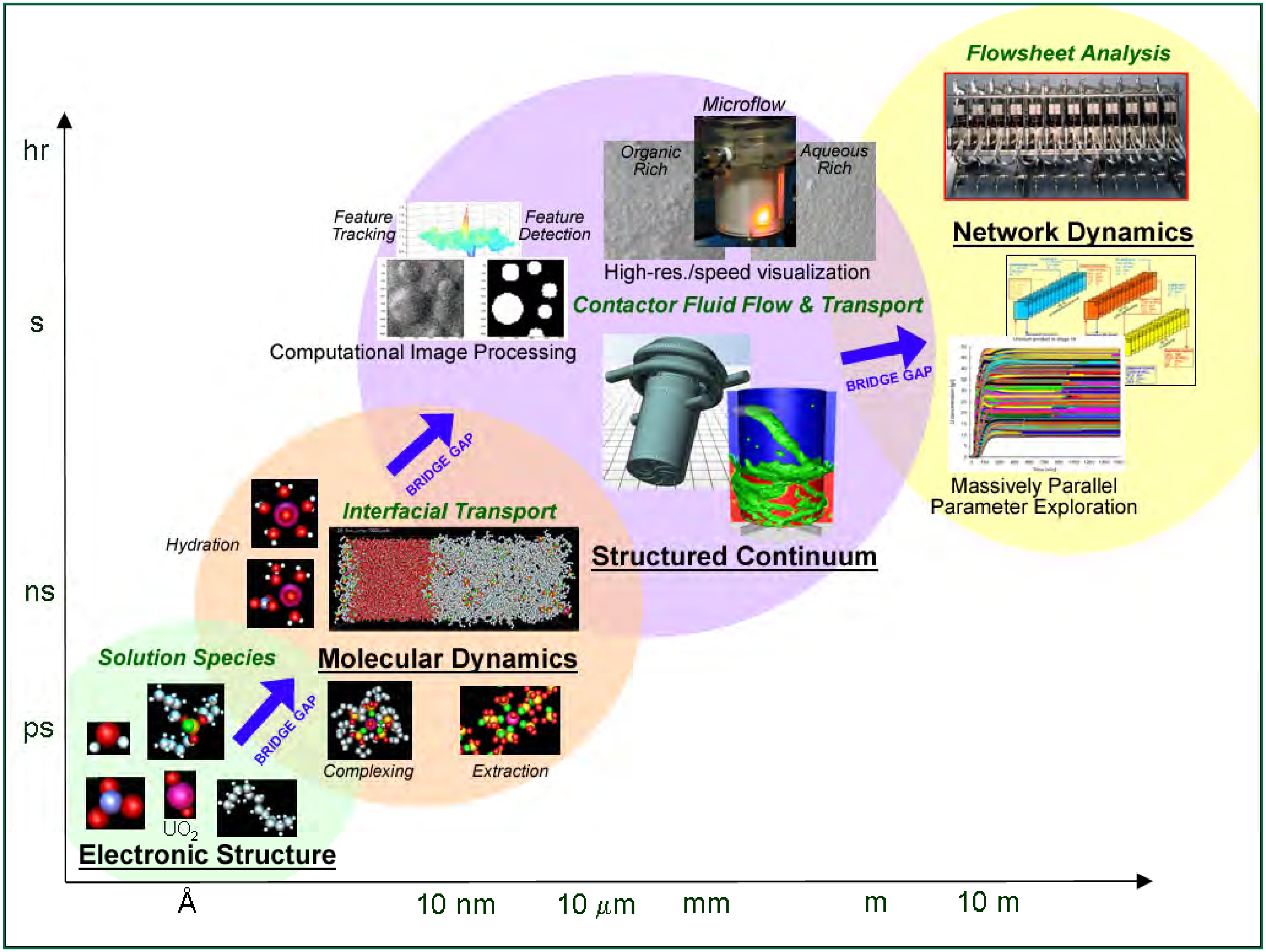
Simulation of Solvent Extraction—How can it all work?

