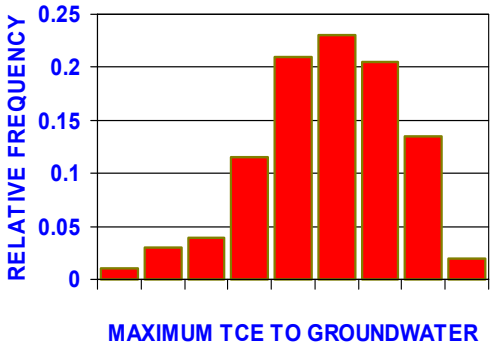
Scientific Computing Within the ORNL Modeling and Simulation Group: Engineering Systems Analysis

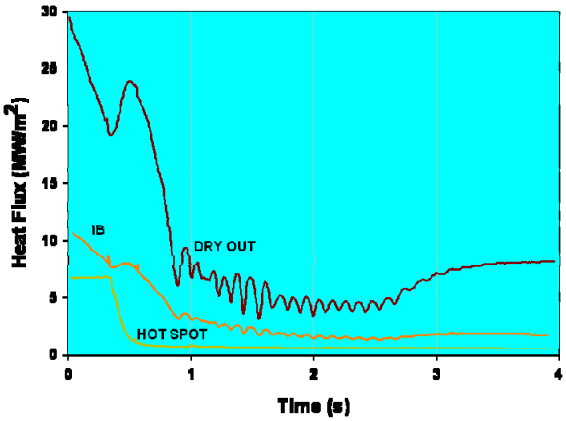
The ORNL Modeling and Simulation Group (MSG) develops sophisticated numerical solutions for a wide range of scientific, engineering, and operational applications. MSG's core competency is computational physics and engineering, and within this context we have considerable expertise with the analysis of large engineering systems. Our problem-solving scope focus on physics/science-based analysis of process components and subsystems, and covers the complete R&D-Engineering-Operations spectrum. This process-oriented expertise includes design optimization studies for equipment upgrades and process reliability; operational support such as calculating process inventories, optimizing plant production, safety and criticality-safety analyses, and site-remediation environmental studies. Prior applications include the following.

- Characterization of the multi-site gaseous-diffusion uranium-enrichment process (GDP) including:
  - simulation of steady-state and transient conditions within the UF_6 process gas, R114 primary cooling, and recirculation cooling water systems;
  - model-based development of Gas Centrifuge (GCEP) and Atomic Vapor (AVLIS) isotope-separation processes including CFD studies to optimize centrifuge flow stability and separative work, systems analysis to define optimal GCEP cascade configurations, and radiation heat-transfer modeling of the AVLIS materials handling development module; and
  - soil-leaching studies at the Paducah and Portsmouth diffusion plants to determine deep-soil and groundwater contamination from legacy industrial chemicals.
- Broad-based support for the ORNL high flux-isotope (HFIR) and spallation neutron source (SNS) research reactors including component design studies, loss-of-coolant accident simulations; and equipment reliability studies.
- Manufacturing support for the DOE Y-12 Weapons plant including model-based R&D of casting and immersion-quench processes, optimization of electroforming cell designs, and development of expert systems.

These applied scientific computing capabilities represent an extremely versatile process engineering resource for a broad range of R&D, industrial, homeland defense, and military applications. We welcome the opportunity to discuss your potential applications and ways MSG can contribute to a solution.



MSG coupled the SESOIL & PRISM codes to determine the most-likely trichloroethylene flows into ground water at the Portsmouth Gaseous Diffusion Plant



MSG utilized RELAP to conduct HFIR loss-of-coolant analysis. Result show maximum calculated heat flux (HOTSPOT) within fuel element is lower than flux required for incipient boiling (IB) or dry out (DRY OUT)

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