COMSOL-Related Activities within the Research Reactors Division of Oak Ridge National Laboratory

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The full outline of the Companion Paper:

- Abstract
- Introduction
- *Why We are Using COMSOL*
- Some Success Stories
- Our Current Applications
- Anticipated Expansion of our Applications
- **Best Practices**
  - Software, License, and Document Management
  - Local COMSOL User Group
  - Joint ORNL / COMSOL Symposia / Workshop
  - Local Tips and Tricks
  - Software Quality Assurance
- Suggestions and Conclusions
- Acknowledgements
- References
My One-Sentence Description of COMSOL:

• COMSOL Multiphysics is a finite-element based computer simulation toolbox
COMSOL is our choice because (part 1 of 2):

• Finite-element methods are the most accurate numerical simulation tool available for deterministic solutions.

• COMSOL is nearly 100%-true finite-element method code for all the physics simulated (some exceptions: ODE solver, Particle Tracing Module).

• COMSOL is the leader, and perhaps, the only true-multiphysics code commercially available (CFD, heat transfer, structural mechanics, PDE mode, etc. on our projects).
COMSOL is our choice because (part 2 of 2):

• If desired, the standard equations solved may be altered on *INPUT* by the *USER* (for example, constitutive equations including turbulence model).

• You can solve your own equations from scratch (PDE, ODE, algebraic, functions, etc.)

• COMSOL provides a convenient GUI in modern computing environments.

• COMSOL continues to provide technical support and code improvements at a remarkable pace (distributed parallel processing, new modules, interface tools, response to user requests, etc.) now at v5.1!

• Application builder now available with base package.
Best Practices: Software, License, and Document Management

• central server for all of these functions
• longer trial period recommended
• floating network license recommended
• combine resources to share licenses
• scripts to quickly update application library, parts library
• share libraries using samba
• network file system for improved sharing and parallel processing of workstations
Best Practices: Local COMSOL User Group

• several attempts at forming a viable user group

• core set of users form a combined user group and project application meeting (always get something done, and improve)

• we found that a user group improves efficiency, helps each other out, adds members to license pool, always learning something new
Best Practices: Joint ORNL / COMSOL Symposia / Workshop

• so far, we have done this about 3-4 times
• many potential users at ORNL
• goal: more users, larger license pool
• some effort required
• outside users find it difficult to visit ORNL
• showcase work, add new customers for analysts using COMSOL
• potentially do this on annual basis
Best Practices: Local Tips and Tricks

- a need exists outside COMSOL tech support to keep track of items unique to the local level
- easy to implement as a .pdf file file-name list on the COMSOL license server (also a web server to the LAN only)
- full paper lists several of the items on our “local tips and tricks”
Best Practices: Software Quality Assurance

- nuclear industry requires SQA, but it is good practice for all
- we separate verification and validation, and require both
- use the COMSOL application library to the extent possible for V&V
- a new validation plan is forthcoming for HFIR-specific needs –continually look to improve
- hope to see more direct V&V support from the COMSOL developers
Suggestions and Conclusions

• no one person knows everything about COMSOL (lots to learn)

• keeping up and learning is a continuous process

• using COMSOL with other users helps the individual to get better with using the code through peer review and constructive criticism and debate

• Questions?
Extra Slides
Success Story: COMSOL on the HFIR Cold Source

COMSOL Multiphysics was the design-basis tool for the cold source pressurizer; now over 50 HFIR fuel cycles operation
Success Story: COMSOL multiphysics simulation of the HFIR cold source pressurizer (part 1 of 2)
Success Story: COMSOL multiphysics simulation of the HFIR cold source pressurizer (part 2 of 2)
Next Success Story: COMSOL on the HFIR Pu-238 Project

V4.2a SQA approved

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COMSOL is the design- and safety-basis tool for the Pu-238 production project
Additional Target Designs have been COMSOL-Analyzed and Irradiated in the Past Year at HFIR
(all temperature contours are shown 135°F → 650°C)

- Additional single bare pellets, also 2nd irradiation cycle, COMSOL 4.2a, 3D, ¼ pie slice

- Reduced-length bare pellets, 1 and 2 irradiation cycles, COMSOL 4.2a, 3D, ¼ pie slice

- Partially-loaded (7 pellets) prototype production target, 1 and 2 irradiation cycles, COMSOL 4.3, 2D axisymmetric

- Fully-loaded prototype production target (52 pellets), 1 irradiation cycle, COMSOL 4.3, 2D axisymmetric (cycle just started)

Individual pellet at maximum temperature in stack:
(note: classic hourglass shape)

3-D Rotated Stress Contour with 10000x Deformation of the 2D Axisymmetric Modeled Volume of the Hot Pellet for the VXF-15 EOC-1 Safety-Basis Conditions at 130% Power.
The Conversion of HFIR to LEU Fuel will be another COMSOL Success Story

• Presently using safety-basis (SB) and best-estimate (BE) models to support the conversion activities.

• Several physics are incorporated and coupled to formulate multiple physics (see separate presentations):
  – turbulent conjugate heat transfer (coolant, clad, fuel, side plates)
  – temperature dependent properties (and pressure for water)
  – structural mechanics
  – thermal-structure interaction
  – irradiation impacts on material properties (limited)
  – fluid-structure interaction (isothermal separate effect only at the present time)

• Additional physics to be included: (1) fully-coupled FSI, (2) additional irradiation impacts including swelling, (3) multi-plate up to entire core, (4) reactor physics, (5) flow blockage, (6) severe accidents.
Franklin Curtis validated separate-effects COMSOL models on data from several sources including ANS and HFIR. ANS test data shown below for aluminum plates up to 40 m/s coolant flow.
Emilian Popov demonstrated through a “proof–of-principal” method that COMSOL can be used to simulate irradiation swelling. Shown below is the Von Mises stress results for a prototypical 2D fuel plate undergoing isotropic (left) and orthotropic (right) swelling.
Prashant Jain and Vaibhav Khane demonstrated that the existing COMSOL single-plate models can be expanded to a multi-plate model.
Additional Physics 4a: Reactor Neutronics by Diffusion Theory

David Chandler, as an integral part of his PhD dissertation used COMSOL PDE equation-based modeling to perform spatially-dependent reactor kinetics of HFIR.

Power shifts to the OFE during control cylinder ejection and then back to IFE during safety plate insertion.
Christopher J. Hurt is currently using COMSOL PDE equation-based modeling to simulate 2D axisymmetric power distribution of the HFIR core as research in support of his PhD dissertation.

HFIR Fission Power (unnormalized and preliminary)