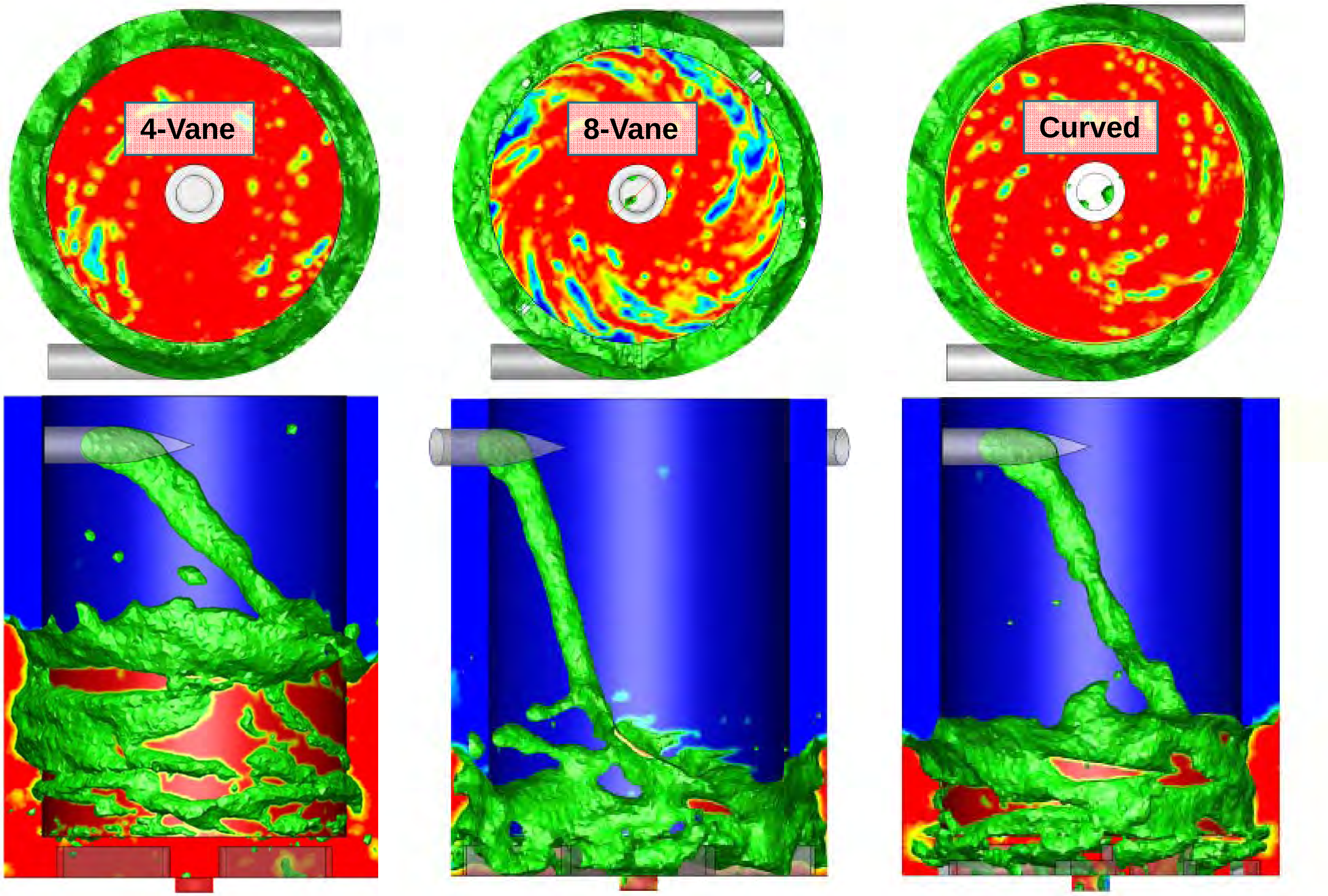


K. Wardle, ANL

Modern M&S for Solvent Extraction



Comparison of effect of vane geometry on mixing



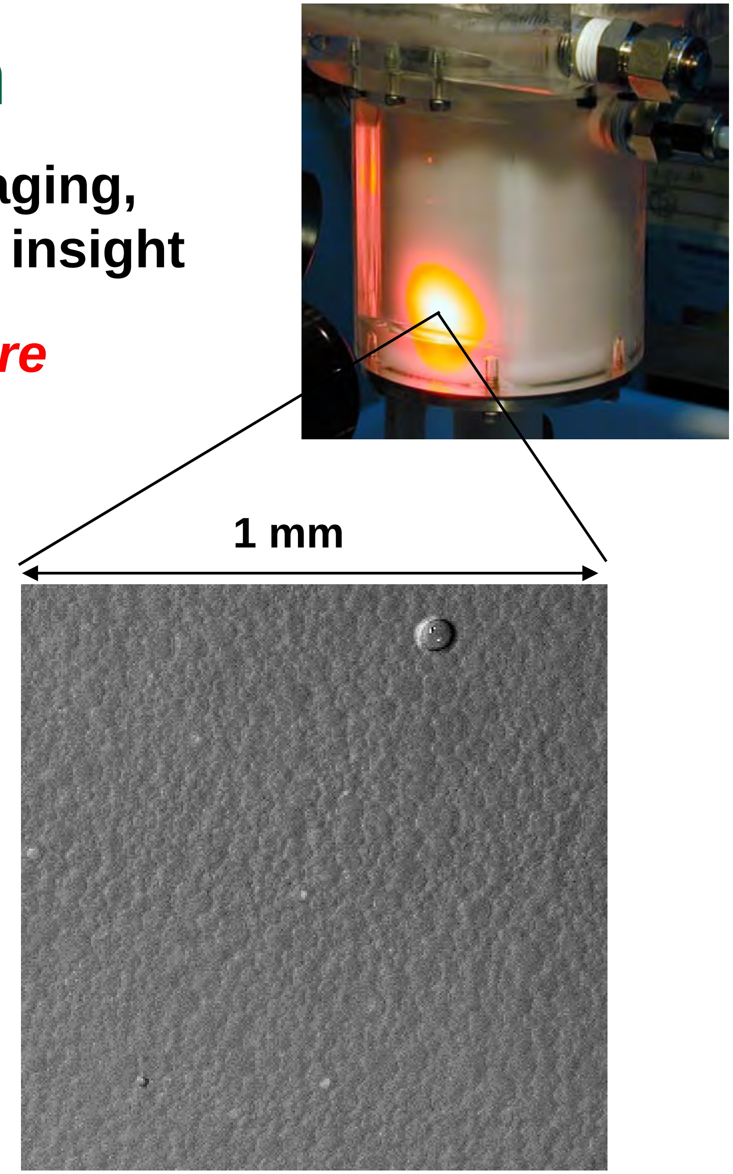
K. Wardle, ANL

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***
- ***Realistic system and operating conditions***

  - **Contactor rotation: 2500 rpm**
  - **Aqueous flow rate:** 300 mL/min
  - **Organic flow rate:** 300 mL/min
  - **Organic:** 30% by volume TBP in dodecane
  - **Aqueous:** 1 *M* HNO_3

  - **Framing:** 5400 fps (185 μs between frames)
  - **Exposure:** 24 μs
  - **Field of view:** ~3.5 mm
  - **Spatial resolution:** ~7 μm
  - **Elapsed time:** 37 ms (200 frames)



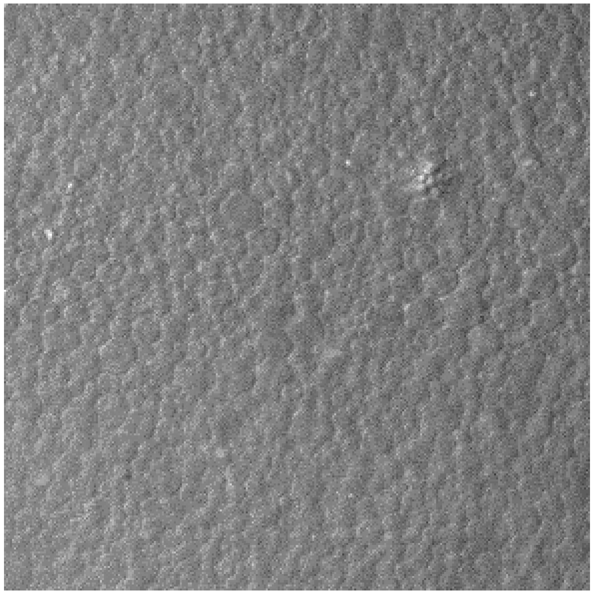
seeing is believing . . .

V. de Almeida, ORNL

Flow Regime Samples

- **1:5 O/A flow ratio**

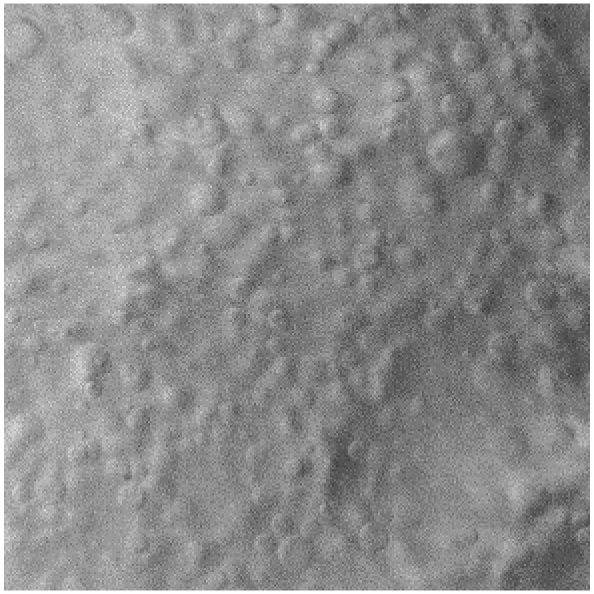
1 mm



• **Elapsed time:** 37 ms (200 frames)

- **5:1 O/A flow ratio**

1 mm



• **Elapsed time:** 18.5 ms (100 frames)

