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

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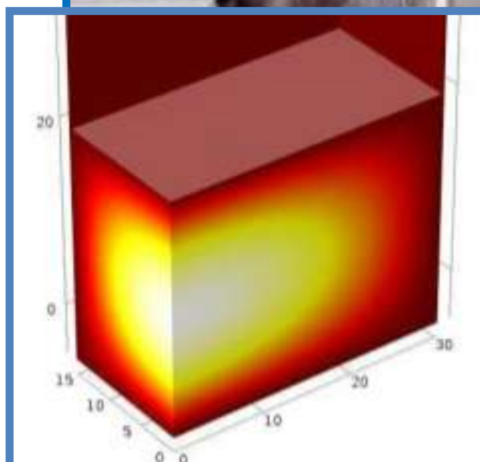
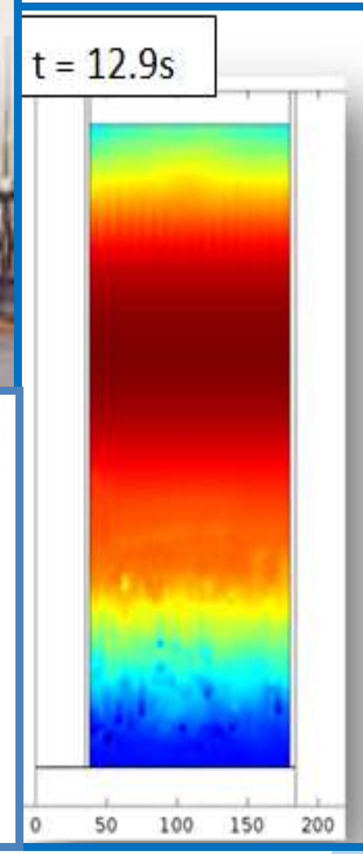
Presented at the





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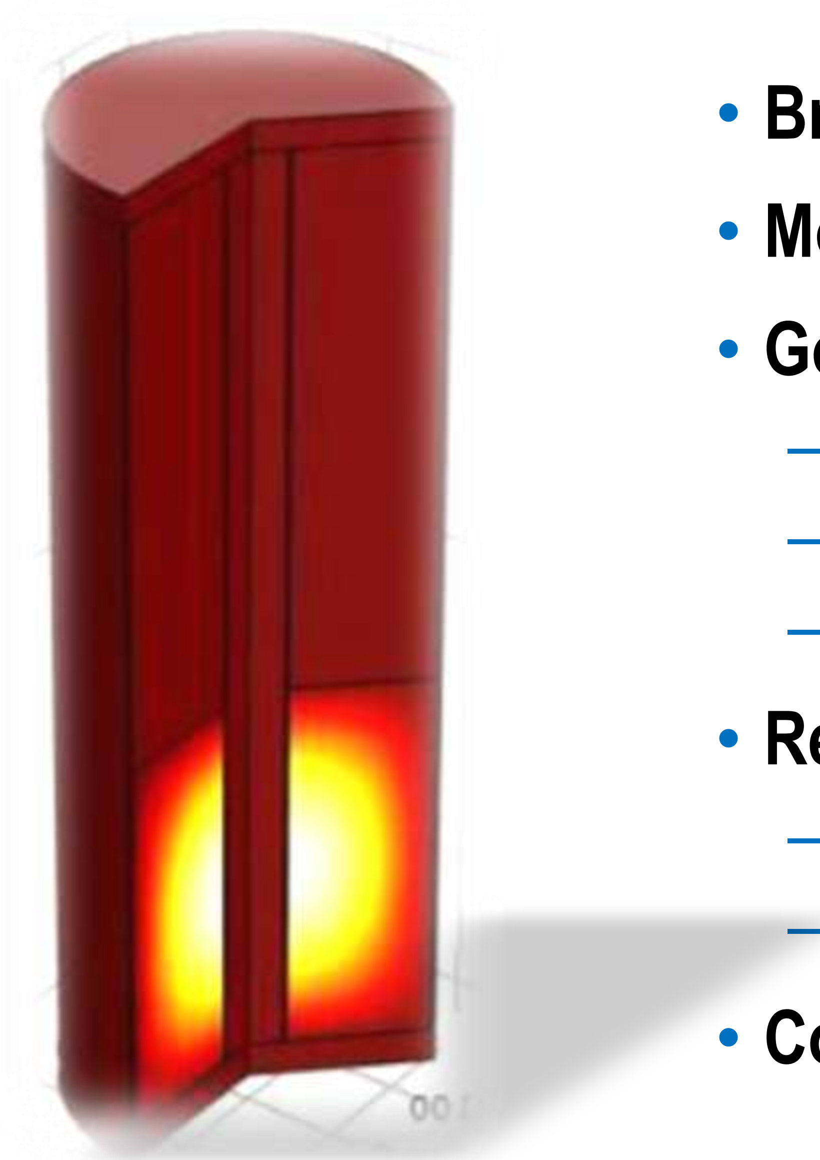
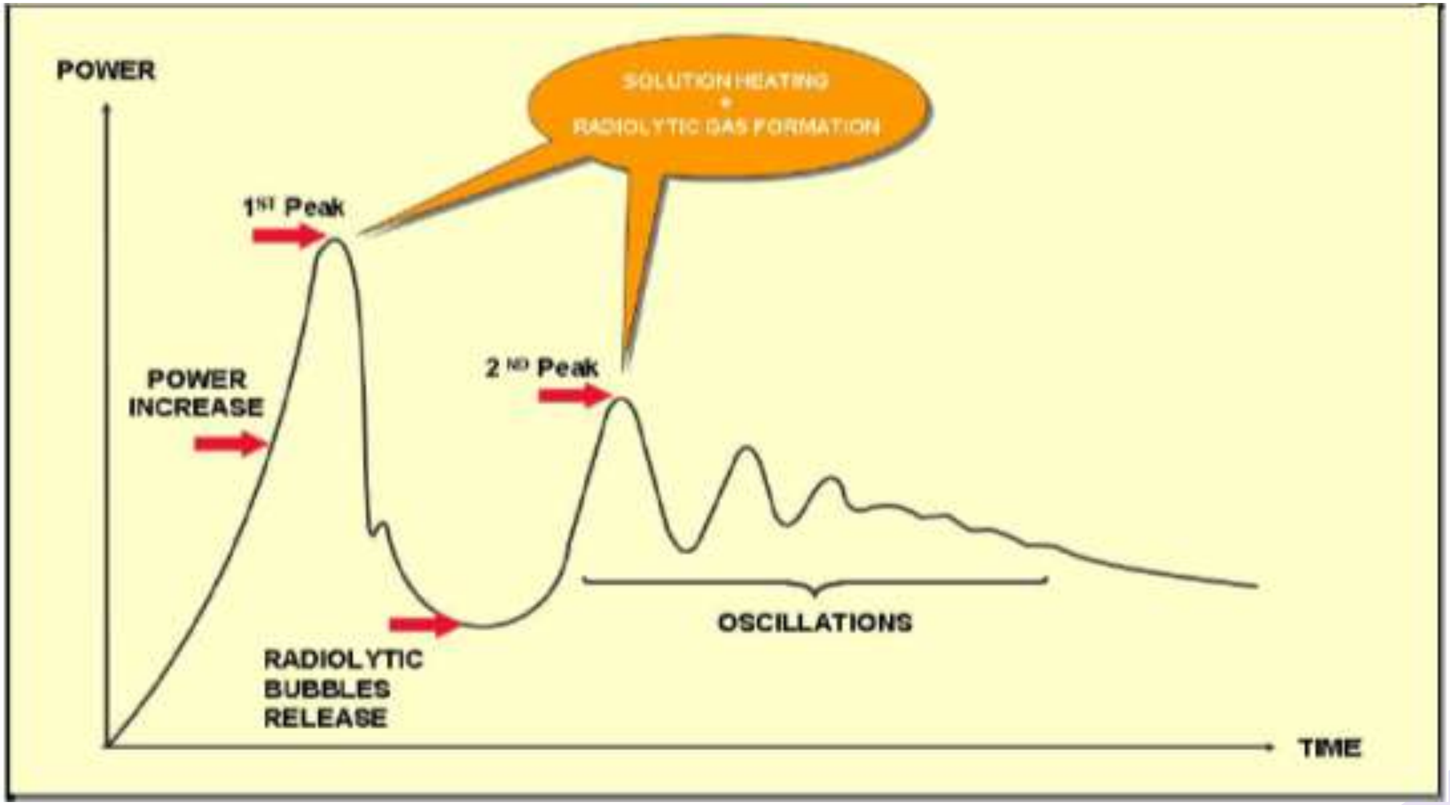
Presentation Outline



