Role of Modeling and Simulation in Used Fuel Recycling

David DePaoli
Nuclear Science and Technology Division
Oak Ridge National Laboratory

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

VISION models the entire fuel cycle and is an important part of the systems analysis activity

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 with varied composition (burn-up, cooling time) leads to products meeting stringent specifications.

Environmental, safety, accountability constraints:
- Shearing
- Dissolution
- Voloxidation
- Feed & accountability

Processes:
- Solvent extraction cycles
- Off-gas treatment
- Recovery systems
- Solidification
- Waste treatment

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 methods to obtain predictions of process performance.

- “Together modeling and simulation do not replace the need for theory or experiments!!
  - enhance understanding of known systems,
  - 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 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
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
Modeling and simulation of nuclear separations has primarily focused on solvent extraction

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

A. D. Ryon, ORNL-3045, 1961
Equations for interphase mass transfer and material balances converted to computer codes

\[
M^{+a_i}_\text{aq} + a_i NO_3^{-}(\text{aq}) + b_i TBP_{\text{org}} \rightleftharpoons M(NO_3)_a_i \cdot b_i TBP_{\text{org}}
\]

\[
K_i = \frac{[M(NO_3)_a_i \cdot b_i TBP]_{\text{org}}}{[M^{+a_i}_\text{aq}] [NO_3^{-}]_{\text{aq}} [TBP]_{\text{org}}}
\]

Overview of SEPHIS model of solvent extraction stages
Existing models are based on empirical fits to experimental data

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

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

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

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

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

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

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

Rainey and Watson, 1975

With good input data, good predictions are obtained – within conditions of fit
AMUSE Models Solvent Extraction

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

M. Regalbuto and C. Pereira, ANL
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**

M. Regalbuto and C. Pereira, ANL
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

M. Regalbuto and C. Pereira, ANL
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 $1.22 \times 10^9$ calculations

- Large impact from different fuel feeds
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)

Segment of UREX Solvent Extraction Module

M. Regalbuto and C. Pereira, ANL
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

B. Cipiti and N. Ricker, SNL
Traditional Accounting Instrumentation (Baseline)

B. Cipiti and N. Ricker, SNL
Additional Accounting Instrumentation (Advanced)

Red  Traditional Accounting
Green Process Monitoring
Blue  Advanced Monitoring

B. Cipiti and N. Ricker, SNL
Pu Inventory Difference

(Baseline)  

(Advanced)  

B. Cipiti and N. Ricker, SNL
Diversion Scenario

(Baseline)

(Advanced)

B. Cipiti and N. Ricker, 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.
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
Sequestering agents are the basis for separations.
Experimental development is slow and expensive

- Identify candidate structures
  - Optimize: binding affinity, selectivity, solubility, stability, cost

- Design criteria

- Ligand synthesis

- Structural characterization including X-ray analysis
  - Thermodynamic studies, binding constant measurement
  - Testing under process conditions

B. Hay, ORNL
Influence of ligand architecture

Large effects on binding affinity:

\[ 10^{10} \quad 10^6 \quad 10^5 \quad 10^3 \]

and significant impacts on selectivity:

\[ \frac{\text{Hg}^{2+}/\text{Cu}^{2+}}{5} \quad \frac{\text{Cu}^{2+}/\text{Hg}^{2+}}{10^4} \quad \frac{\text{Eu}^{3+}/\text{Al}^{3+}}{13} \quad \frac{\text{Al}^{3+}/\text{Eu}^{3+}}{500} \]

B.Hay, ORNL
Computer-aided ligand development

- Identify candidate structures
- Computational screening
- Molecular modeling
- Design criteria
- Ligand synthesis
- Structural characterization including X-ray analysis
- Thermodynamic studies, Binding constant measurement
- Testing under process conditions

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)
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

- Structure Generator
- Identify candidate structures
  - Computational screening
  - Molecular modeling
  - Design criteria

- Ligand synthesis
  - Structural characterization including X-ray analysis
  - Thermodynamic studies, Binding constant measurement
  - Testing under process conditions

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
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
Improving Our Vision into Complex Physical Processes

Understanding of Complex Physical Process

Start
Limited Insight Gained from Theory, Experiments and Empirical Based Modeling and Simulation