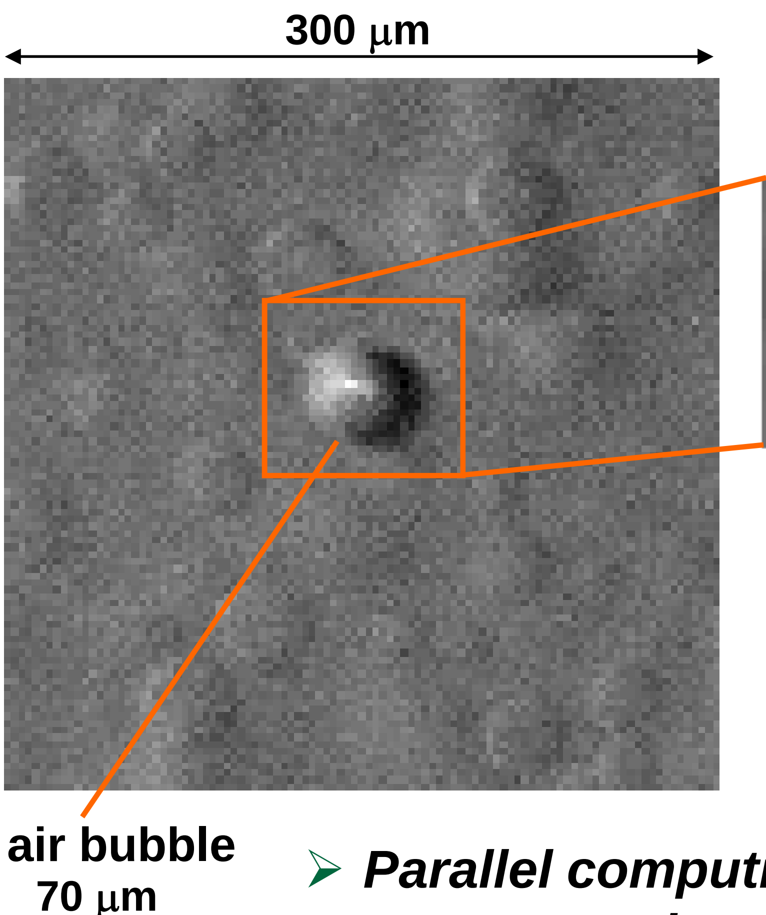
- ***Organic-rich flow regimes possess greater air entrainment***

- ***Identified significant air entrainment in realistic operation for most of the corresponding flow rate ratios***
- ***These videos provide more than insight for modeling . . .***

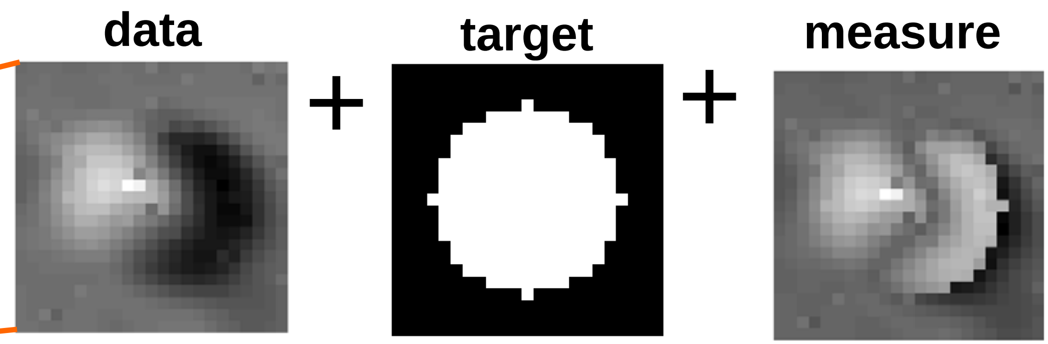
V. de Almeida, ORNL

Computer-Aided Image Analysis for Data

- **Large data sets are obtained (8 GB for 1-s elapsed time)**
- **Can utilize powerful tools of computer image analysis (machine vision)**
  - **Algorithms (filters) and open-source code**



- **Reduce noise and preserve edges**

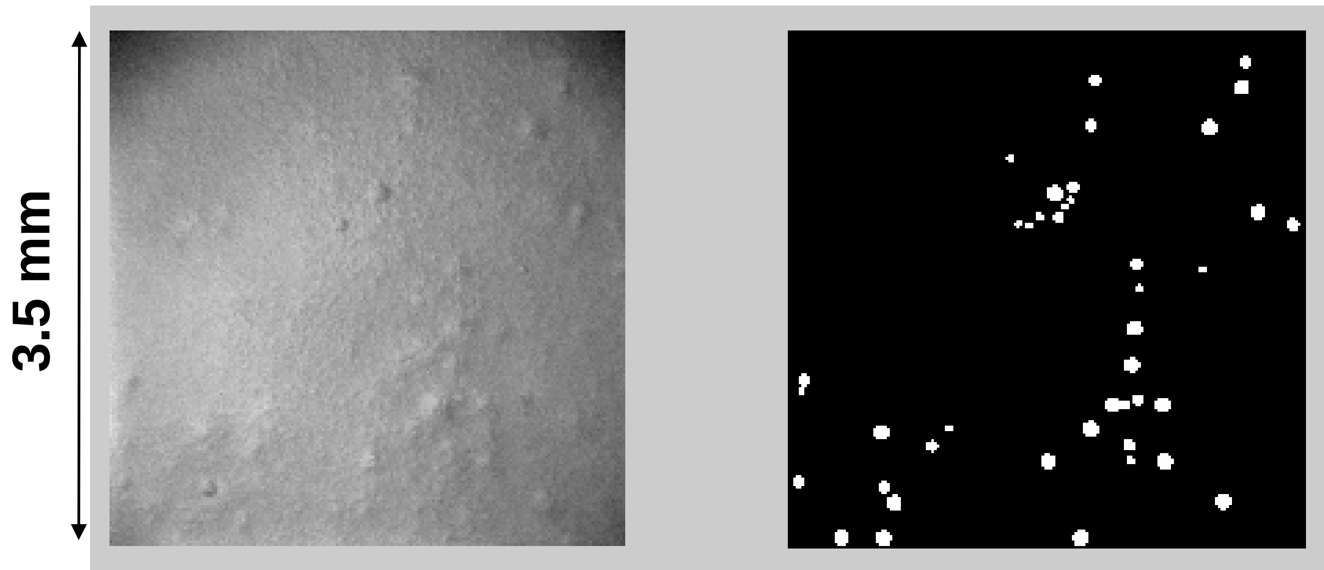


- **Computing intensive**
  - **Need to inspect every pixel and its neighborhood**
  - **Repeat for every target size for every frame**