- Brief background
- Model Introduction
- Governing Equations
  - Point Kinetics
  - Conjugate Heat Transfer
  - Radiolytic Gas Transport
- Results
  - SILENE benchmark
  - “Methodological” Exercise
- Conclusions

Criticality Transients in Solution

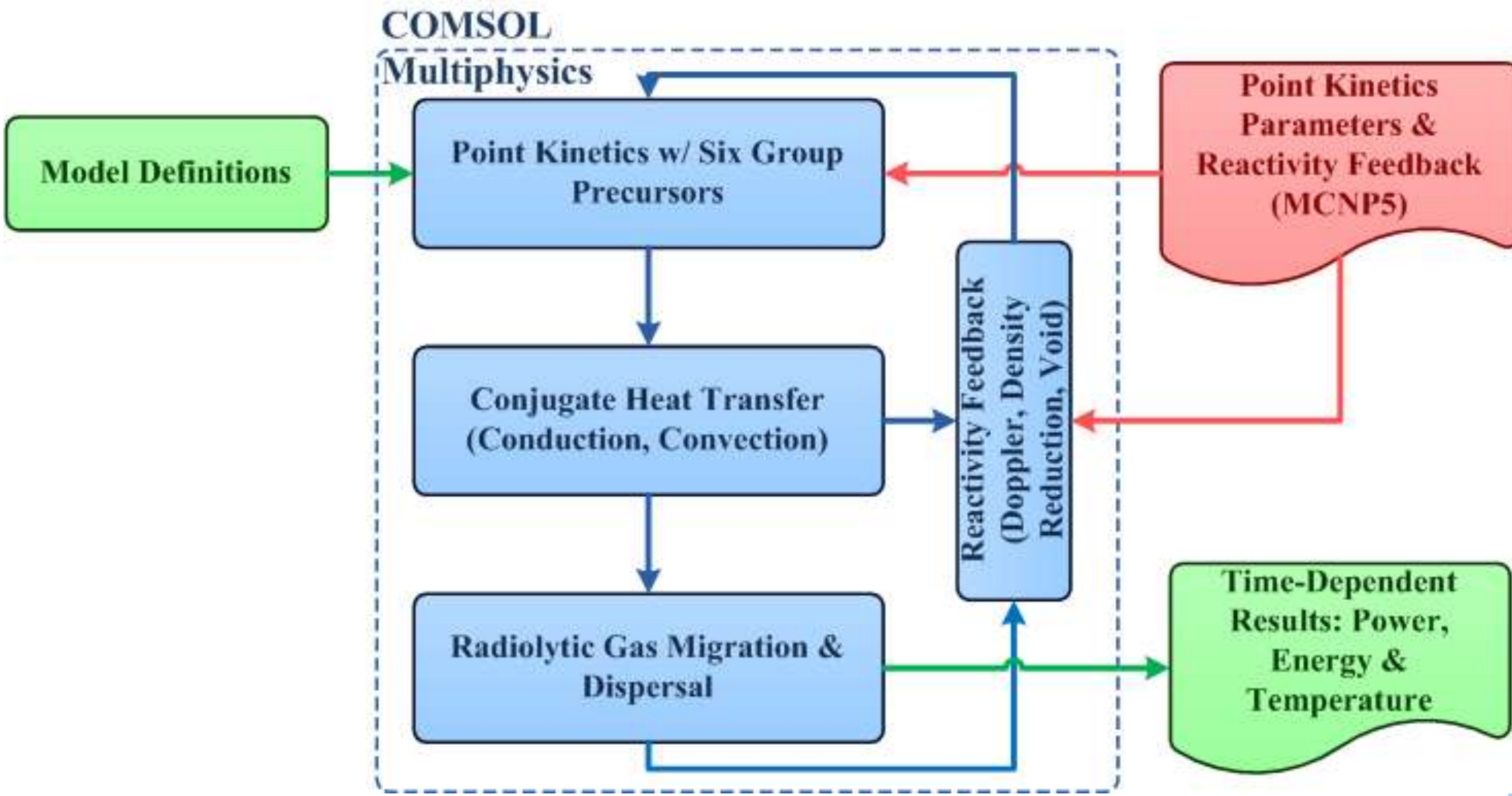
- **Typical Multiphysics Reactivity Feedbacks:**
  - **Included in Model: Radiolytic Gas, Thermal Expansion, Temperature (Cross Sections)**
  - **Not included: Solution Ejection, Sloshing, Boiling, etc.**



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



Point Kinetics

Neutron Kinetics Balance

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

Delayed Neutron Precursor Concentration

$$\boxed{\frac{dC_i(t)}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t)} \boxed{i = 1:6}$$

Reactivity

$$\boxed{\rho(\mathrm{t}) = \rho_0 + ramp(t) + \alpha_T \Delta T + \alpha_V \Delta V}$$

