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Modeling the Thermal and Structural Response of Engineered Systems to Abnormal Environments

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Introduction

Sandia National Laboratories (SNL) is engaged actively in research to improve the ability to accurately predict the response of engineered systems to thermal and structural abnormal environments. Abnormal environments that will be addressed in this paper include: fire, impact, and puncture by probes and fragments, as well as a combination of all of the above. Historically, SNL has demonstrated the survivability of engineered systems to abnormal environments using a balanced approach between numerical simulation and testing. It is necessary to determine the response of engineered systems in two cases: 1) to satisfy regulatory specifications, and 2) to enable quantification of a probabilistic risk assessment (PRA). In a regulatory case, numerical simulation of system response is generally used to guide the system design such that the system will respond satisfactorily to the specified regulatory abnormal environment. Testing is conducted at the regulatory abnormal environment to ensure compliance.

In conducting a PRA, risk is determined by the product of probability and consequence. Therefore, it is often necessary to evaluate many low-probability, but high-consequence, abnormal environments. Two types of numerical simulation tools are required to predict system response for PRA's: 1) PRA-compatible numerical tools that can be exercised over a large accident parameter space within computational constraints, and 2) high-fidelity deterministic numerical simulation tools that are used to develop and verify the PRA-compatible tools. Both types of numerical simulation tools are used to predict system response over a range of accident parameter values for which limited test data are available. Testing is conducted to validate the simulation tools, particularly at high-risk abnormal environment conditions. Expert opinion is used when neither test data nor numerical simulation results are available.

Figure 1 shows the relationship between a suite of deterministic models used to support a probabilistic risk assessment. The models are exercised by running them hundreds to thousands of times with different values of accident parameters. In order to be computationally feasible, these models

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must be simplified, yet must correctly simulate the dominant transport mechanisms. The accident parameters are characterized in terms of probability distributions. Each model must accept as input the accident parameters and the output from the previous model. The accident parameters and model output variables must be carefully chosen so that all important parameters affecting system response are included.

Thermal Response

Figure 2 categorizes the information that is necessary to model the thermal response of a system to a crash followed by fire. It is necessary to describe the distribution of fuel and the fire environment, which are discussed in the paper, "Development and Experimental Validation of Computational Methods to Simulate Thermal and Structural Environments." This paper will describe areas of research that are required to predict the response of the system, categorized as follows: predicting the coupling between a fire and the response of a container, the response of a container, the characterization of critical material response, the simulation of radiation-intensive transport for very large, complex geometries, and the reponse of a device within a container.

Coupling Between a Fire and the Response of a Container

When a container is subjected to a fire environment, the thermal response of the container and the fire may become coupled. This complex environment requires a model that solves the coupled radiative transport, energy and momentum equations for the flowfield in addition to the energy equation within the container. A combustion model and soot production model must also be included. Although significant detail is required to obtain a predictive capability, radiative transport normal to the surface of the container is the dominant mode of energy transfer in these problems. Convective effects are typically limited to 25% or less of the total surface heat flux acting on the container. Recent efforts have focused on developing PRA-compatible deterministic models that incorporate a simplified formulation of the dominant heat transfer mechanisms. Since the dominant mechanisms associated with varying fire conditions are modeled, object response trends can be estimated over an expanded range of conditions.

PRA-compatible models have been developed for geometries including a vertical flat plate, an inverted flat plate (that is, a plate oriented such that the surface is horizontal and is subjected to impinging flames), and a cylinder in cross flow. All of the simplified models include radiative heat transfer between a gray-diffuse surface and a gray gas, and advection of energy by the buoyant gas plume. Radiative heat transfer is considered only in a direction normal to the object surface. Scattering of radiative energy is neglected, since these models are intended for hydrocarbon pool fires. Flow fields are modeled using solutions from potential flow theory and correlations are included to model convective effects. Other transport issues are represented by empirically determined parameters. Computational times are consistent with assessing a number of scenarios within a PRA.

These models have sucessfully illustrated the coupled responses between the object and the fire environment that have been observed in experimental data. When used in conjunction with a conduction code to model the object thermal response, these simplified models have been used to identify a regime specified by nondimensional parameters within which the fire can be reasonably approximated as a blackbody radiant heat source. When the blackbody approximation applies, the thermal response of the object and the fire environment are not coupled. Outside of this regime and early in the transient, reductions in net heat fluxes up to 65% are predicted by the coupled model as compared to results obtained using the blackbody approximation (see Figure 3). This reduction in the initial heat flux produces lower surface temperature predictions from the coupled model. Due to the initially reduced surface temperatures, the coupled model net heat flux exceeds the blackbody net heat flux with increasing time. For radiation Biot numbers, Bi_{rad}, greater than 5, or values of the radiation parameter, N_{rad}, less than 10^{-2}, the differences inherent in treating the media as a participating media or a blackbody are negligible and the use of uncoupled thermal reponse models for the object and fire environment is valid.

