Simulating Hostile Electrical Environments

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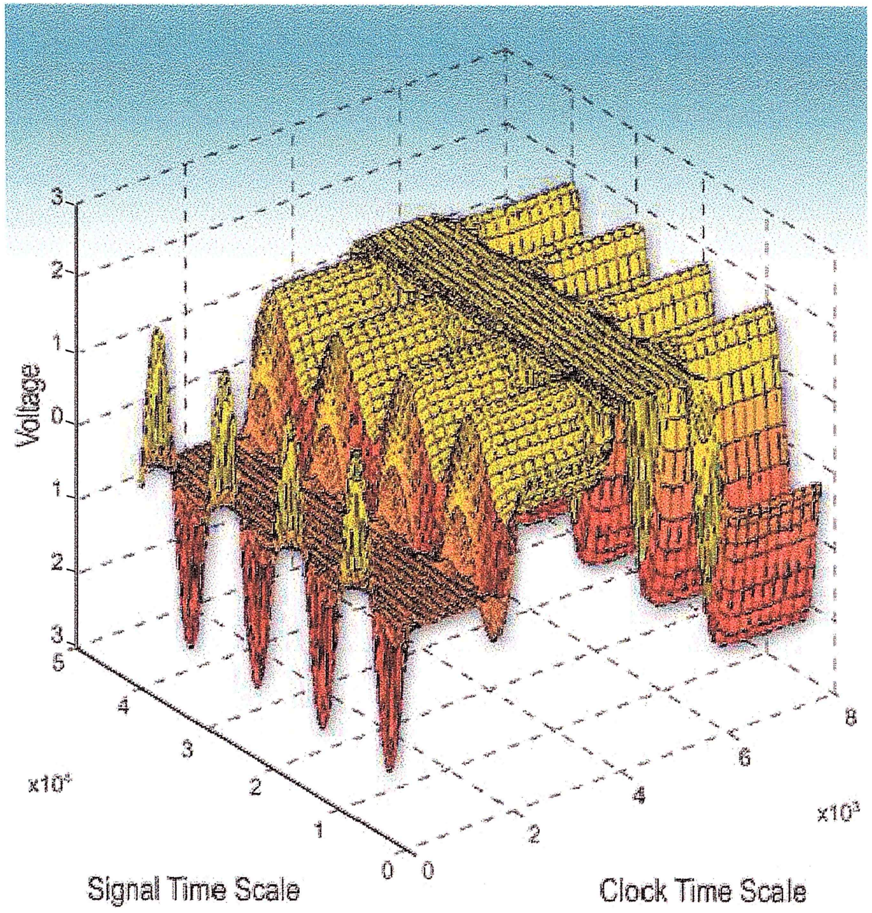


RIGHT: With the Xyce™ circuit code, novel methods are used to solve multiple-time partial differential equations, as shown here. At the milestone review in May 2003, the external review panel was "impressed with the work being done on time-parallel, multi-time partial differential equations within Xyce™."

Description

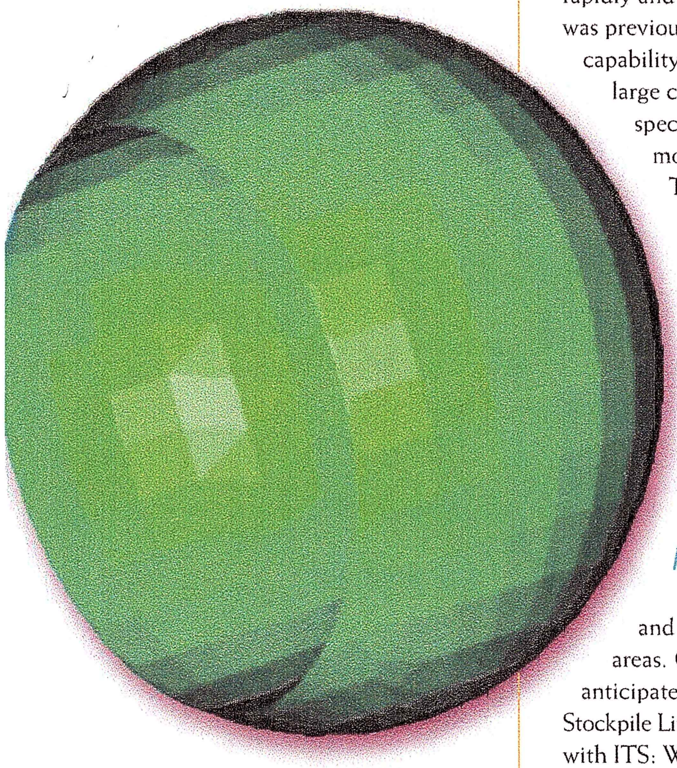
The completion of an FY03 ASC Level 1 Milestone, *"Stockpile-to-Target Sequence hostile environment simulation for cable SGEMP and electrical response to x-rays,"* demonstrated simulation capability for transient x-ray radiation response of electrical components, representative of weapon components in hostile environments. This new capability was demonstrated for a circuit of the replacement arming, fuzing, and firing (AF&F) unit for the W76-1. The Integrated-TIGER-Series (ITS) Monte Carlo code predicted dose rate for locations on circuit boards corresponding to the locations of radiation-sensitive semiconductor devices. Using the ITS dose-rate data, the Xyce™ circuit code predicted the response of the circuit under radiation.