T temperature

V void volume

$$\alpha_k = \frac{\partial \rho}{\partial k}$$

P fission rate (fission/s)

ρ reactivity

Λ mean neutron generation time (s)

C_i DNP concentration (neutrons/m^3)

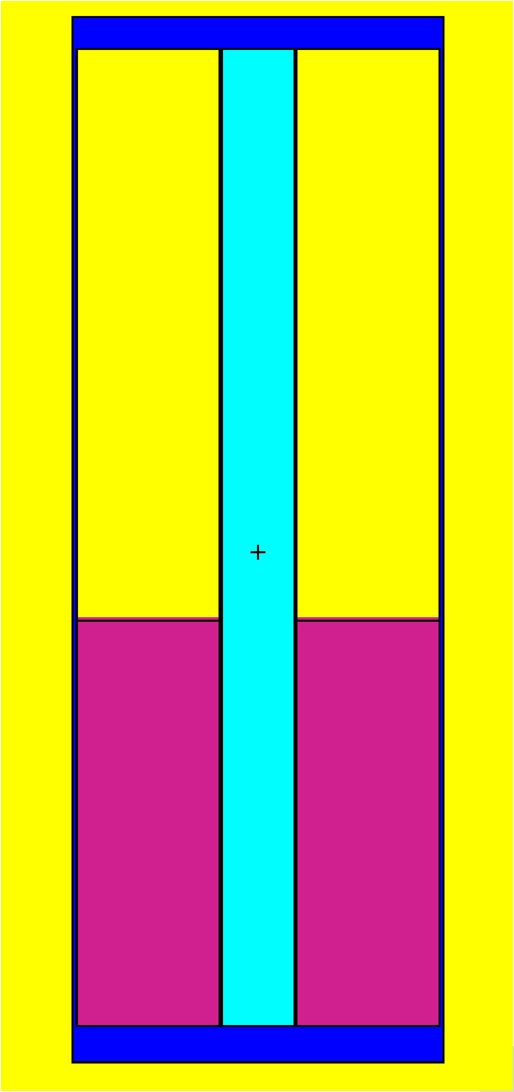
λ_i decay constant (1/s)

β_i delayed neutron fraction

$$\beta_{eff} = \sum_{i=1}^{6} \beta_i$$

Use of MCNP5

- Point Kinetics Parameters
  - Using MCNP5-1.6's KOPTS card precursor decay rates and delayed neutron fractions (λ_i's & β_i's) along with mean neutron generation time (Λ) can be calculated using
- Reactivity Feedback
  - Step changes in reactivity vs. feedback parameters (void, temperature) are used to inform reactivity feedback coefficients (α_k's)



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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/m³)
$\dot{\rho}$	material density(kg/m³)
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 (m³)
x_i, L_i, δ_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

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

p pressure (Pa)

μ material dynamic viscosity (Pa-s)

F external body force (N/m³)

Mass Continuity

$$\boxed{\frac{\partial\dot{\rho}}{\partial t}+\nabla\cdot\left(\dot{\rho}u\right)=0}$$

B.C.'s

- No slip at solution/cointainer walls
- Outlet at external surface

Radiolytic Gas Transport

Radiolytic Gas Bubble Volume

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

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 → 1)

Radiolytic Gas Concentration

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

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)
τ	dissolution rate (s)

B.C.'s

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

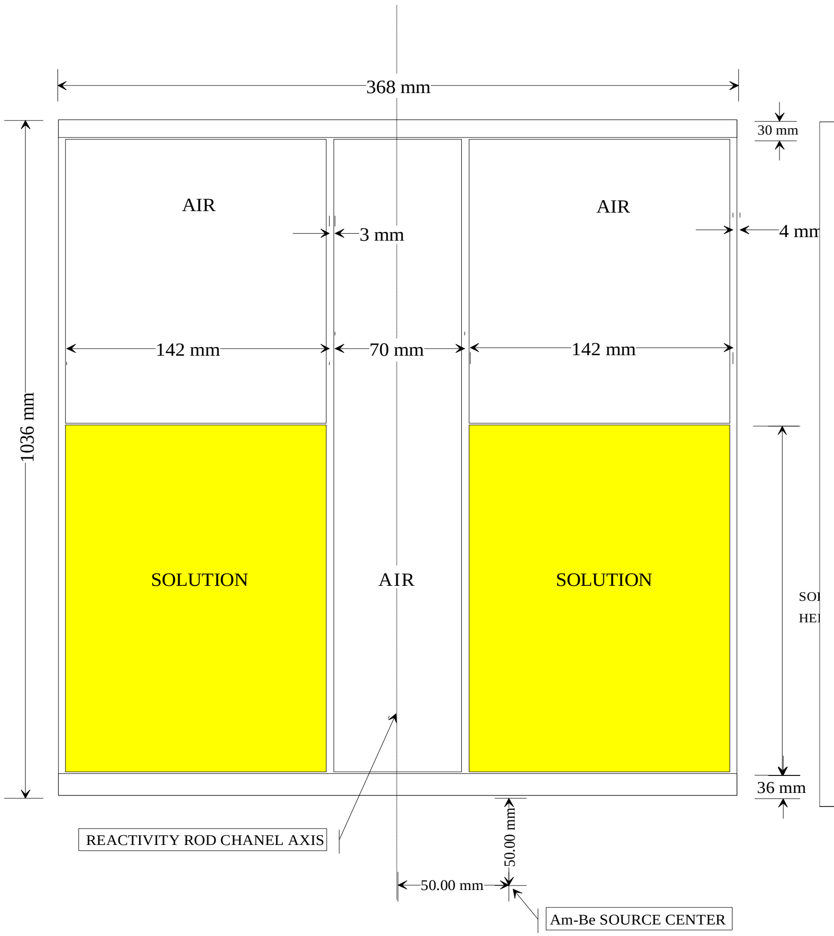
COMSOL's built-in mesh generator used to discretize the geometry and Direct solvers are utilized