Response of a Container

A suite of high-fidelity finite element codes have been developed to simulate system response to the abnormal environments defined above, including a three-dimensional thermal code, and several mesh and visualization tools. An advanced finite element code has been developed for the solution of steady-state and time-dependent, multidimensional, nonlinear heat conduction problems and related diffusion problems. Multiple materials are allowed with heterogeneous, isotropic or orthotropic behavior and properties that vary with time, spatial location and temperature. Coupled heat and mass transfer problems, heat and enclosure radiation, and heat and chemistry can be solved. Current development activities are focused on coupling structural and thermal codes to simulate combined abnormal environments involving structural deformation and failure followed by fire. Advanced solvers are under development to include moving boundaries, birth and death of elements, and phase change.

Similar to the PRA-compatible models described for the fire/response coupling, PRA-compatible system response models have been developed and exercised tens of thousands of times over a broad parameter range. An example of predictions for the thermal response of a transporter van in a fire are shown in Figure 4. In general, predictions from the PRA-compatible code agree reasonably well with that from the detailed model, and run approximately 3000 times faster.

Characterization of Critical Material

The characterization of material response to abnormal environments is critical to predict the response of the system. Numerical models are being developed to predict the nonlinear thermal and structural behavior of materials, including decomposition of organic materials and melting of metallic materials. Our approach is to conduct tightly coupled numerical and experimental investigations that will characterize the dominant physical processes needed to develop a comprehensive predictive tool. The model describing the heat and mass transfer within the decomposing material consists of a series of coupled, partial differential equations with a sizable number of material parameters. The governing equations are based on the following assumptions: 1) local thermal equilibrium exists between the fluid and the solid, 2) the material devolatization and oxidation can be represented by Arrhenius relationships, 3) decomposition gases can be represented as a single ideal gas, 4) decomposition gases are nonreactive, and 5) the fluid motion can be governed by the Darcy-Forcheimer equation. Materials studied to date include: rigid polyurethane foam, ceramic fibers, wire mesh, woods including redwood and balsawood, carbon phenolic, and aluminum honeycomb. Pyrolysis and oxidation rates and heat transfer through the thermally degraded materials are of interest.

Radiation-Intensive Transport and Device Response

In order to accurately predict the response of objects within containers subjected to a fire environment, it is necessary to model the radiative transfer that occurs between a large number of surfaces (greater than 5000) within the enclosure. Specialized numerical tools have been developed to enable the solution of this complex problem within the constraints of computer resources and time. One tool calculates .he surface-to-surface view factors using the hemicube algorithm, given a three-dimensional finite element data structure. An internal database is used to efficiently store and access the view factors. The database incorporates several user-selectable compression/decompression techniques such as byte run length encoding, word run length encoding, and Limpel-Ziv encoding, which allows very large view factor matrices to be stored in core memory while minimizing large disc input/output. The radiosity matrix equation can be solved using the traditional Gauss-Siedel algorithm or a progressive refinement algorithm.

When both conduction and radiation are important transport mechanisms, the use of the sequential, or Picard, iteration technique does not always converge. An algorithm has been developed to solve fully coupled nonlinear heat conduction and enclosure radiation problems. The problem is cast as a single, fully-coupled system of nonlinear algebraic equations in which both the nodal temperatures and the radiative fluxes are kept as unknowns. The system is solved using Newton's method with a sparse iterative solver, providing better stability and faster convergence, but at the expense of increased memory requirements.

Structural Response

To determine the structural response of an engineered system in a severe crash environment it is first necessary to describe the initial conditions. These are the velocities, orientations and target hardness for the impact problem, and in addition, characterize of the probes and fragments for the penetration problem. This was discussed in the paper, "Development and Experimental Validation of Computational Methods to Simulate Thermal and Structural Environments." The response simulation is primarily dependent upon the computer code capability for transient dynamics of nonlinear solid mechanics. In the following we describe the computing environment at SNL, and the research being conducted in transient dynamics codes. Then, two examples are presented that are representative of impact and penetration calculations.