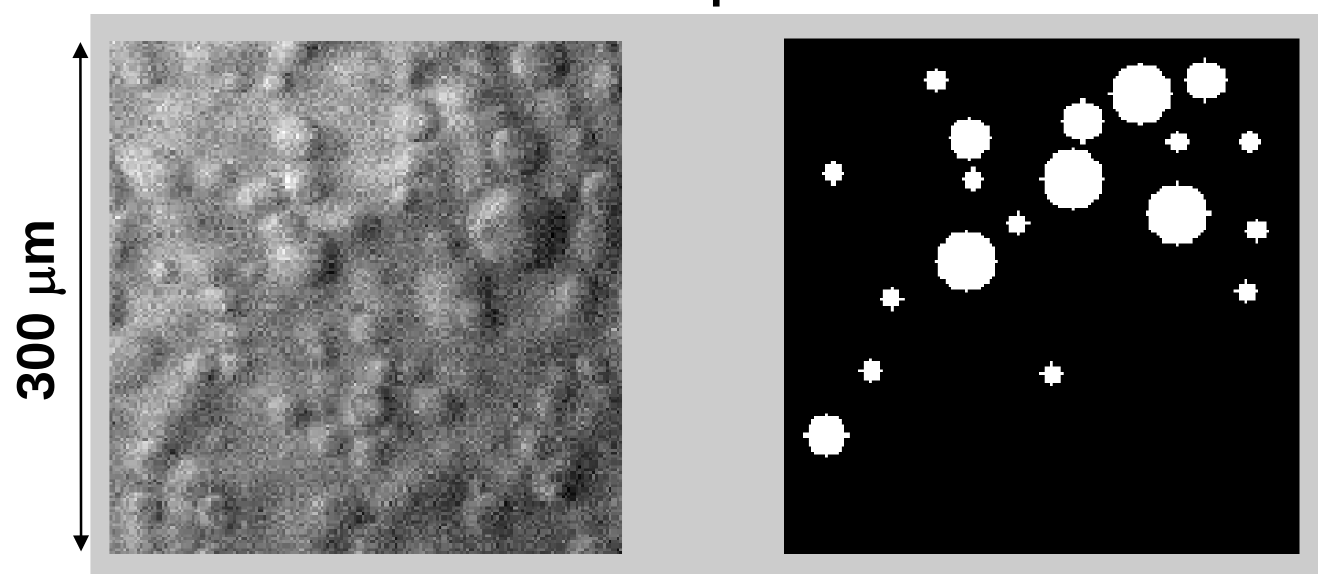
- ***Parallel computing can process large data sets on modest clusters***

V. de Almeida, ORNL

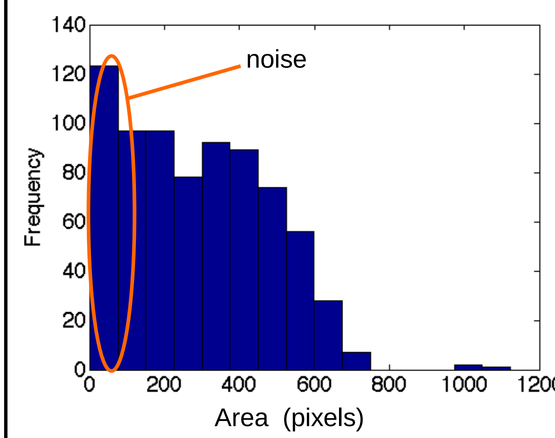
bubbles



drops



Generate data useful for model development



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

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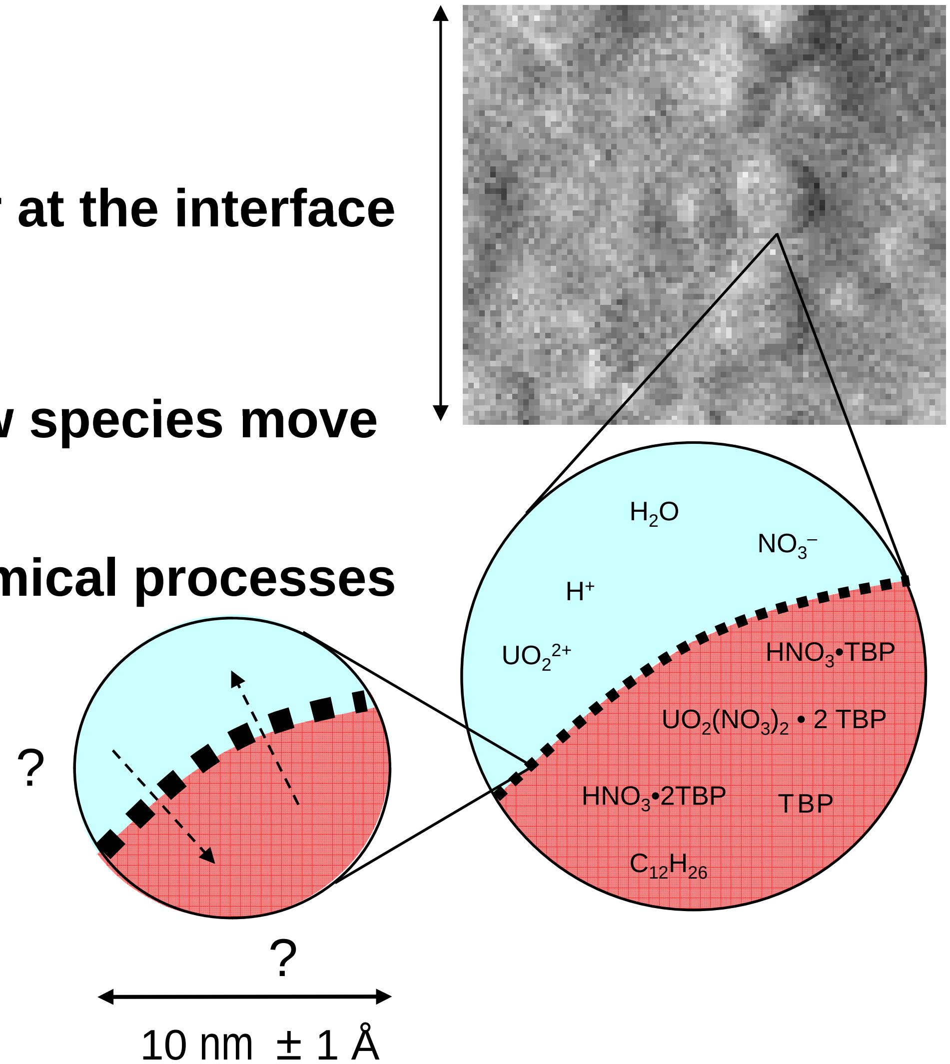
Chemical Transport

- **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

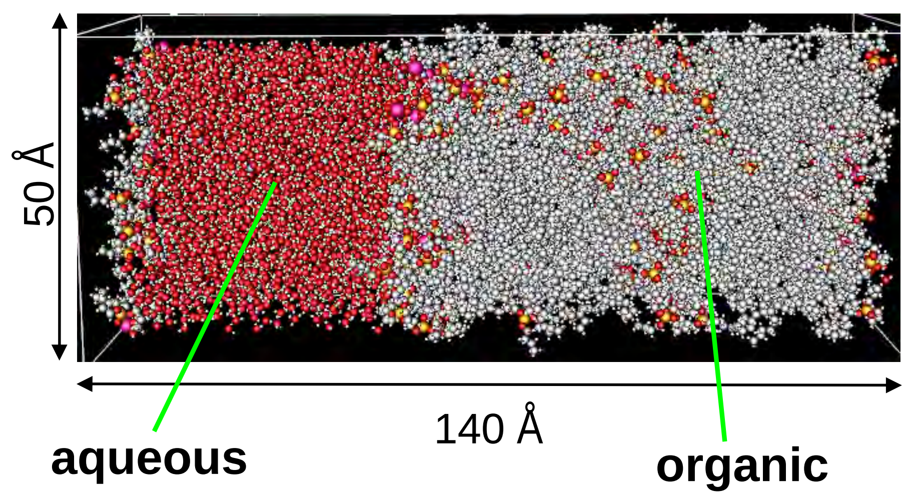
- **Molecular dynamics simulation**
- **Calibration from experimental data**
- **Insight from molecular quantum chemistry calculations when experimental data are not available**