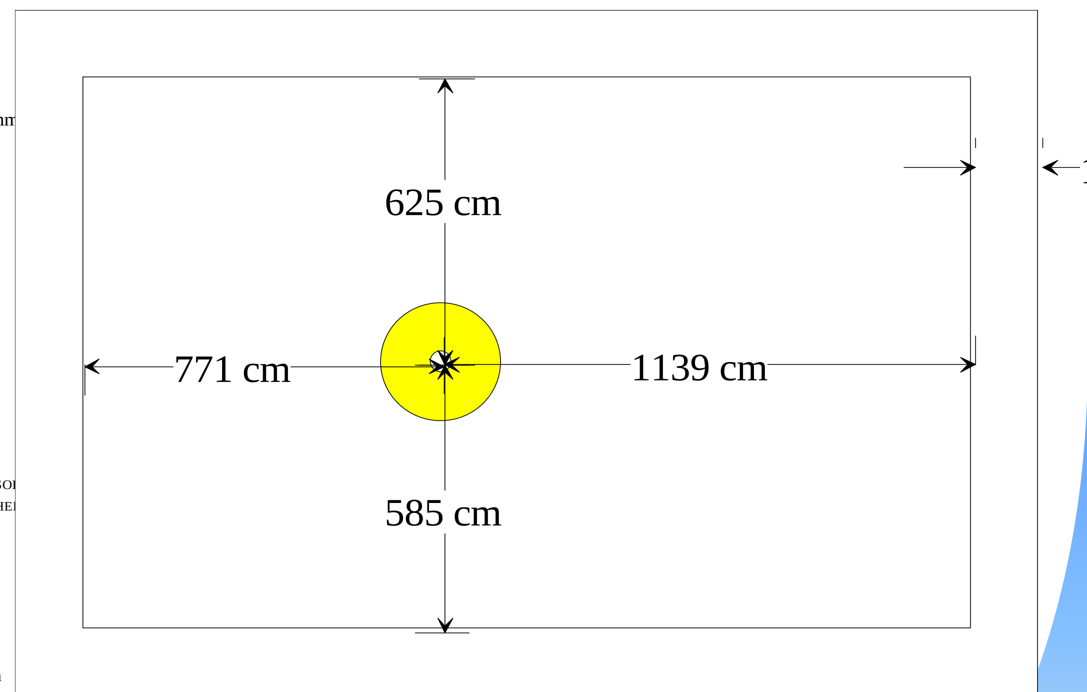
- Boundary layers in narrow domains located near steep flux gradients and/or fissile solution boundaries
- Free triangular mesh elsewhere
  - "fine"-"extra fine" in core region (+refinements)
  - "coarse"-"normal" elsewhere
- Each model set up with ~10-30k elements
  - ~20 thousand DOF → <12 hr solution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

Transient: SILENE LE1-641

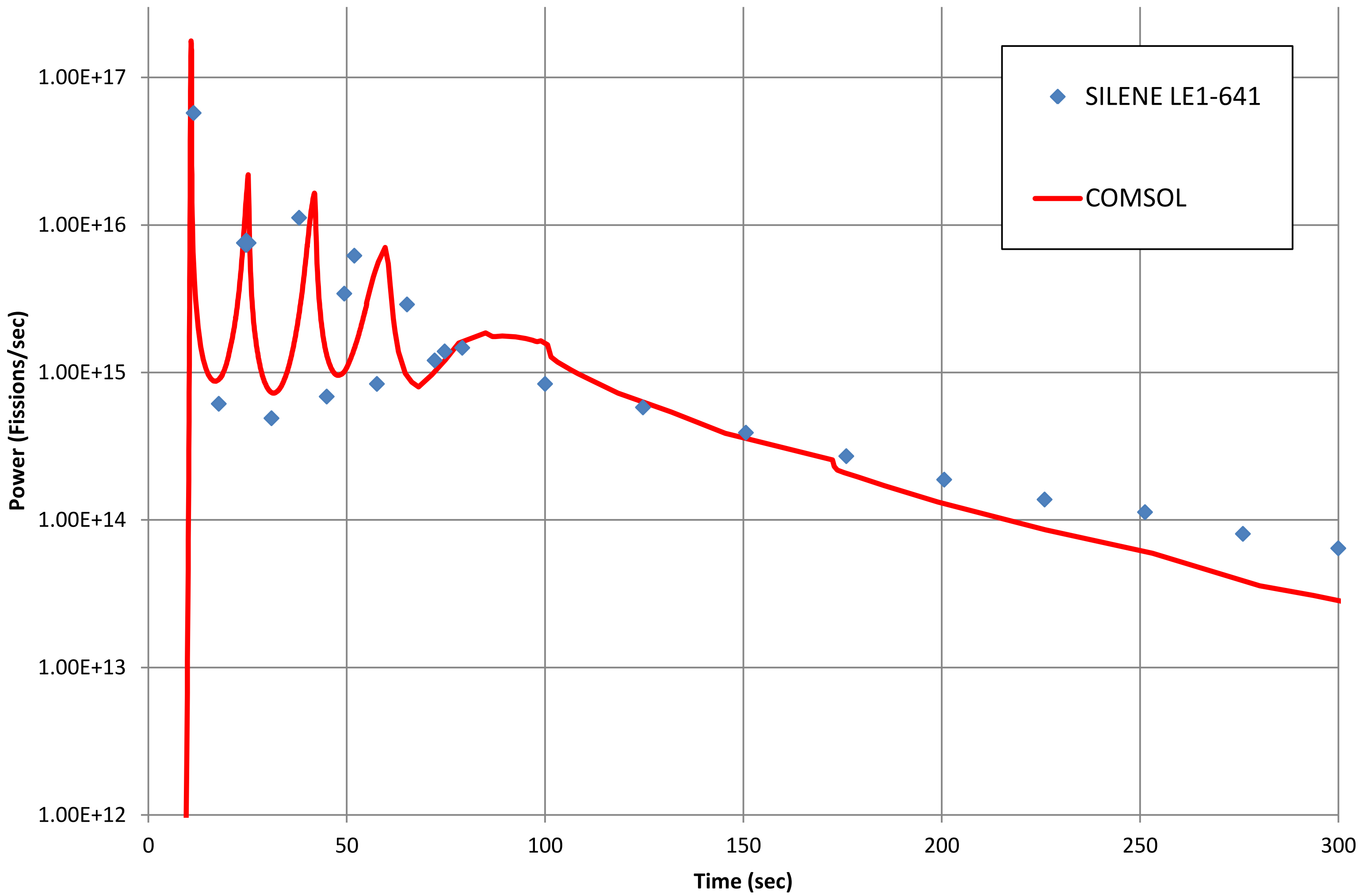
- Background
  - Part of a series of criticality benchmarks performed at the Valduc facility in France
  - Annular, cylindrical stainless steel reactor with control rod chamber
  - 93% Enriched Uranyl Nitrate (~71 g U/l) Solution
  - 2 $ reactivity ramp over t=0:20 seconds
- Model
  - 2-D Axisymmetric
  - Variable time-stepping, error < 1e-2

Transient: SILENE LE1-641 (cont'd)