Finite Element Transient Dynamics

The computing environment for structural analysis consists of several different components tailored to provide maximum efficiency. At the desktop, engineers are provided with a SUNworkstation which is used only to display results. The local workstations are used primarily as an X-Window display device for data generated elsewhere. The local workstations are networked to a compute server cluster consisting of one HP 755, and two HP 735 computers. The compute servers are used for preprocessing and postprocessing all analysis data and for documentation. The compute servers are equipped with considerable memory and a 12 Gigabyte disk farm. All of the actual analyses are performed on supercomputers. Currently all production analyses are run on either the Cray YMP/864 or the Cray YMP/264. Analyses are archived on one of the two Network Storage Servers (NSS) which provide over 1 Terabyte of disk space.

Research is being conducted in the general area of transient dynamics algorithms for use in finite element computer codes. Two-dimensional and three-dimensional codes are employed to simulate large deformations of highly nonlinear materials subjected to extremely high strain rates. These Lagrangian finite element programs use an explicit time integration operator to integrate the equations of motion. Four-node, uniform-strain, quadrilateral elements are used. These include an adaptive time step control algorithm for improved stability, a robust hourglass control scheme, and an efficient contact algorithm for interacting and sliding material surfaces. All constitutive models are cast in an unrotated configuration defined by the polar decomposition of the deformation gradient.

The robustness and the efficiency of these transient dynamics codes is greatly dependent on automatic mesh generation of arbitrary solid geometries. Previous work has resulted in the development of a two-dimensional automatic meshing algorithm called PAVING. This algorithm is capable of automatically meshing a completely arbitrary two-dimensional surface with an all-quadrilateral mesh. Research is currently being conducted at Sandia to extend the PAVING algorithm to mesh three-dimensional surfaces. Called PLASTERING, this algorithm is capable of meshing an arbitrary three-dimensional solid with an all-hexahedron mesh. These new meshing algorithms are expected to generate very large databases for three-dimensional problems, thus the transient dynamics codes need to be implemented on massively parallel computers. One of the main problems with massively parallel computing is domain decomposition, a strategy for deciding which processor will process which elements.

It is critical to have efficient contact surface algorithms because nonlinear structural problems for abnormal environments usually involve multi-body impact, self-contacting surfaces, and tearing and eroding surfaces. We have develop a new algorithm that uses a fast, efficient memory search to determine proximity of surfaces, and a detailed contact check using projected movements of surfaces. This algorithm is implemented as a serial process for the Cray vector machines. For the massively parallel implementation, a different, global parallel contact search is needed.

Example of Calculation for Impact

This transient dynamics calculation considers the end-on impact of a shipping container onto an unyielding target at an impact velocity of approximately 140 m/s. The container has a cylindrical geometry, and is constructed of radial and longitudinal layers of redwood placed inside a highly ductile stainless steel outer container. The orthotropic behavior of the redwood is modeled using alternating layers of hard and soft crushable materials, with contact surfaces defined between each layer. The results of the calculations are shown in Figure 5. Note the numerous locations where redwood layers have separated from their inital neighboring layers, and where the ductile outer container wall has folded back onto itself.

Example of Calculation for Penetration

This transient dynamics calculation considers the penetration of steel plates by maraging steel rods at 100 to 400 m/s impact velocities. A maximum equivalent plastic strain criteria is employed to govern the progressive failure process in the target plate. When the strain criteria is reached, the element is removed from the model and a new surface is created. A dissipative viscous pressure is introduced to allow energy to be dissipated as new surfaces are formed. Calculated results are shown in Figure 6. Under these impact conditions, little damage is inflicted on the marging steel rod while the steel target fails by shear-induced plugging.

Combined Environments

The tools being developed for analyzing combined thermal/structural environments include loosely-coupled and tightly-coupled thermal—mechanical analysis codes. A loosely-coupled analysis is performed in a serial mode. First, one calculation (thermal or structural) is performed for a certain period of time. Then, relevant data (temperatures or displacements) are transferred to the second computer code and calculations are continued using the new data from the first code. This process can be repeated indefinitely, but all calculations are performed in a serial mode. In a tightly-coupled analysis, both the thermal and structural calculations are performed simultaneously and communication of the relevant data between the two codes is fast. It may be possible to write codes which directly solve the mathematically coupled thermal and mechanical governing equations, but the resulting finite element formulation would be very complicated and most likely not applicable to large, multi-dimensional, complex geometries.

The loosely-coupled codes will be used to perform multi-step thermal--mechanical analyses including:

- Thermal stress calculations of a system which experiences quasistatic heating followed by transient dynamics from ignition of an energetic material.
- Thermal response calculations of a system which is deformed or damaged prior to the thermal event.
- Structural response calculations arising from energy release (pressure) due to material chemical reactions and from material loss due to melting, burning, or degradation.