Well Understood Initial Conditions
Limited Theoretical and Experimental Insight Into Physical Processes

Well Characterized Effects

Finish
A. Larzelere, DOE-NE
Improving Our Vision into Complex Physical Processes

Understanding of Complex Physical Process

Start
Improved Insight by Adding Science (1st Principles) Based Advance Modeling and Simulation to Theory and Experiments

Finish

Well Understood Initial Conditions
Advanced Science Based
Limited Theoretical and Experimental Insight Into Physical Processes
Modeling and Simulation
Well Characterized Effects

Level of Possible Insight

It is Important to Note That Advanced Modeling and Simulation Does Not Replace the Need for Theory or Experiments

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.

- 3D, 2D, 1D
- Science Based Physical Behaviors
- High Resolution
- Integrated Systems
- Advanced Computing

- Low Dimensionality
- Test Based Physical Behaviors
- Low Resolution
- Uncoupled Systems
- Workstation Computing

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

- **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
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**
    • Solvent extraction
      – Continuum
      – Molecular-level
    • Visualization with interactive models
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.

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
    - Solvent extraction
      - Continuum
      - Molecular-level
    - Visualization with interactive models
Simulation of Solvent Extraction—How can it all work?

Fluid flow simulation

Liquid–liquid flow simulation

Solvent Extraction = liquid–liquid flow simulation + chemistry

↑ continuum scale

↓ molecular scale

Molecular model development & MD simulation

Liquid–liquid MD simulation → Mass transfer coefficients

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 HNO₃
  - 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 . . .
Flow Regime Samples

- **1:5 O/A flow ratio**
  - Elapsed time: 37 ms (200 frames)

- **5:1 O/A flow ratio**
  - 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
3.5 mm
bubbles

Generate data useful for model development

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

300 μm
drops

Noise

V. de Almeida, 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**
    • Solvent extraction
      – Continuum
      – **Molecular-level**
    • Visualization with interactive models
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

<table>
<thead>
<tr>
<th>species</th>
<th># units</th>
<th># computational atoms/unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>tributyl phosphate</td>
<td>230</td>
<td>17</td>
</tr>
<tr>
<td>dodecane</td>
<td>350</td>
<td>12</td>
</tr>
<tr>
<td>uranyl</td>
<td>18</td>
<td>3</td>
</tr>
<tr>
<td>nitrate ion</td>
<td>36</td>
<td>3</td>
</tr>
<tr>
<td>water</td>
<td>3,490</td>
<td>4</td>
</tr>
<tr>
<td>total</td>
<td>4,124</td>
<td>18,778</td>
</tr>
</tbody>
</table>

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

V. de Almeida, ORNL
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, $t = 10$ ns

- All uranyl adsorbed on interface
- Some nitrate ion also adsorbed
- $\text{H}_2\text{O}$ hidden
- Onset of extraction of $\text{UO}_2^{2+}$, $\text{NO}_3^-$, $\text{H}_2\text{O}$
- Species have crossed the TBP surfactant layer
Equatorial coordination of uranyl after crossing the interface

$\text{UO}_2^{2+} (\text{NO}_3^-)(\text{H}_2\text{O}) \cdot 3\text{TBP}$

$t = 9:8$ ns

"TPB interface thickness" $\sim 10 \text{ Å}$

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

V. de Almeida, 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
    - Solvent extraction
      - Continuum
      - Molecular-level
    - Visualization with interactive models
Photorealistic and Physics-Realistic Interactive Models for Test, Evaluation and Analysis

K. Michel, LANL
• 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
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

K. Michel, LANL
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, 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.
Acknowledgments

Ben Cipiti
Valmor de Almeida
Ben Hay
Bob Jubin
Alex Larzelere

Kelly Michel
Candido Pereira
Monica Regalbuto
Kent Wardle

Prepared by Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, Tennessee 37831-6285, managed by UT-Battelle, LLC, for the U.S. Department of Energy under contract DE-AC05-00OR22725.

The submitted manuscript has been authored by a contractor of the U.S. Government under contract DE-AC05-00OR22725. Accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U.S. Government purposes.

This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.