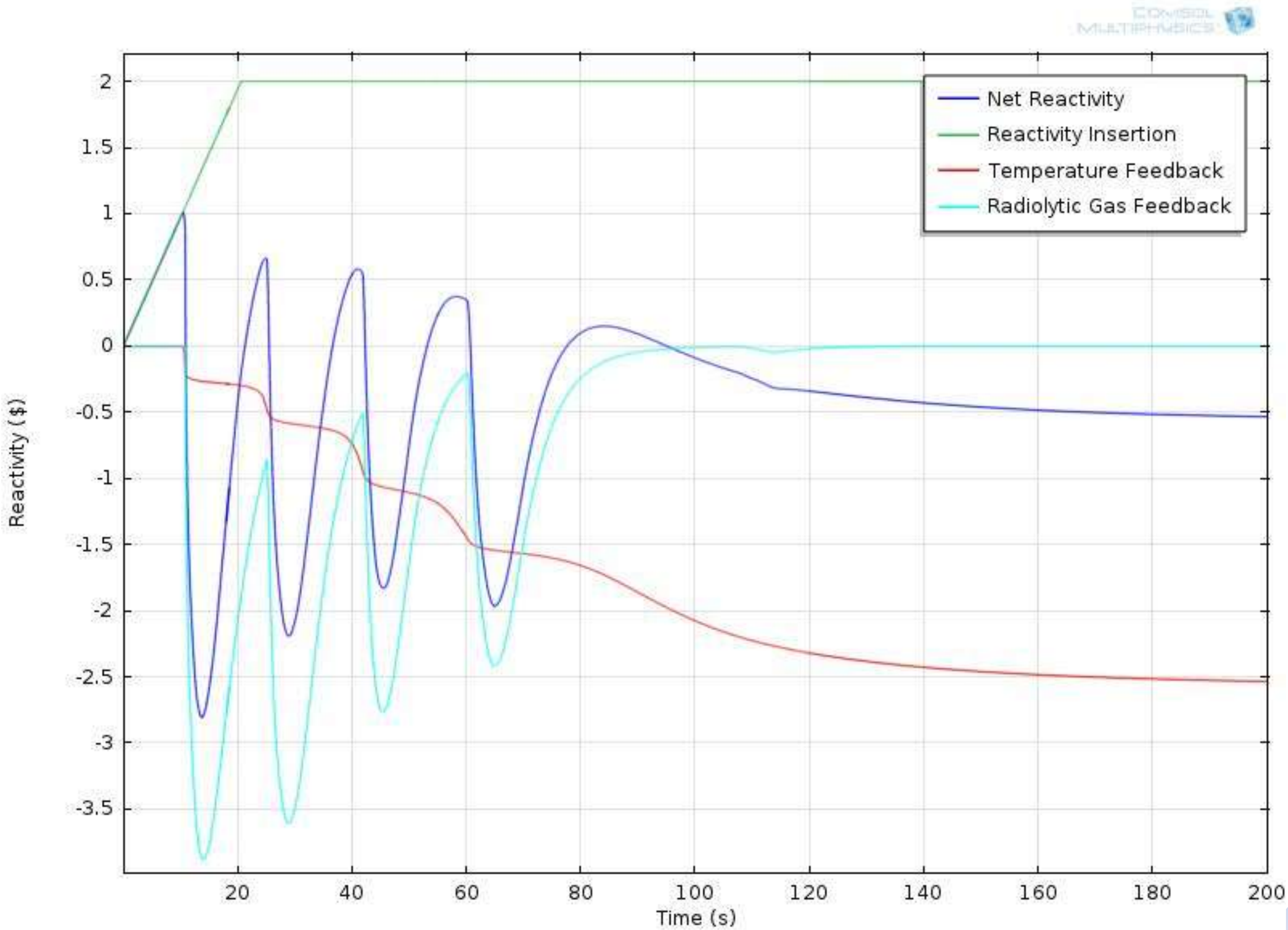




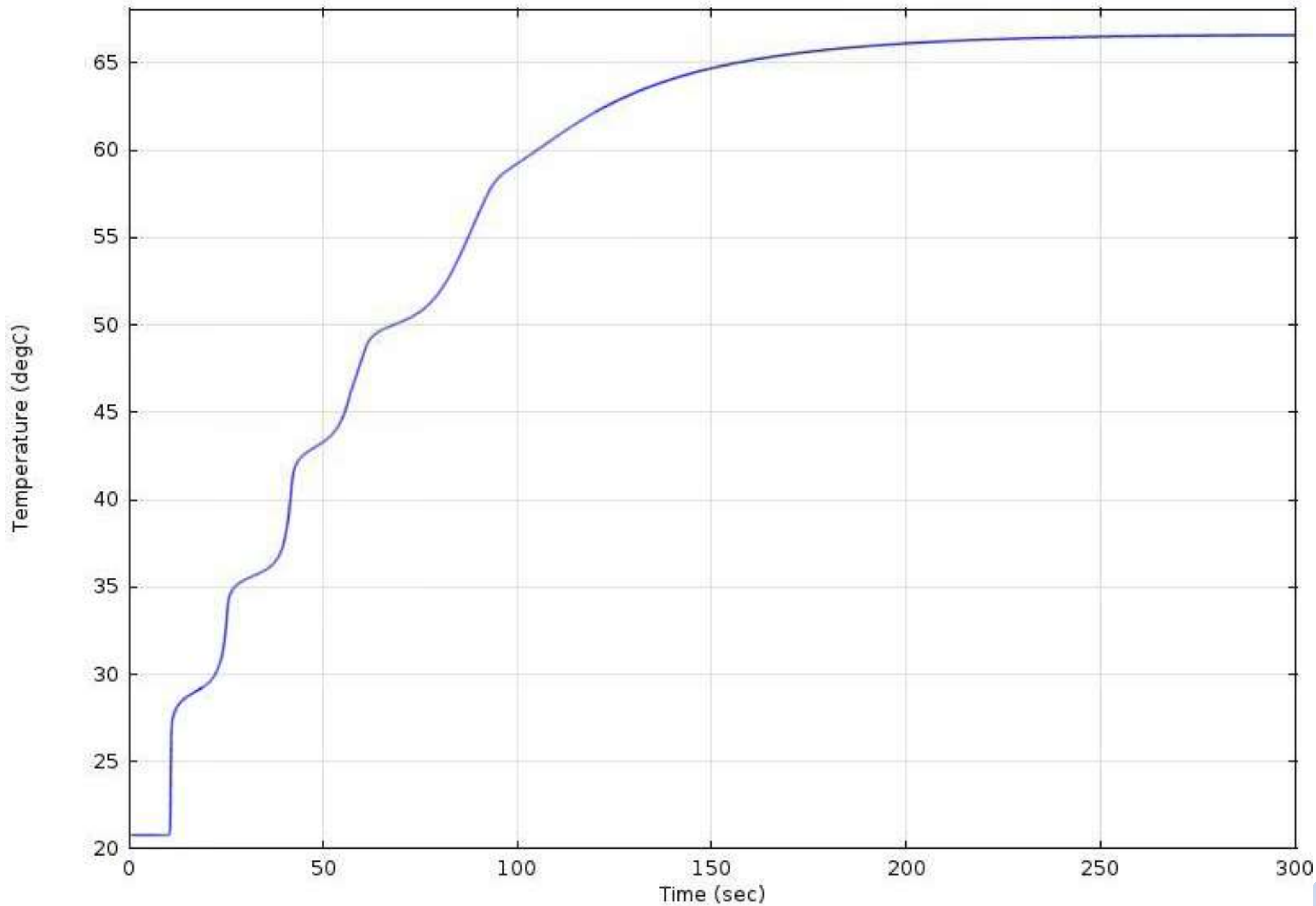
Comparison to Benchmark



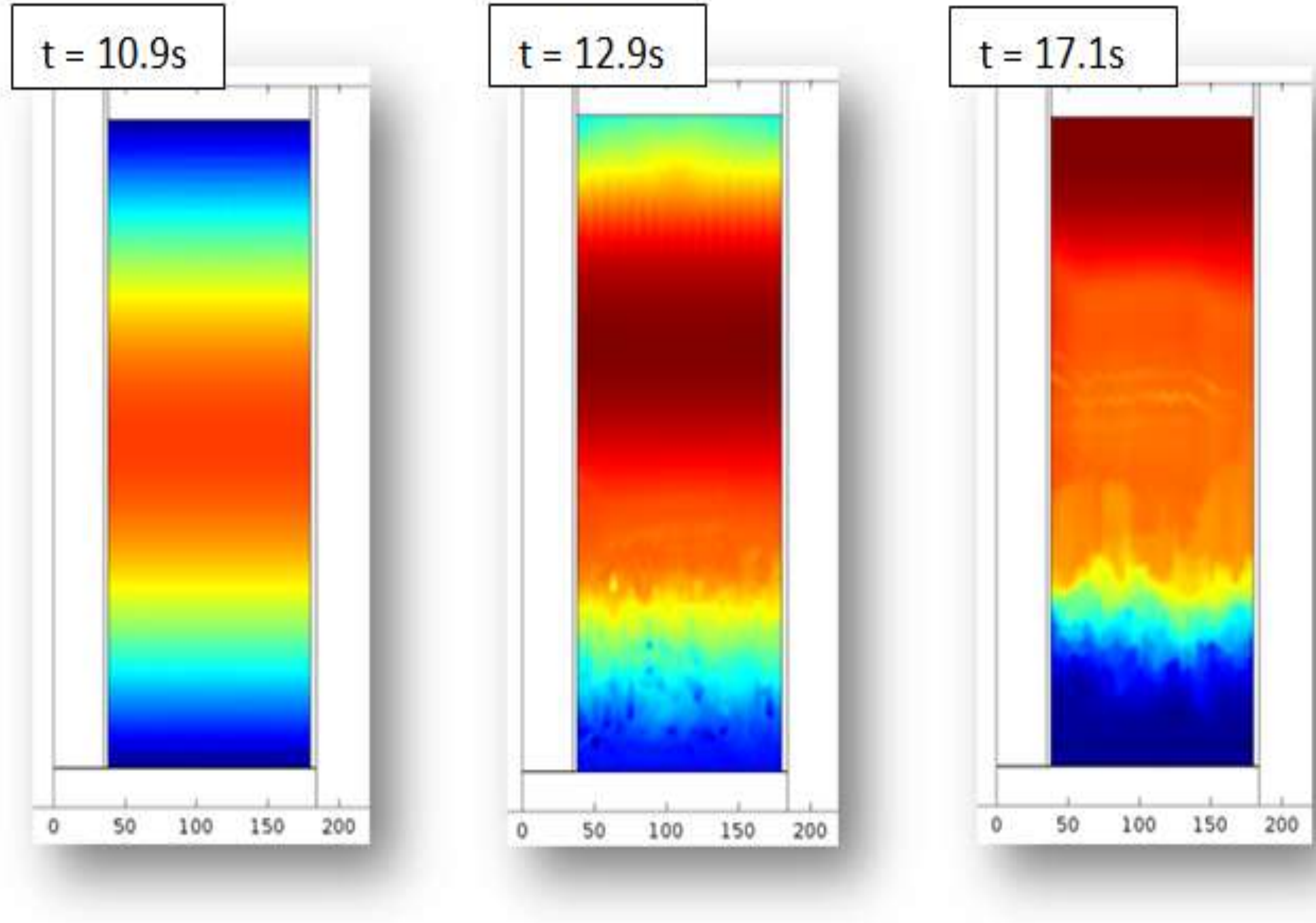
SILENE LE1-641: Reactivity Contributions