The tightly-coupled codes will be used to perform analyses in which there is a strong and necessary communication between the thermal and mechanical response. An example of a tightly-coupled process is the cookoff response of foaming propellants in which extreme temperature causes degradation of binder and oxidizer with associated gas generation and void formation. Gas generation leads to pressure buildup, which imposes stresses on both the propellant and the confining material. In some cases, this can lead to large deformations and possible breaching of the confinement. The violence, or degree of the confinement breaching, is directly related to the pressure and pressure rise at the time of rupture. Development of tightly-coupled codes is also being done for other potential applications including welding, single-phase and multiple-phase porous flow, and electromechanics.

Another research effort in coupling mechanics phenomena uses a numerical method developed in the astrophysics community called smooth particle hydrodynamics (SPH). This is a gridless Lagrangian hydrodynamic technique. Requiring no mesh, SPH can model materials with zero shear strength, such as gases, fluids and explosives bi-products. It can also be used to model material fracture, large shear flows, and penetration. Material is modeled as particles that have their masses smoothed in space. The density is computed at a point by summing the contributions of the smoothed particle masses in the vicinity of the point. The SPH technique is currently being implemented within existing transient dynamics codes for solids and structures; the SPH particles are simply an additional element type in the code. This coupling of SPH and structures codes will allow analysis of fluid/solid interaction problems, such as an airplane crash into a lake. The solid materials would be modeled using quadrilateral solid elements, and the fluid would be modeled using SPH methods. A simple calculation which illustrates this coupling of fluid and structural mechanics is shown in Figure 7.

Opportunities for Collaborative Research

Develop an ability to predict burn-through.

Material Decomposition:

The ability to predict smoke generation, devolatization and oxidation rates as a function of heating rates, and the effects of aging on material performance.

Data is needed to develop an empirical/theoretical relationship that predicts the thermal conductivity or density of the foam as it decomposes.

Determining the evolution of the pore structure as a function of heating rate is key in predicting the mass flow rate of pyrolysis gases. In particular, the pore structure of the foam is of considerable importance for both heat and mass transfer. The experimental data is needed to develop empirical/theoretical relationships describing pore structure/permeability evolution as a function of time, temperature, and mass fraction of volatiles.

Experimental data is needed to develop representative chemical reaction rates.

In addition to the phenomenological experiments, data from larger-scale experiments are needed to investigate global behavior, such as mass-loss rate as a function of specimen size, heating rates, environmental conditions and foam orientation. This data are also needed to validate the system response model.

Mechanical property data on foams and other materials at high strain rates and temperatures is needed. Material constitutive models need to be developed for implementation in finite element codes.

Numerical Techniques:

Research is needed to extend algorithms in finite element codes in the areas of mesh generation and visualization, contact surface algorithms, adaptive analysis methods, and massively parallel implementation.

Research is needed to extend capability to perform tightly coupled simulations involving thermal, structural, fluid and chemical processes.

Full- and scale-model test data to validate calculations.

Analytical, or database management, methods to construct simplified structural models in the PRA codes.

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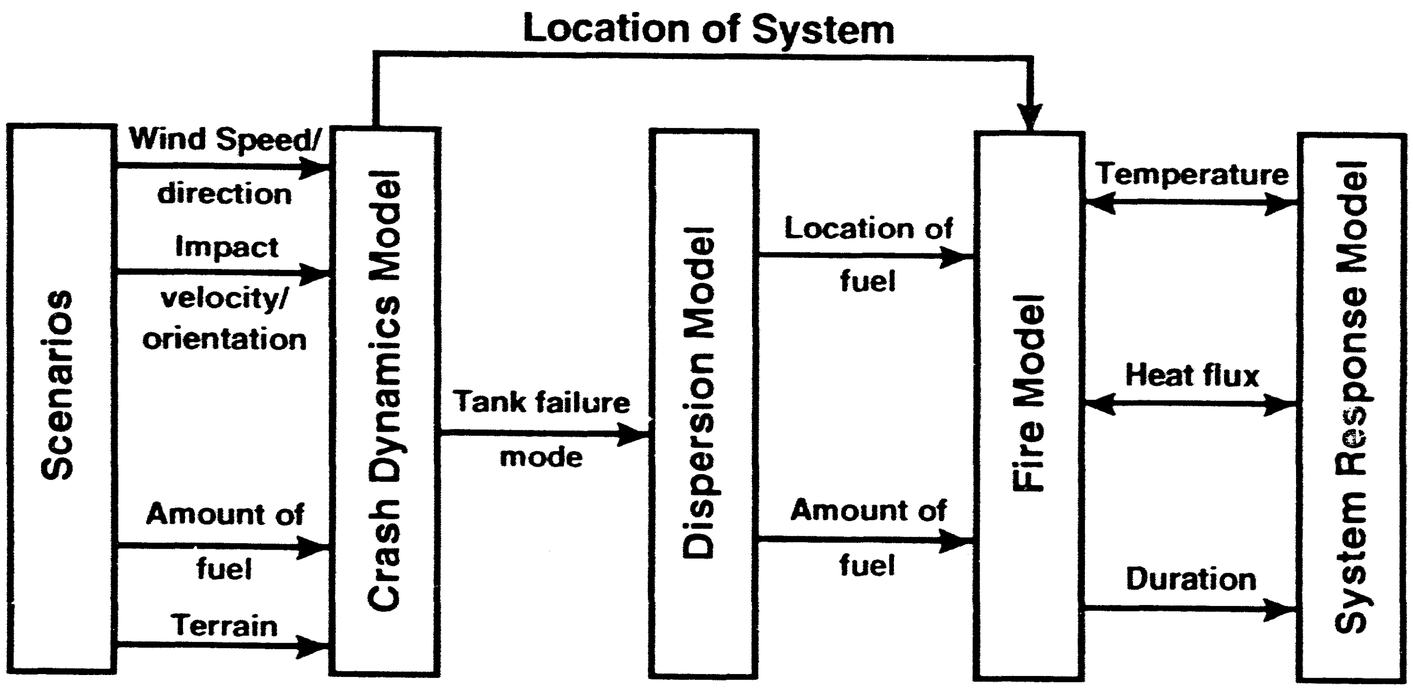


