Simulation of Criticality Accident Transients in Uranyl Nitrate Solution with COMSOL Multiphysics

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Presentation Outline

• Brief background
• Model Introduction
• Governing Equations
  – Point Kinetics
  – Conjugate Heat Transfer
  – Radiolytic Gas Transport
• Results
  – SILENE benchmark
  – “Methodological” Exercise
• Conclusions
Criticality Transients in Solution

- Typical Multiphysics Reactivity Feedbacks:
  - Included in Model: Radiolytic Gas, Thermal Expansion, Temperature (Cross Sections)
  - Not included: Solution Ejection, Sloshing, Boiling, etc.
Model Introduction

• Importance:
  • Fissile solution transients often introduce a strongly time-dependent radiation source term for emergency planning, characterization of which is motivated by ANSI/ANS-8.23-2007, *Nuclear Criticality Accident Emergency Planning and Response*.
  • LA-13638 R2000, *A Review of Criticality Accidents* documents the nature and high frequency of process accidents in fissile solution or slurry.

• Purpose: Develop a “Level 1.5” model of criticality transients in solution
  – Serve as flexible & powerful intermediary between “Level 2” models with full radiation transport & CFD (FETCH) and less exhaustive “Level 1” models (AGNES, CRITEX, TRACE)
Multiphysics Model Structure

- Model Definitions
- Point Kinetics w/ Six Group Precursors
- Conjugate Heat Transfer (Conduction, Convection)
- Radiolytic Gas Migration & Dispersal
- Time-Dependent Results: Power, Energy & Temperature

COMSOL Multiphysics

Point Kinetics Parameters & Reactivity Feedback (MCNP5)

Reactivity Feedback (Doppler, Density Reduction, Void)
# Point Kinetics

## Neutron Kinetics Balance

\[
dP(t) = \frac{\rho(t) - \beta_{\text{eff}}}{\Lambda} P(t) + \sum_{i=1}^{6} \lambda_i C_i(t)
\]

## Delayed Neutron Precursor Concentration

\[
dC_i(t) = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t)
\]

## Reactivity

\[
\rho(t) = \rho_0 + \text{ramp}(t) + \alpha_T \Delta T + \alpha_V \Delta V
\]

- \(P\) fission rate (fission/s)
- \(\rho\) reactivity
- \(\Lambda\) mean neutron generation time (s)
- \(C_i\) DNP concentration (neutrons/m^3)
- \(\lambda_i\) decay constant (1/s)
- \(\beta_i\) delayed neutron fraction
- \(\beta_{\text{eff}}\) = \(\sum_{i=1}^{6} \beta_i\)

- \(T\) temperature
- \(V\) void volume

\[
\alpha_k = \frac{\partial \rho}{\partial k}
\]
Use of MCNP5

• Point Kinetics Parameters
  – Using MCNP5-1.6’s KOPTS card precursor decay rates and delayed neutron fractions ($\lambda_i$’s & $\beta_i$’s) along with mean neutron generation time ($\Lambda$) can be calculated using

• Reactivity Feedback
  – Step changes in reactivity vs. feedback parameters (void, temperature) are used to inform reactivity feedback coefficients ($\alpha_k$’s)
## Point Kinetics

### Neutron Kinetics Balance

\[
\frac{dP(t)}{dt} = \frac{\rho(t)}{\Lambda} - \beta_{\text{eff}} P(t) + \sum_{i=1}^{6} \lambda_i C_i(t)
\]

### Delayed Neutron Precursor Concentration

\[
\frac{dC_i(t)}{dt} = \frac{\beta_i n(t)}{\Lambda} - \lambda_i C_i(t)
\]

### Reactivity

\[
\rho(t) = \rho_0 + \text{ramp}(t) + \alpha_T \Delta T + \alpha_V \Delta V
\]

- \( P \): fission rate (fission/s)
- \( \rho \): reactivity
- \( \Lambda \): mean neutron generation time (s)
- \( C_i \): DNP concentration (neutrons/m\(^3\))
- \( \lambda_i \): decay constant (1/s)
- \( \beta_i \): delayed neutron fraction
- \( \beta_{\text{eff}} = \sum_{i=1}^{6} \beta_i \)

\( T \): temperature
\( V \): void volume
\( \alpha_k = \frac{\partial \rho}{\partial k} \)

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**MCNP5**

**KOPTS card**
Conjugate Heat Transfer

Heat Conduction & Convection

\[ \dot{\rho} C_p \left( \frac{\partial T}{\partial t} + u \cdot \nabla T \right) = \nabla \cdot (k \nabla T) + Q \]

- \( T \) temperature (K)
- \( u \) fluid velocity (m/s)
- \( t \) time (s)
- \( Q \) volumetric heat source (W/m\(^3\))
- \( \dot{\rho} \) material density (kg/m\(^3\))
- \( k \) material thermal conductivity (W/m-K)
- \( C_p \) material specific heat capacity (W/kg-K)

Volumetric Heat Source

\[ Q = \frac{P w_e}{V} \prod_{i=1}^{n} \cos \left( \frac{\pi x_i}{L_i} - \delta_i \right) \]

- \( P \) power (fission/s)
- \( w_e \) fission energy release (J/fission)
- \( V \) fissile solution volume (m\(^3\))
- \( x_i, L_i, \delta_i \) \( i^{th} \) dimensional position (m), length (m) and phase shift