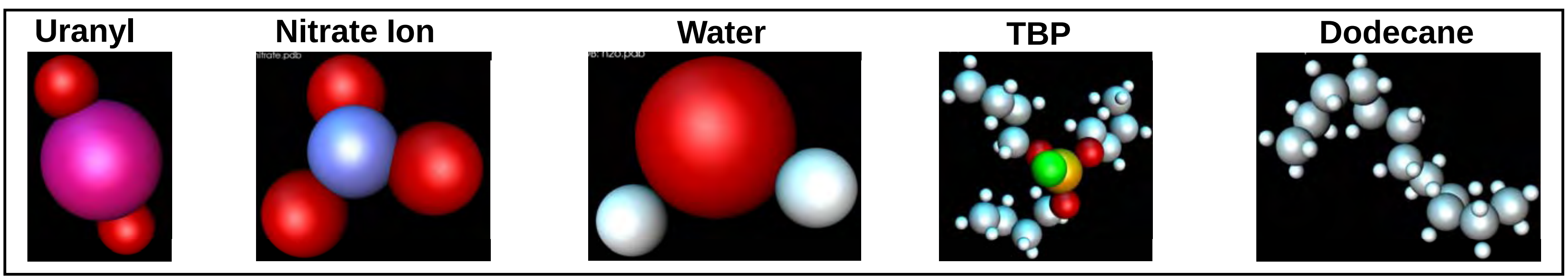
Interfacial Transport "Visualization" by Molecular Dynamics Simulation

- Insight on uranyl nitrate extraction into tributyl phosphate diluted in dodecane

species		# units	# computational atoms/unit
tributyl phosphate	$(BuO)_3PO$	230	17
dodecane	$C_{12}H_{26}$	350	12
uranyl	UO_2^{2+}	18	3
nitrate ion	NO_3^-	36	3
water	H_2O	3,490	4
total		4,124	18,778

- 298.15 K





- All molecular models are of flexible type; no bond constraints

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Status of MD Modeling and Simulation

- **No published MD work on this TBP system in the open literature**
  - **There are similar systems that have different diluents with smaller molecules (e.g. SC CO_2 and $CHCl_3$)**
  - **Dodecane has a different interaction with TBP; the molecule is larger therefore less packing**

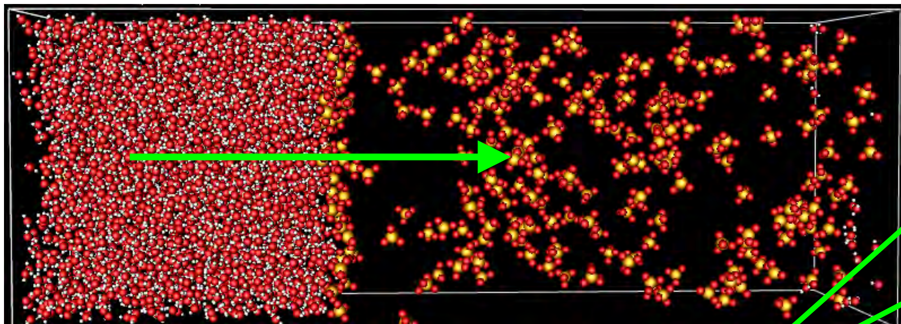
- **Force field for TBP in the literature only from G. Wipff's group; tested with only a few systems**
  - **Charges assigned to atoms from QM electrostatic potential obtained on an isolated molecule**
  - ***A systematic experimental calibration of the MD model is still lacking***

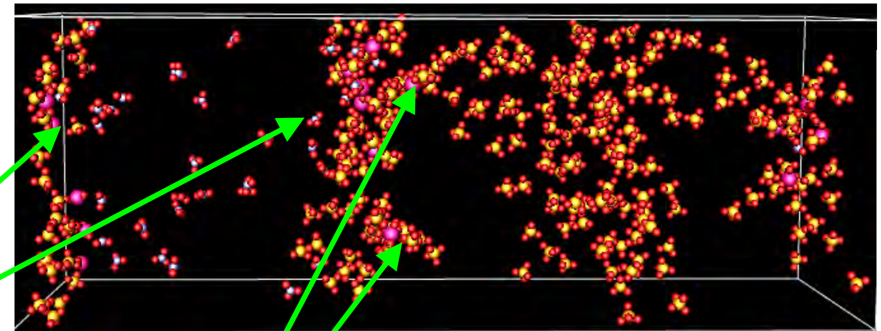
- **Simulations performed so far (mostly, if not only, by G. Wipff's group) are still quite limited in the number of atoms (~4000 atoms)**