Figure 1. Technical Approach to Predict System Response to Accident Scenarios

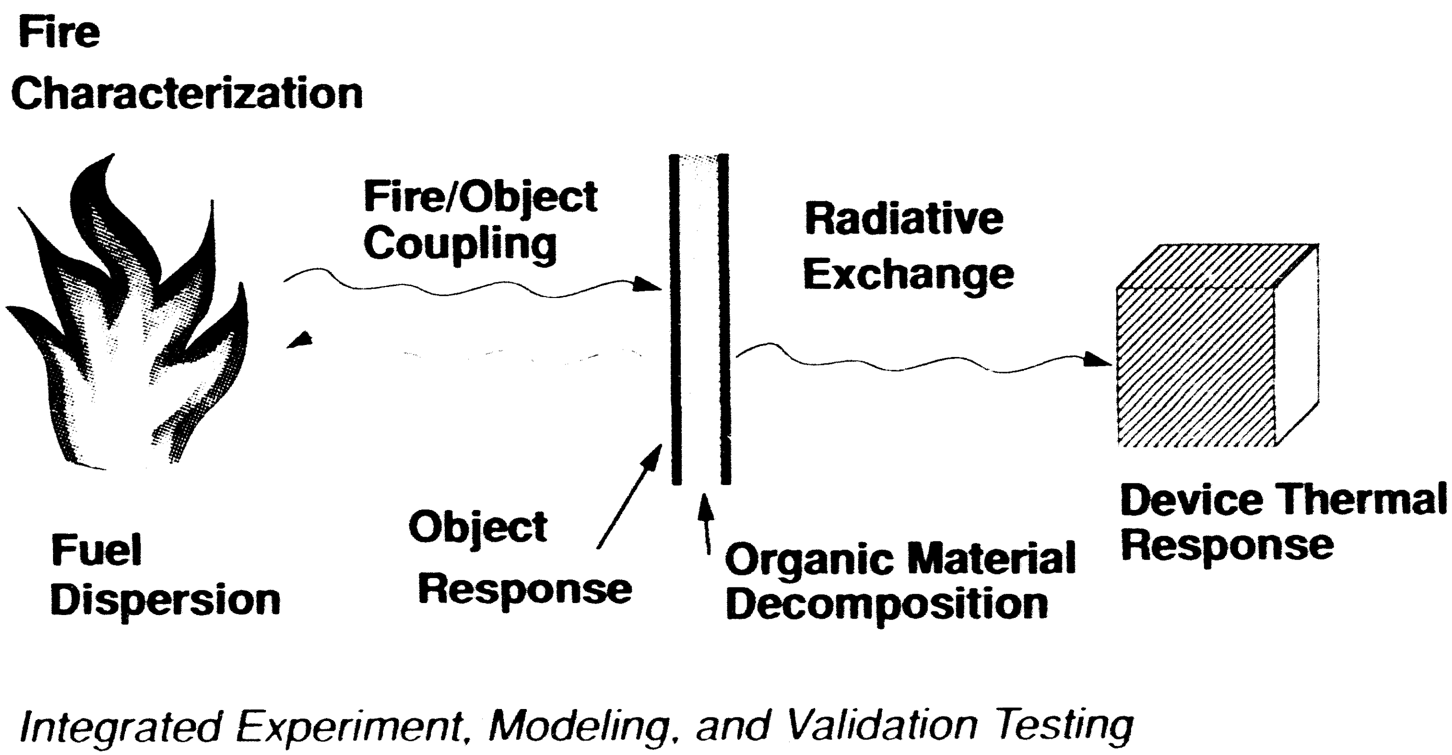
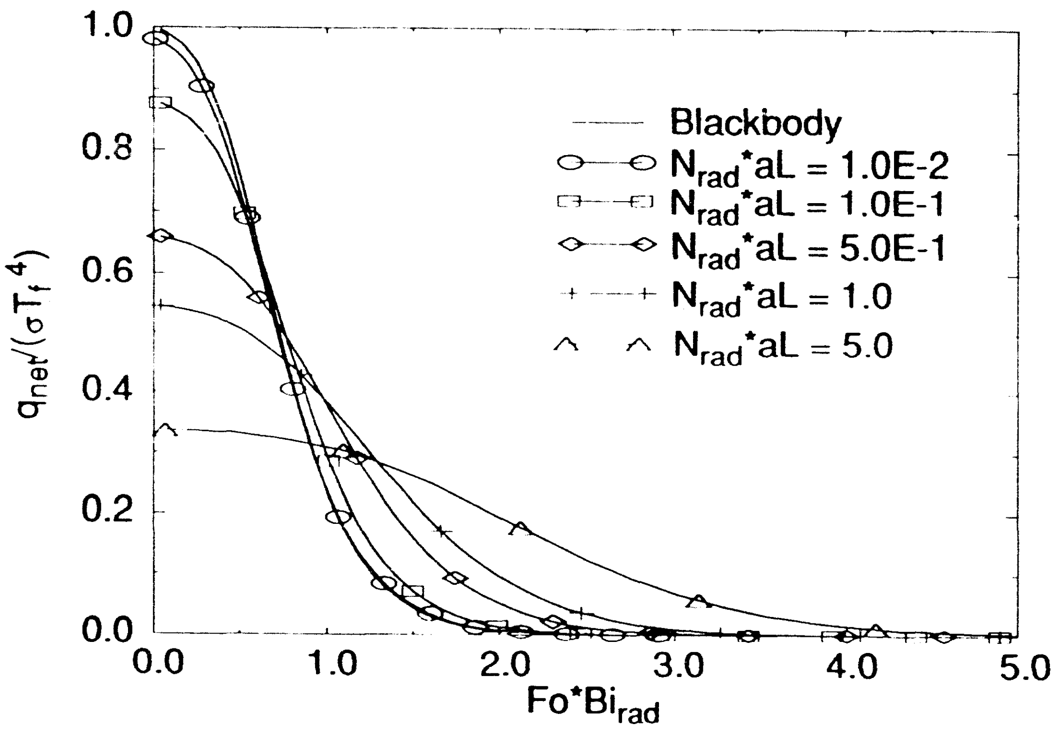


Figure 2. System Response to a Crash Followed by Fire



Transient Nondimensional Heat Flux, $T_{i,w}/T_f = 1/4$, $Bi_{rad} = 0.1$

$$N_{rad} = \frac{\sigma T_f^3}{\rho_f c_p u_\infty}$$

$$Bi_{rad} = \frac{\sigma T_f^3 w}{k_s}$$

- **Response Approaches a Blackbody for N_{rad}*aL < 1.0E-2**
- **65% Reduction in Net Heat Flux Early in Transient for N_{rad}*aL=5.**

Figure 3. Predictions by PRA-Compatible Fire Model Showing Coupled Object/Fire Thermal Response