SILENE LE1-641: Temperature

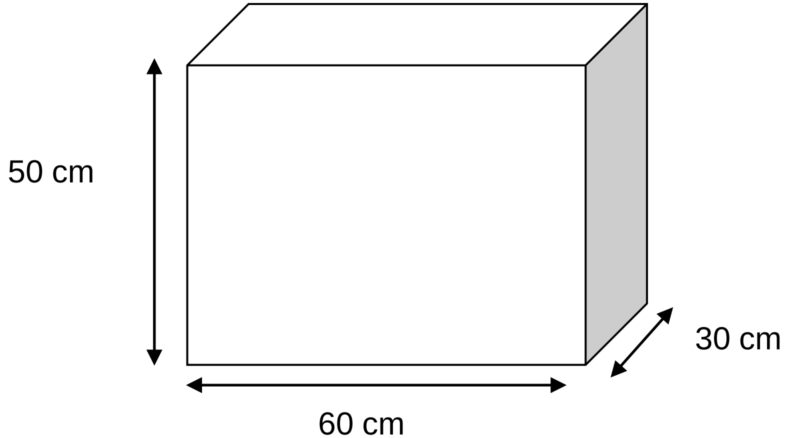


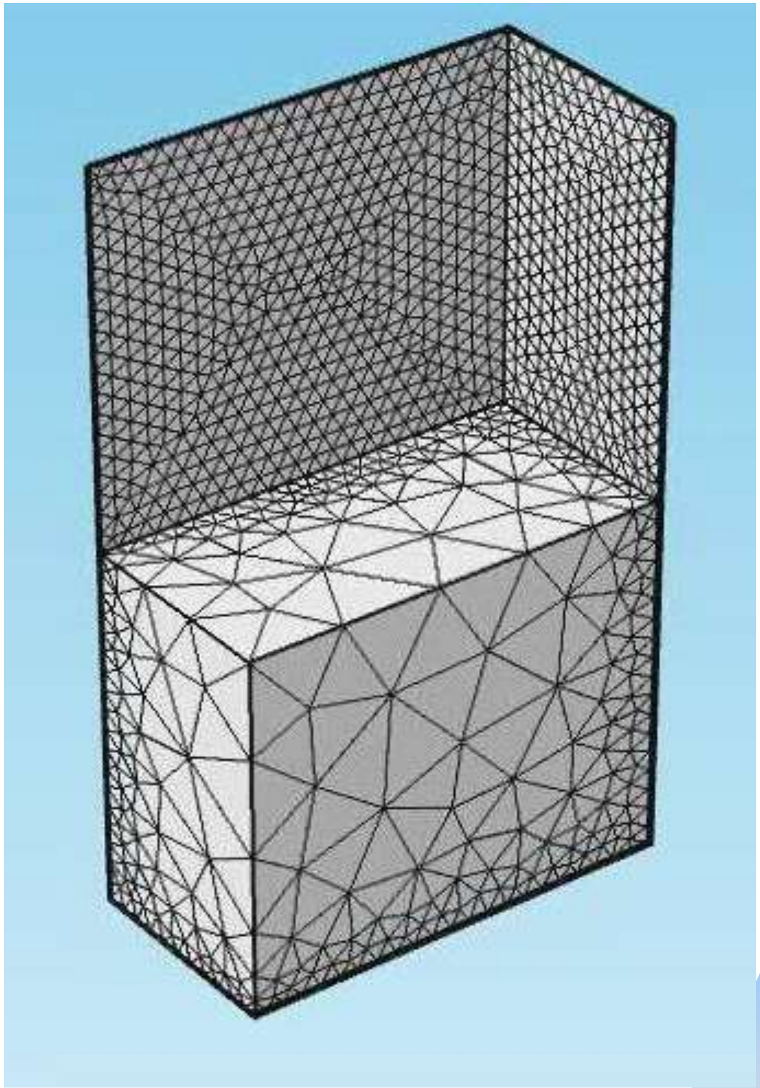
Distribution of radiolytic gas around the first excursion peak