B.C.’s

- Heat continuity at internal boundaries
- Natural Convection to air at external boundaries
- Insulation/Symmetry at center boundaries
Conjugate Heat Transfer (cont’d)

Incompressible Navier-Stokes momentum

\[
\dot{\rho} \left( \frac{\partial u}{\partial t} + (u \cdot \nabla) u \right) = -\nabla p + \nabla \left( \mu \left( \nabla u + (\nabla u)^T \right) - \frac{2}{3} \mu (\nabla \cdot u) I \right) + F
\]

\[p\] pressure (Pa)

\[\mu\] material dynamic viscosity (Pa-s)

\[F\] external body force (N/m³)

### Mass Continuity

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\dot{\rho} u) = 0
\]

### B.C.’s

- No slip at solution/container walls
- Outlet at external surface
Radiolytic Gas Transport

Radiolytic Gas Bubble Volume

\[
\frac{\partial V}{\partial t} + (v \cdot \nabla)V = v_e P(t) w_e (C - C_0) \theta(C - C_0)
\]

\( V \) bubble gas volume (m\(^3\))

\( v \) bubble velocity (m/s)

\( v_e \) energy-void transfer coefficient (m\(^6\)/mol-J)

\( P \) power(fission/s)

\( w_e \) energy released per fission=> (J/fission)

\( \theta(x) \) heavyside function (x>0 \rightarrow 1)

B.C.’s

- Insulation/"Reflection" at container walls
- Outlet at solution surface

Radiolytic Gas Concentration

\[
\frac{\partial C}{\partial t} + (v \cdot \nabla)C = G_H Q - \frac{C}{\tau}
\]

\( C \) radiolytic gas concentration (mol/m\(^3\))

\( C_0 \) saturation concentration (mol/m\(^3\))

\( G_H \) gas molecular energy yield (mol/J)

\( Q \propto P \) heat source (W/m\(^3\))

\( \tau \) dissolution rate (s)
COMSOL’s built-in mesh generator used to discretize the geometry and Direct solvers are utilized

- Boundary layers in narrow domains located near steep flux gradients and/or fissile solution boundaries
- Free triangular mesh elsewhere
  - “fine”-”extra fine” in core region (+refinements)
  - “coarse”-”normal” elsewhere
- Each model set up with ~10-30k elements
  - ~20 thousand DOF → <12 hr solution time
  - 1 core computer, 4 GB RAM
- Direct Solver: COMSOL’s MUMPS & PARDISIO algorithms
  - Extendable to multi-node parallel runs
Transient: SILENE LE1-641

**Background**
- Part of a series of criticality benchmarks performed at the Valduc facility in France
- Annular, cylindrical stainless steel reactor with control rod chamber
- 93% Enriched Uranyl Nitrate (~71 g U/l) Solution
- 2 $ reactivity ramp over t=0:20 seconds

**Model**
- 2-D Axisymmetric
- Variable time-stepping, error < 1e-2
Transient: SILENE LE1-641 (cont’d)
Comparison to Benchmark

![Graph showing Comparison to Benchmark](graph.png)
SILENE LE1-641: Reactivity Contributions
SILENE LE1-641: Temperature
Distribution of radiolytic gas around the first excursion peak

$t = 10.9s$

$t = 12.9s$

$t = 17.1s$
Transient: “Methodological” Exercise

- Theoretical situation postulated by the OECD/NEA Criticality Excursion Analyses Experts Group at the 2011 International Conference on Nuclear Criticality
  - 93% Enriched Uranyl Nitrate (~71 g U/l) Solution
  - Rectangular stainless steel tank with no lid, surrounded by air
- COMSOL: 3-D quarter-slice, Error < 1e-2
50¢ Reactivity Step: Excursion History

Exercise 1, 50 cent Step: Excursion Power History

Temperature vs. Time (sec):
- Blue line: Energy (fissions)
- Green line: Power (fissions/sec)
50¢ Reactivity Step: Reactivity Feedback

Exercise 1, 50 cent Step: Reactivity Contributions

- Net Reactivity
- Radiolytic Gas Feedback
- Temperature Feedback
- Reactivity Insertion

Graph showing the reactivity of a nuclear reactor over time, with contributions from net reactivity, radiolytic gas feedback, temperature feedback, and reactivity insertion.
50¢ Reactivity Step: Temperature

Exercise 1, 50 cent Step: Solution Temperature
Summary and Conclusions

• COMSOL-based models of UN solution transients were created via built-in & equation-based modeling
  – 3 coupled physics phenomena: neutronics, conjugate heat transfer & radiolytic gas transport
  – 3-D & 2-D axisymmetric geometries
  – Nuclear data derived from MCNP5-1.60 & KOPTS card

• Results are encouraging
  – Expected power excursion behavior observed for all cases
  – Good agreement between referenced benchmark SILENE LE1-641

• Plenty of room for improvement
  – Solution Sloshing (surface distortion, moving mesh)
  – Space-time neutron kinetics methodology (few-group diffusion)
  – Extension to other benchmarks (different geometries & solutions)
  – Solution boiling
Questions??

- CHANDLER, D., Spatially-Dependent Reactor Kinetics and Supporting Physics Validation Studies at the High Flux Isotope Reactor, PhD Diss., University of Tennessee (2011)
- STACEY, W., Nuclear Reactor Physics, p. 147, WILEY-VCH, Berlin, Germany (2007)