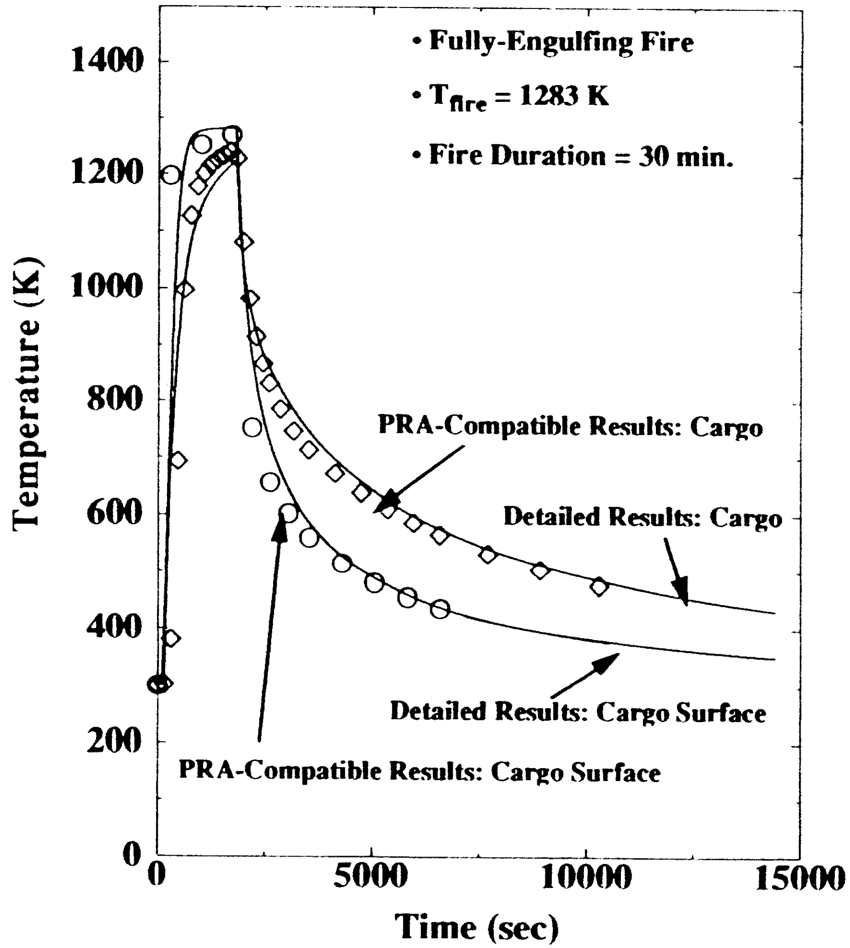


Figure 4. Comparison of PRA-Compatible and Detailed Model Results for Transporter Trailer