➢ Aqueous and organic: TBP butyl tails hidden

t = 0 ns

t = 10 ns





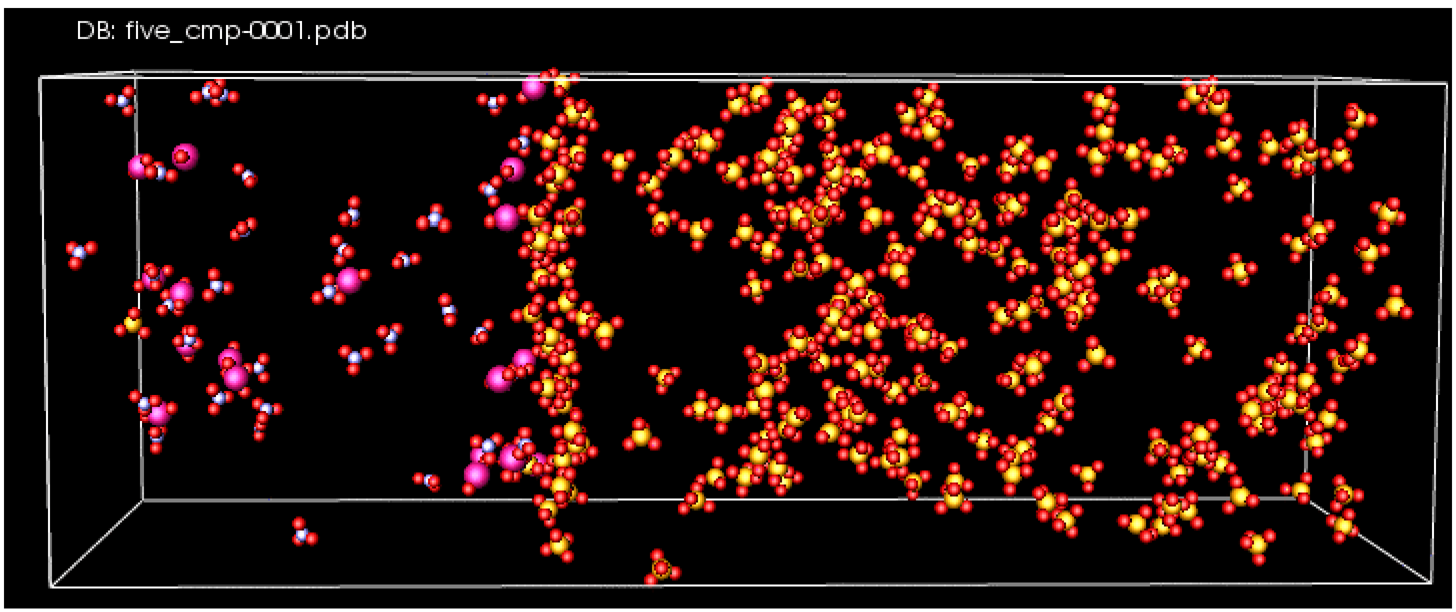
➢ H_2O hidden

➢ 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



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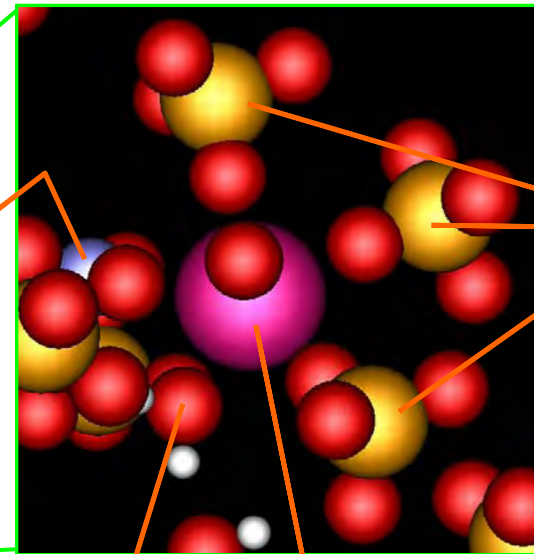
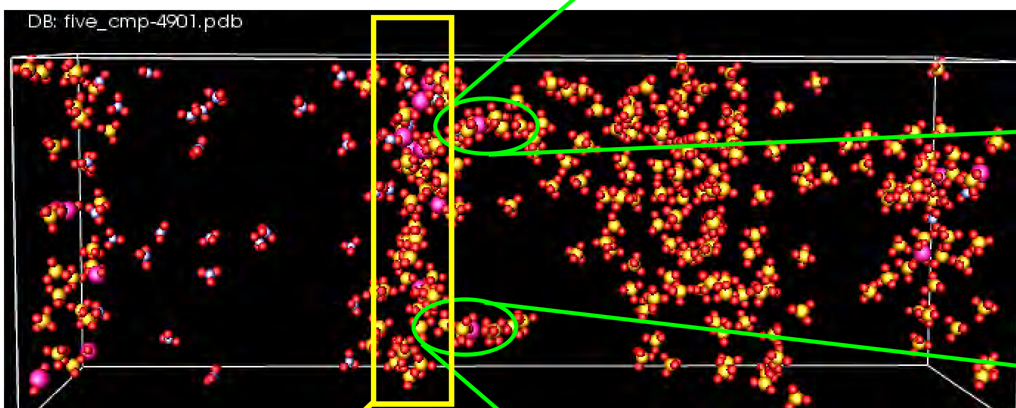
➢ Equatorial coordination of uranyl after crossing the interface

$UO_2^{2+}(NO_3^-)(H_2O)\bullet 3TBP$

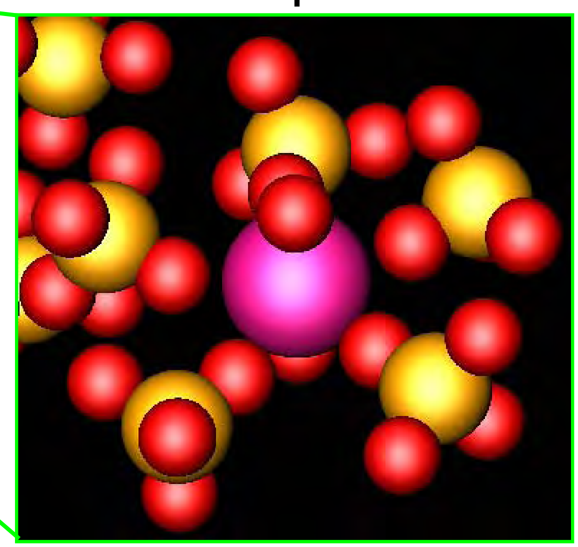


t = 9:8 ns



- “TPB interface thickness” ~10 Å

$UO_2^{2+}\bullet 5\ TBP$



- Bridging mechanism for transporting into the bulk region of the organic phase?