On May 29, 2003, an external review panel concluded that the ITS team had successfully met its part of the FY03 milestone. The Xyce™ calculations were completed before the due date of September 30, 2003, and were reviewed by the external review panel on November 3 and 4, 2003.

Technical Significance

For this milestone, a new computer-aided-design (CAD)-based transport capability for Sandia's Monte Carlo radiation transport code, the ITS, was demonstrated. Before ASC, the legacy version of ITS required construction of a geometrical model specifically tailored for the radiation-transport code. This time-consuming method involved Boolean combinations of solid primitives. For complex weapon systems, more than a year of effort was required to assemble geometry models. For this milestone, the ITS radiation-transport modeling team demonstrated a new capability developed under ASC that allows radiation to be transported on a three-dimensional CAD model of a re-entry body. Thus, CAD models created by weapon designers can now be leveraged by radiation transport analysts.

The Xyce™ circuit calculations also showcased several new capabilities. The Xyce™ code is part of the ASC code-development effort of High Performance Electrical Modeling and Simulation (HPEMS) team. The development of new, predictive, radiation-aware device models and their integration into Xyce™ was



With the ITS radiation transport code, investigation of radiation transport to faceted surfaces, like the one shown here, is under way. At the milestone review in May 2003, the external review panel said that it "applauds the ITS team's effort to develop alternative geometry representation for ITS such as the faceted surfaces."

demonstrated. These photocurrent models for semiconductor devices can be more rapidly and less expensively created than was previously possible. Also, the new capability of Xyce™ to simulate very large circuits, including application-specific integrated circuit (ASIC) models, was demonstrated. Together, these two new capabilities allow Sandia circuit modelers to achieve unprecedented high fidelity in their circuit simulations, vastly surpassing the capabilities available from commercial software tools.

Contribution to the Stockpile Stewardship Program (SSP)

Both the ITS Monte Carlo and Xyce™ codes support SSP areas. Over the next two years, we anticipate supporting as many as five Stockpile Life Extension Programs (SLEPs) with ITS: W76-1 AF&F, W78 neutron generator (NG), W87 NG, W80, and B61. Such extensive support of the SSP would have been impossible without the new CAD capability of ITS. In FY04, we are performing calculations to assess the internal x-ray radiation in the W76-1 AF&F and the W78 NG. We anticipate doing the same for the W87 NG in the near future. Moreover, the ITS code (along with the Presto, Andante, and Salinas codes) is used to predict thermomechanical shock and structural effects in systems that need to be designed to cope with hostile radiation threats. We are also beginning simulations with ITS for the W80 and the B61 to predict a normal environment phenomenon, the internal radiation environment that occurs because of the intrinsic radiation from the nuclear explosives package. The Xyce™ circuit code is being used to analyze electrical systems for the W80, W76, and B61.

Benefits to ASC and to Sandia

The improved CAD version of ITS can be used to assess rapidly radiation-hardness design issues (the design-to-analysis process was reduced from a year to weeks with this CAD capability). This will allow more rapid, improved designs of radiation-hardened components for qualification. The better coupling between radiation-transport and circuit-analysis codes will also allow circuits and ASICs to be designed with significantly less margin, greater robustness, and reduced expense. Larger, more complex circuits can be simulated than ever before, so interface issues can be addressed without hardware fabrication. When functional blocks are simulated separately, design flaws or parasitic coupling (cross-talk) can be missed. If the flawed designs are fabricated, extra costs (hundreds of thousands of dollars) to the customer and inability to meet Department of Energy (DOE) / Department of Defense (DoD) production deadlines can result. Xyce™ can simulate large (>250K) transistor count circuits rapidly in days (not weeks) and aid the ASIC designers at Sandia.

Future Developments

The new ITS CAD capability will support the simulation of other phenomena that arise under hostile environments, including thermo-structural response and cavity system-generated electromagnetic pulse effects. Efforts are under way to improve the computational efficiency of CAD-based simulations, possibly through faceted representations of surfaces generated by the Cholla component of CUBIT. Improvements in ITS physical and numerical algorithms are also under way.