- Large deformations
- Non-linear material response
- Numerous contact surfaces

Figure 5. Prediction of Shipping Cask Impact onto Unyielding Target

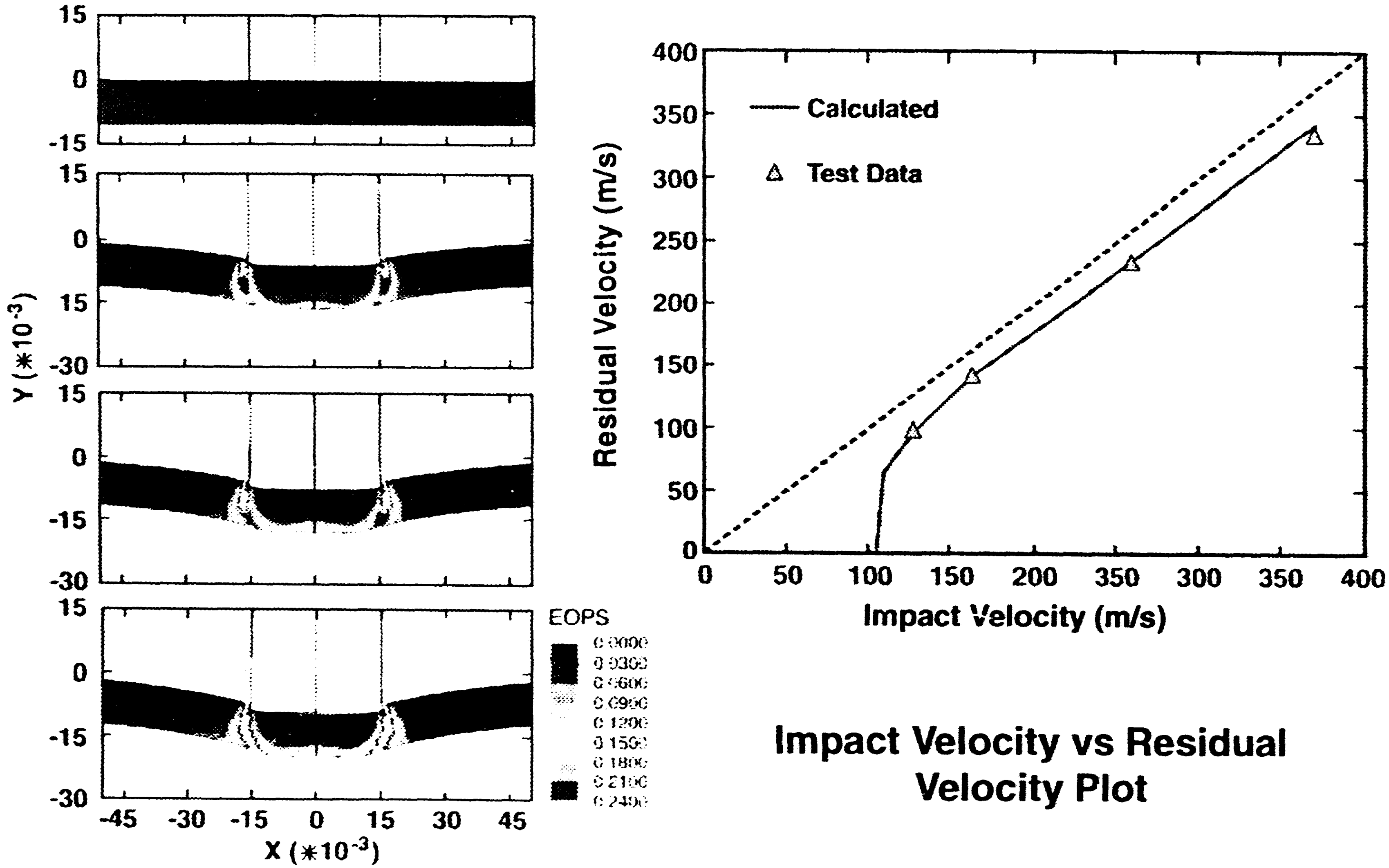


Figure 6. Prediction of Steel Plate Penetration by Steel Rod