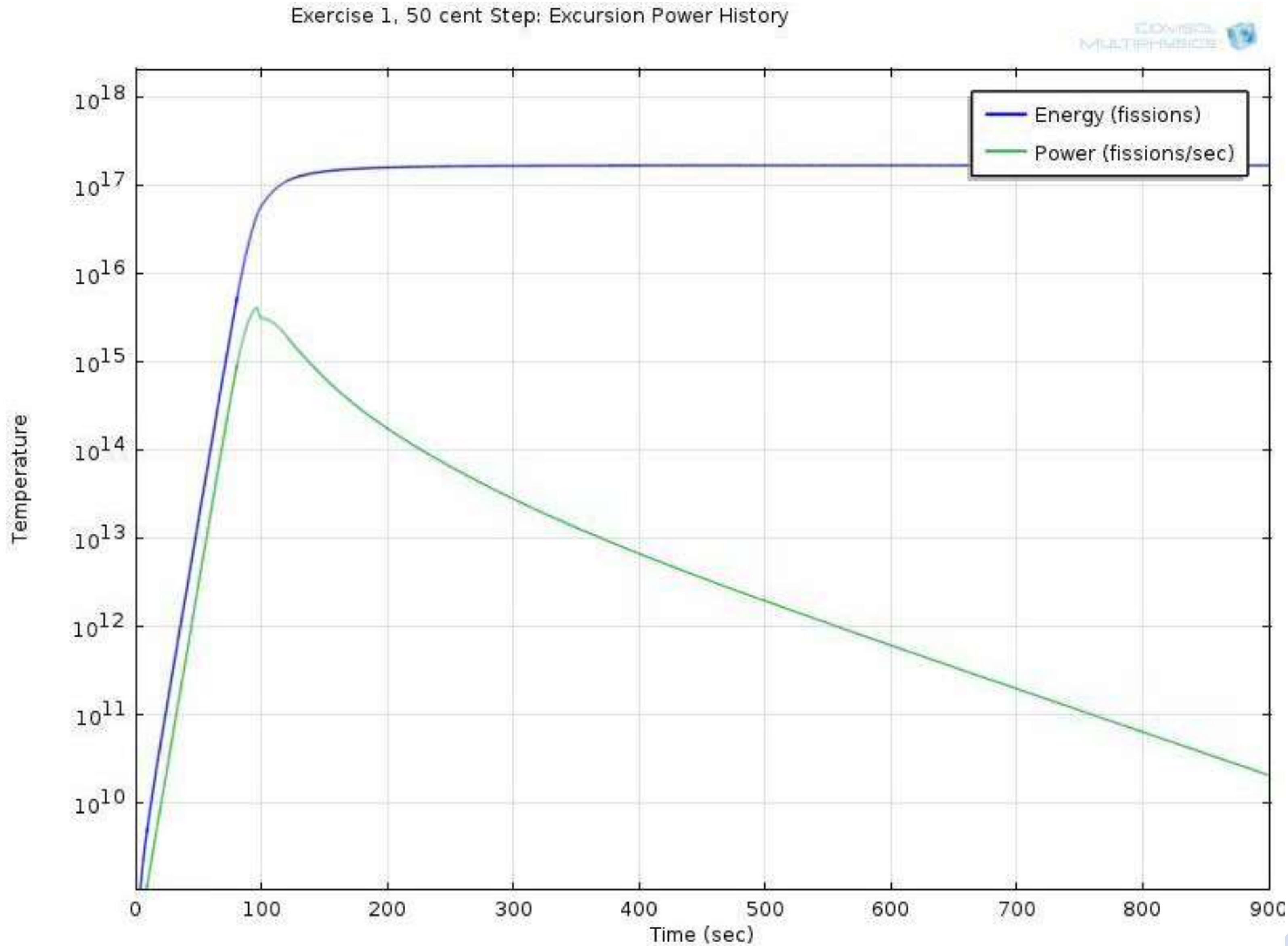
Transient: "Methodological" Exercise

- 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

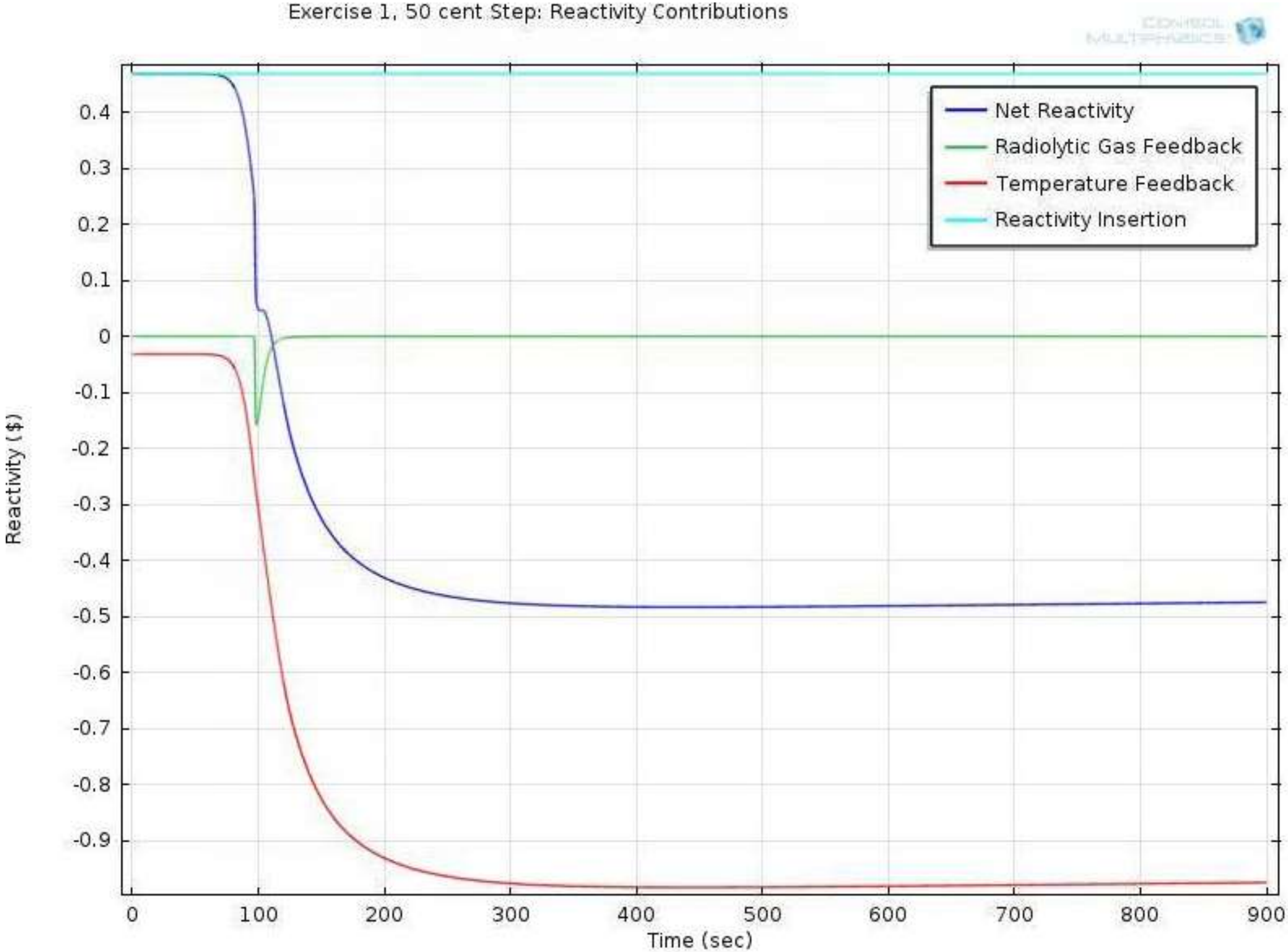




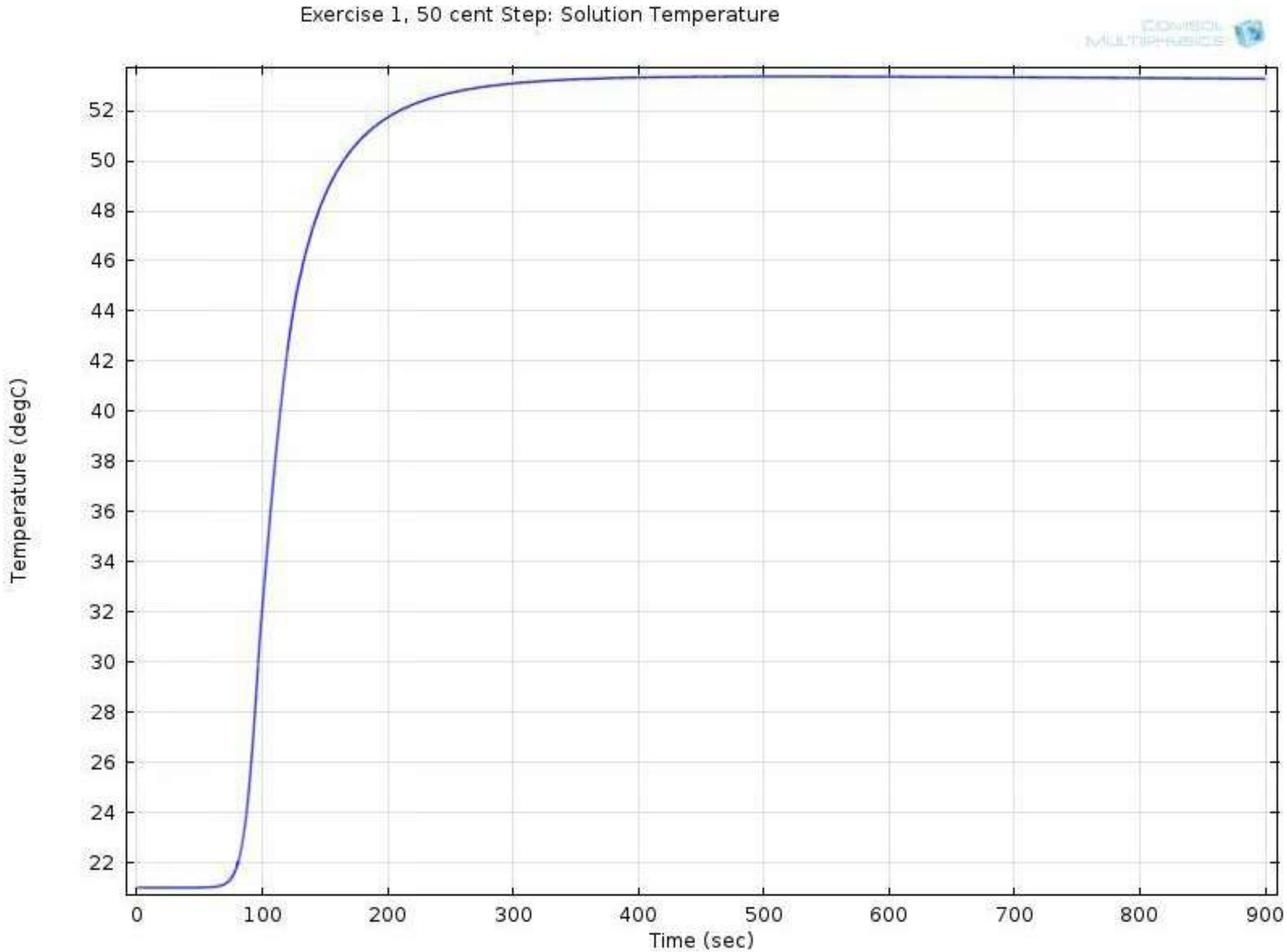
50¢ Reactivity Step: Excursion History



50¢ Reactivity Step: Reactivity Feedback



50¢ Reactivity Step: 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??

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