For the Xyce™ code, future work includes (1) the development of radiation-response models for ASICs and their inclusion in a complete circuit model, (2) more accurate determination of parasitic elements, and (3) enhanced linear solvers and preconditioning methods from the Trilinos library. Finally, we will continue to improve validation of both ITS and Xyce™ for radiation effects through our important links to Campaign 7 experimentation.

Modeling Removable Epoxy Foam to Support the W76 and W80

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This work demonstrates how ASC can conduct leading-edge research while developing useful models to solve today's problems.

Description

Both the W76 and W80 AF&F use a Removable Epoxy Foam (REF) for encapsulation. Safety concerns and design guidance necessitate the

1. Development of a decomposition chemistry and response model to predict this response and an
2. Understanding of the thermal, chemical, and mechanical response of REF to abnormal thermal environments, such as fire.

A Simplified Removable Epoxy Foam (SREF) chemistry model has been developed to describe decomposition of polymeric foam exposed to high heat fluxes. The SREF model considers polymer fragments that subsequently evolve into the gas-phase based on vapor-liquid-equilibrium constraints. Percolation theory is used to describe the fragment distribution. The SREF chemistry model was implemented into the ASCI code Calore to describe the macroscopic response of the foam. Figure 1a shows calculations done with Calore. Calore is a thermal/chemistry code that uses element death and dynamic radiation enclosures to describe the developing enclosure. Calore does not solve the momentum transfer and therefore material relocation due to flow. The flow simulations include chemical kinetics, phase transitions, and material flow based on the developing viscosity. The coupled-physics model is solved using a multi-physics, finite-element code Goma capable of tracking moving liquid-vapor and solid-liquid interfaces. Figure 1b shows a 2-D snapshot of foam degradation when heated on the side.

Technical Significance

Modeling flow of decomposing foam including phase transitions is challenging. In this work, the model is further complicated by several factors: complex polymeric materials, radiation heat source, gravity-induced flow, and pressurization. In the past, liquefaction of the foam was considered negligible for modeling unconfined decomposition of polyurethane foam. This was not adequate for REF100, especially when the decomposition products were confined, since liquid formation was significant. Solid material dissolves at elevated temperatures (T > 300 °C) partially because of the rigid polymeric network becoming soluble by its own lightweight decomposition fragments. The complex physics associated with flow of decomposed foam has not been addressed in detail in the published literature.