- Boat impacting water
- Fluid/structural interaction
- Large structural deformation
- Gridless fluid model

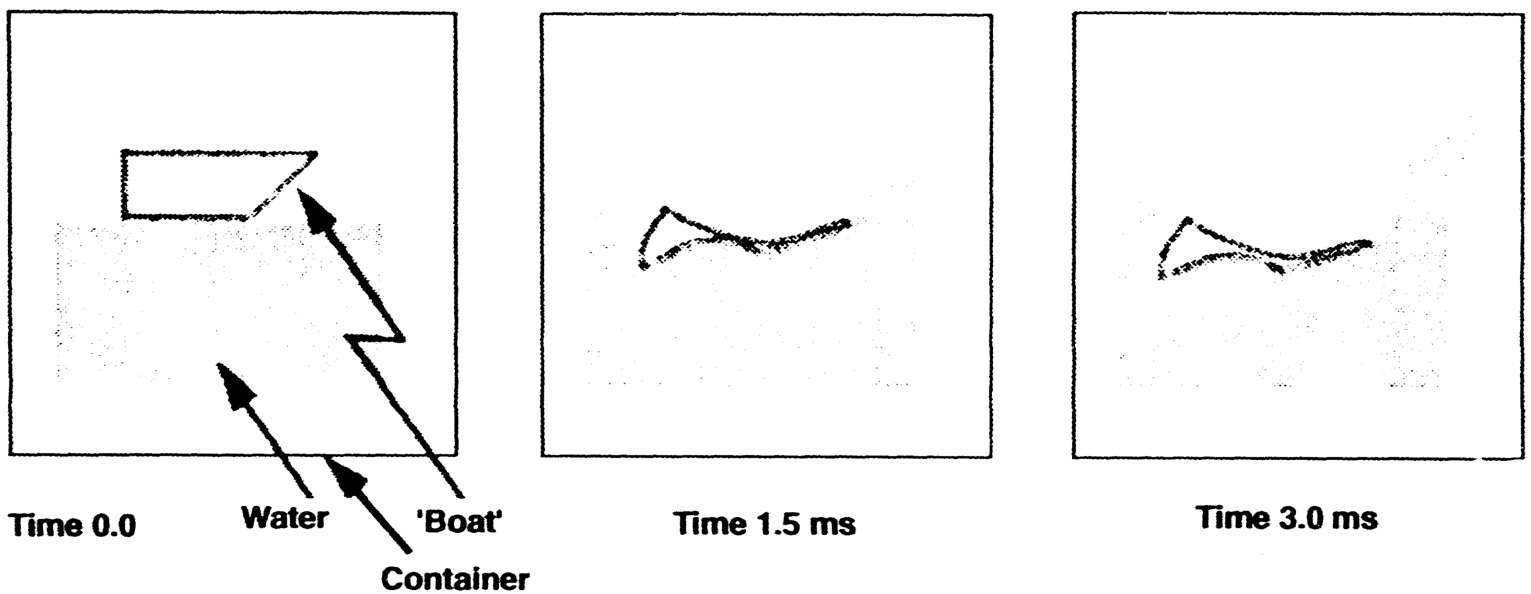


Figure 7. Example Calculation of Coupled Fluid and Structural Mechanics

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