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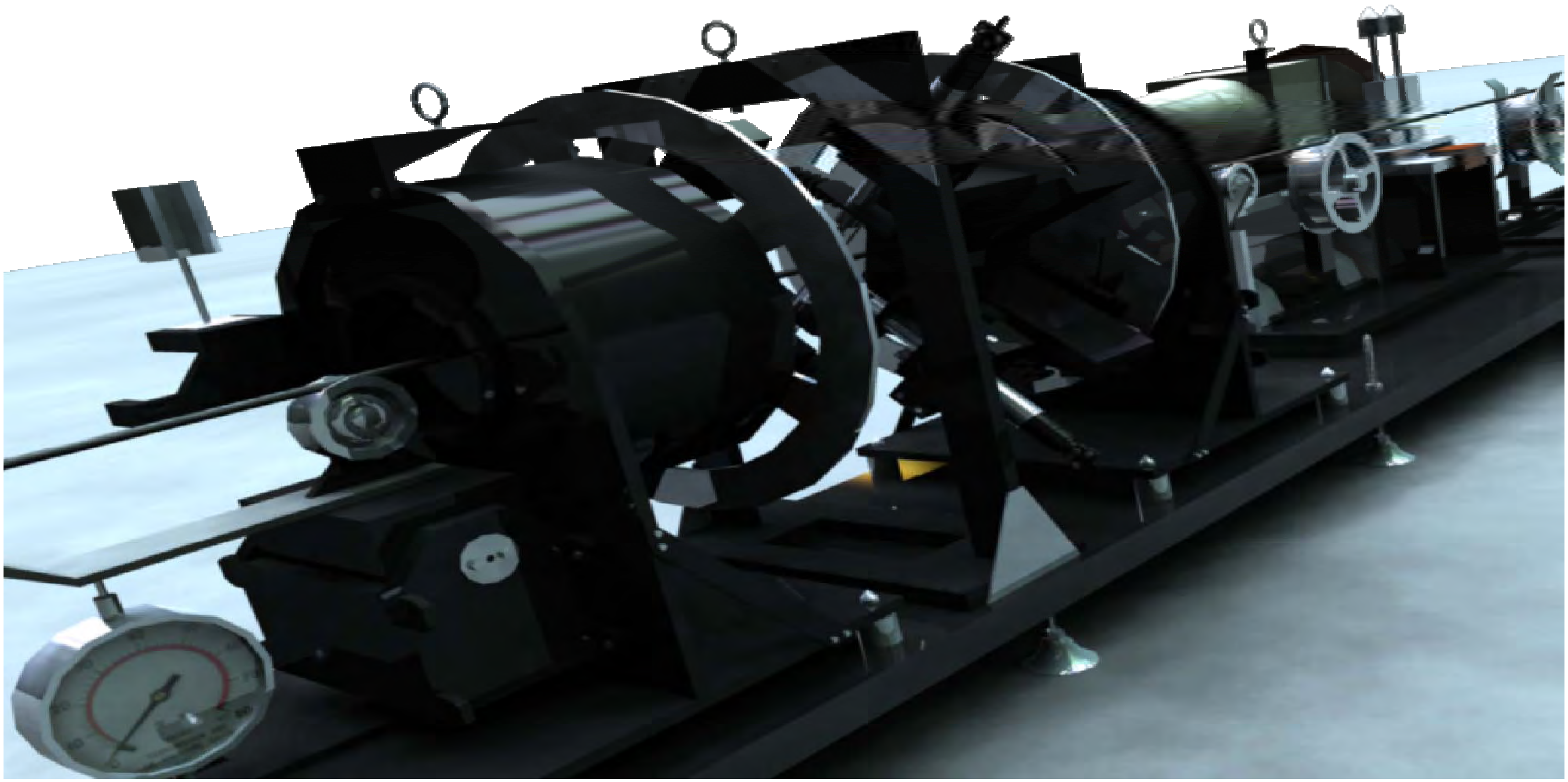
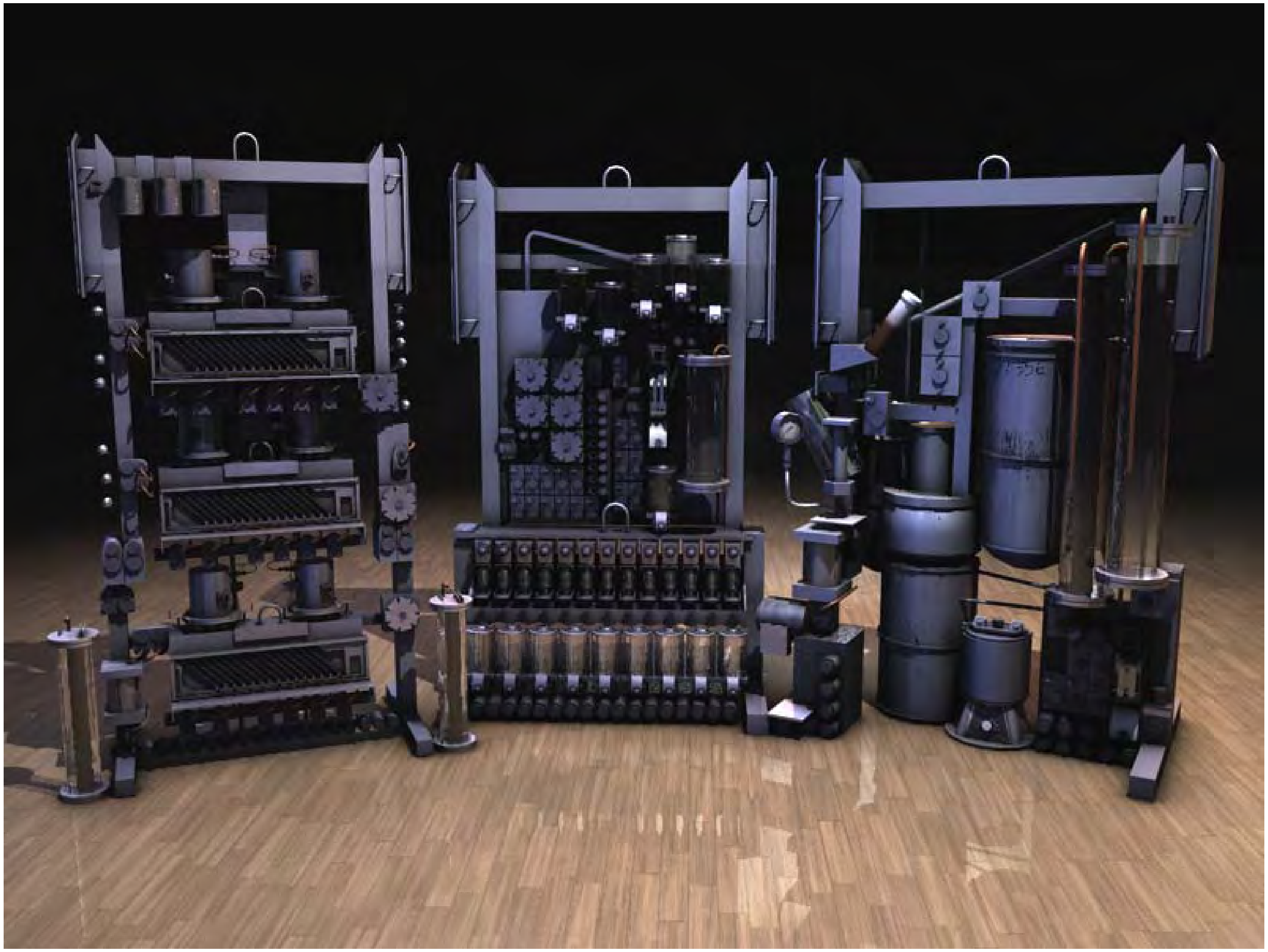
Photorealistic and Physics-Realistic Interactive Models for Test, Evaluation and Analysis



K. Michel, LANL

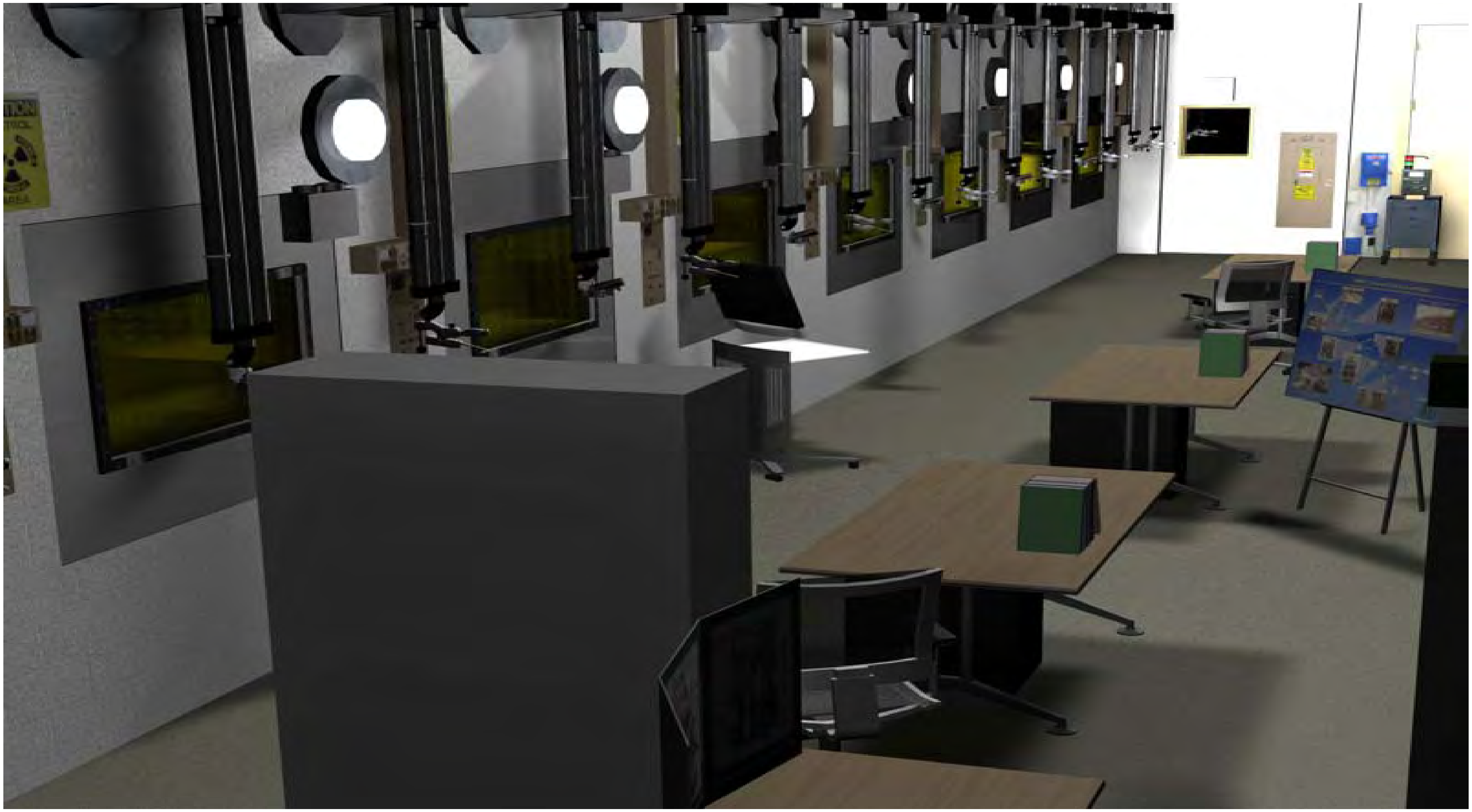
Mixer/Settler Equipment Computer Graphics 3-D Model