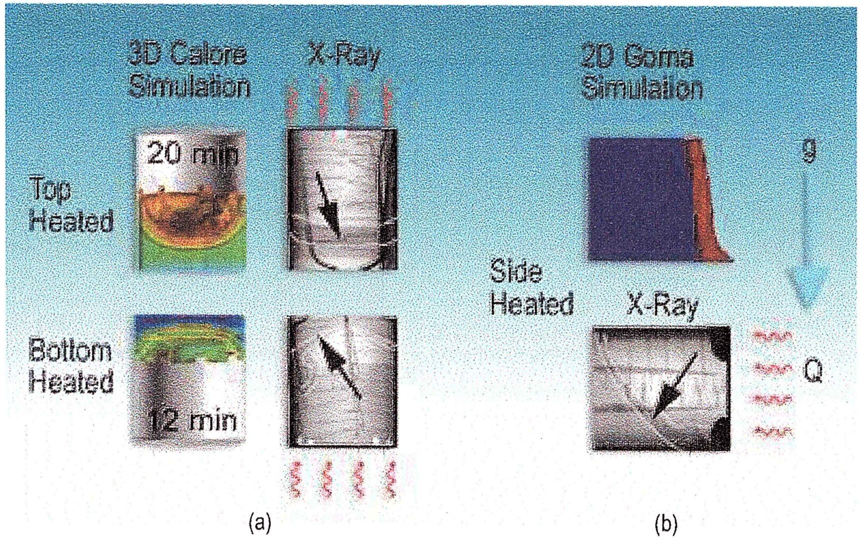
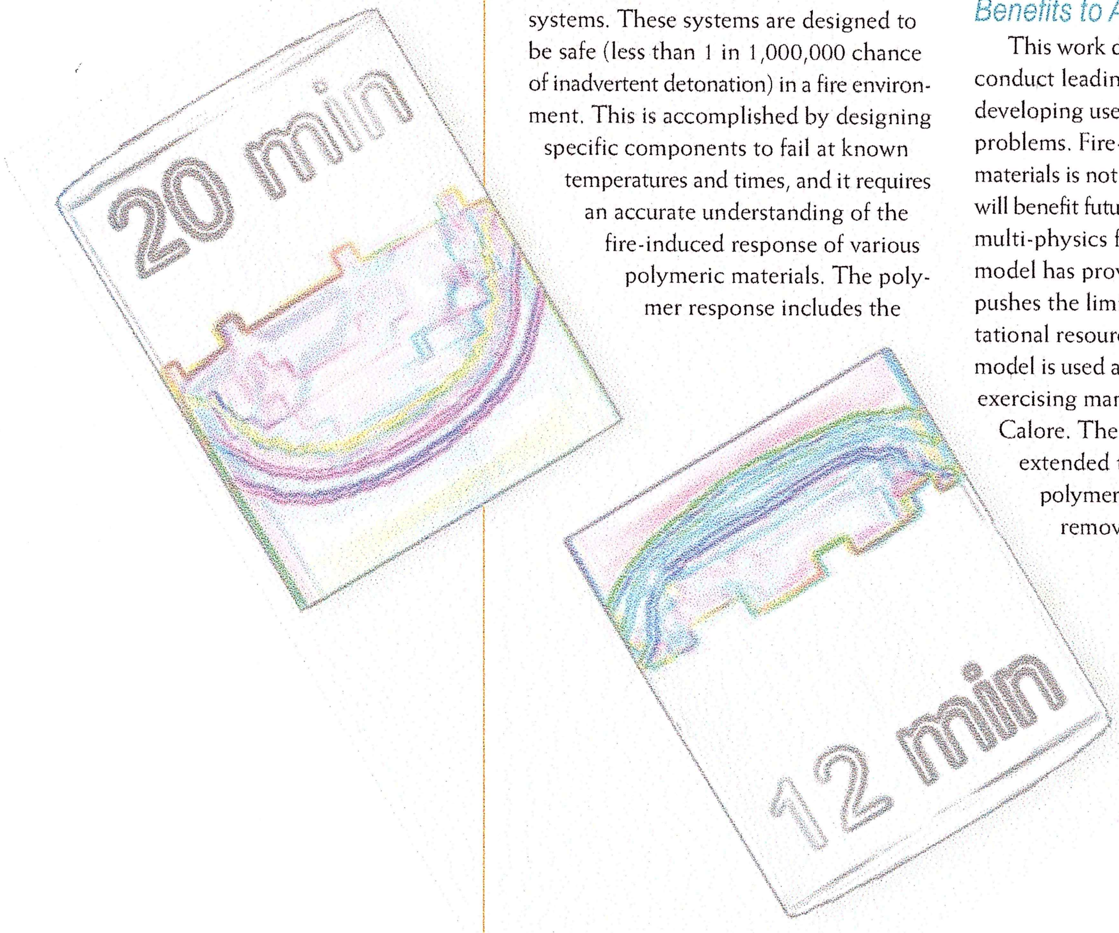


Figure 1. Comparison of REF in a 9-cm-diameter can exposed to fire-like heat fluxes at various orientations. Three-dimensional Calore modeling results and their corresponding x-ray images are shown on (a) while 2-D Goma modeling results are shown on (b). The decomposition front location is highlighted in the x-rays, using a thick black arrow. White lines indicate estimates of phase interfaces by visual judgment. Significant flow effects are observed for the bottom- and side-heated experiments.



Contribution to the Stockpile Stewardship Program (SSP)

REF encapsulates thermally and mechanically sensitive components within the firing set of the W76-1 and W80-3 systems. These systems are designed to be safe (less than 1 in 1,000,000 chance of inadvertent detonation) in a fire environment. This is accomplished by designing specific components to fail at known temperatures and times, and it requires an accurate understanding of the fire-induced response of various polymeric materials. The polymer response includes the decomposition front velocity/location, pressurization of sealed systems, formation of liquids, relocation of polymeric liquids, etc.

Benefits to ASC and to Sandia

This work demonstrates how ASC can conduct leading-edge research while developing useful models to solve today's problems. Fire-induced liquefaction of materials is not limited to foam. This work will benefit future modeling of multi-phase, multi-physics flow problems. The SREF model has proved extremely useful and pushes the limits of the ASC computational resources, especially when the model is used at full grid resolution, while exercising many of the capabilities of Calore. The methodology can be extended to other decomposing polymers of interest to Sandia (e.g., removable syntactic foams).

Future Developments

The near-term goal of the REF model research is to address pressurized systems that may have different modes of decomposition. In the long term, this analytical capability (software and engineering knowledge) is expected to apply to safety studies of all polymeric-based foam candidates. Results of the SREF model will be compared to real-time x-rays of foam in a can exposed to fire-like heat fluxes. Pressurization of sealed systems will also be considered. The model will be extended to syntactic removable foam, which is expected to behave similarly except for the substitution of glass microballoons for bubbles created using the blowing agent.