- 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

Screenshot from an immersive virtual model



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Visualization in Safeguards

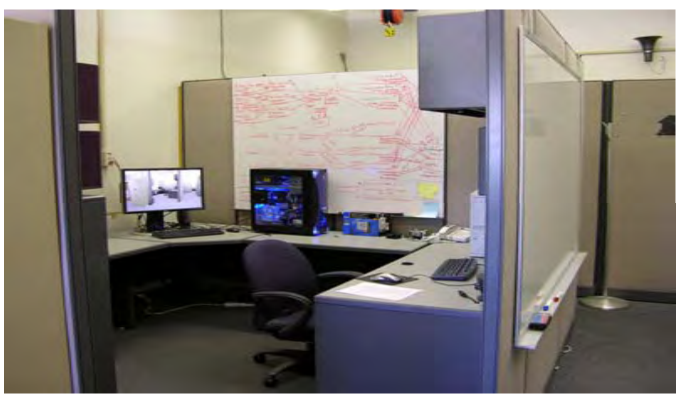
- 3-D models already employed in safeguards
  - Experiments, micro scale - High Performance Computing
    - Power walls
  - IAEA Training
    - Mock Inspection exercises
- Visual models could provide a cost-effective safeguards design and test of a facility design
  - Drop-in toolkit for safeguards implements
  - Integrate numeric models that characterize materials, chemical processes, instruments, detectors
  - Challenge safeguards in virtual environment
    - Where are the planned safeguards weak or effective?
    - Where should the safeguards be improved?
    - Multi-player engagement in an integrated virtual computer locale

Broader Application

- Process design
  - Integrated process simulation with imagery
  - Utilize existing process simulation codes from across DOE complex in a virtual modeled framework
- Training

Real-world vs. Virtual World

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



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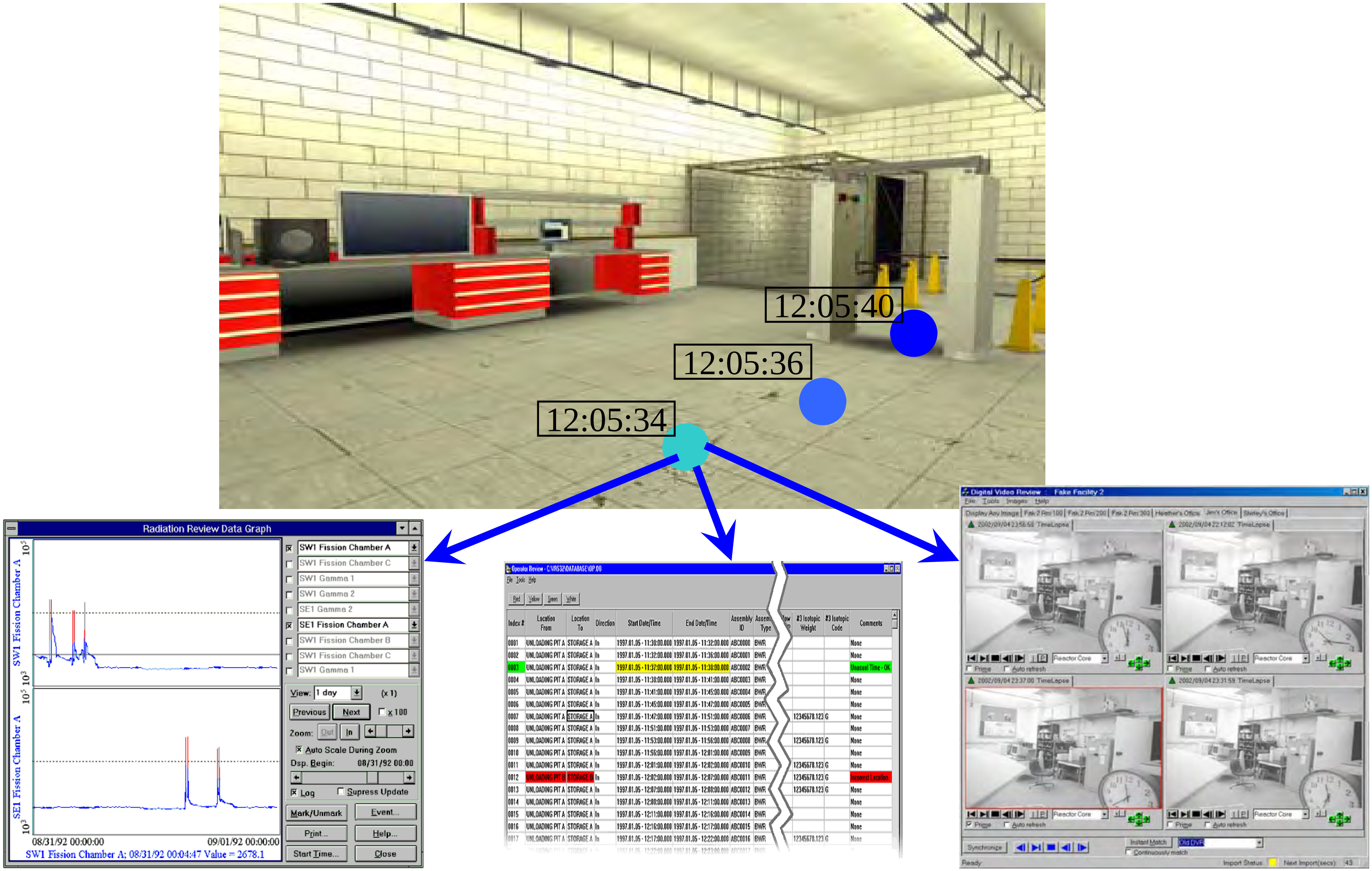
Future Safeguards Data Review Interface: Safeguards Data Shown in Context for Evaluation and Analysis of Events



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.**

Acknowledgments

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Monica Regalbuto

Kent Wardle

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