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COMPUTATIONAL METHODS FOR SIMULATING ROCKET MOTOR COOKOFF

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ABSTRACT

To qualify for transportation, munitions are normally subjected to a fire environment in conditions in which they are shipped. They are required to meet specified target conditions to allow the occurrence of an accident to be mitigated, and to minimize further loss. Tests that are conducted are expensive, and they are difficult to instrument in a way that can inform safety engineers regarding system performance. To aid this effort, modeling and simulation tools can be leveraged. Here, we describe an activity to simulate the behavior of a booster rocket in an engulfing fire. Some of the complexities associated with the simulation effort are described. Conjugate heat transport is simulated. Models include heterogeneous properties and algorithms for thermal decomposition. Several methods of coupling between the solid phase and gas phase simulation tools are explored. We believe this activity represents a good example of the current state of the community in terms of modeling and simulation capabilities. Results suggest the models can give a bounded prediction of the test environment, and potentially aid in safety assessment activities. However, some discussion on the current modeling approach is warranted so that a roadmap for future model development activities can be developed.

INTRODUCTION

Munition and munition-related material transportation can be risky because transportation accidents can be severe. The energy of the accident has the potential to release additional energy contained in the shipment package. Prior to receiving approval to ship munitions and related materials, there is a process to approve the packages that is based in part on qualification activities. This may involve demonstration tests that create hazardous environments. The two principal environments of concern are structural and thermal. One thermal hazard postulates a fire that engulfs the package. This is a credible accident scenario, as transportation fuels can be a source for fire hazard.

Experiments that are performed with munitions or boosters in fires are difficult to instrument because measurement equipment tends not to survive the environment. Thus, the interpretation of the tests is a challenge, which can be ameliorated through use of numerical models. Numerical models are improving in their capability, but have some challenges that relate to missing physics, and the difficulty associated with modeling a variety of time and length scales.

Sandia National Labs (SNL) develops and maintains the SIERRA suite of codes. SIERRA is an architecture under which engineering models are deployed that permit simulation of environments and system responses to those environments. The thermal and structural environments are a particular focus of these tools. The fluid mechanics modules in SIERRA consist of Fuego (which is a low-Mach number reacting flow code for predicting fire environments) and Aria (a multi-mechanics code, which for this project is a heat transport and generalized low Reynolds number flow code). Part of the philosophy of having the codes under a similar architecture is that this will enable code coupling. SIERRA manuals are generally available as unlimited release documents [1-4].

The activity that produced the material in this report was part of a joint collaborative effort between the Naval Surface Warfare Center Dahlgren Division (NSWCDD) and SNL. NSWCDD has the responsibility to perform assessments of munitions for safety. SNL produces the simulation tools, and has experienced users familiar with the tools' capabilities. The collaborative activity was for SNL to add fidelity and capability to the simulations for making assessments for this type of burn scenario. The context for the study was a rocket booster, placed inside of a shipping canister, which had previously undergone a fire test with associated transducer data available for comparison. We have been asked not to release data from the test, so the data will not be a component of this report. The activity leveraged the computing infrastructure at SNL to produce fire simulations relevant to a 15-minute cookoff assessment. The ongoing activity has progressively added fidelity to the model, with the final intent of having the best available representative model for simulating thermal environments. As fidelity is added, the results become the grounds for assessing the significance of model assumptions, and an improved understanding of model uncertainties. Parametric analysis gives a sense for the significance of model methods and assumptions. This paper exhibits some of the results, and evaluates the quantitative effect of some of the model assumptions. In particular, mesh resolution, convection, and radiation approximations are explored.

METHODS

The problem to be investigated includes a fuel-filled pool, 9.1 m by 9.1 m (30 ft by 30 ft) with a depth of 30 cm (1 foot). The test item is suspended above the surface of the pool such that the bottom of the canister is 61 cm (2 ft) above the surface of the fuel. The surrounding region is flat ground for a large distance. The ambient conditions should be considered 1 atm pressure, 26.7 ºC (80ºF) air temperature, and no wind. The pool contains 7570 ℓ (2000 gal) of kerosene fuel that is consumed in 20 min. The kerosene fuel is modeled using a surrogate fuel (octane; C_8H_{18}).

For this report, details of the modeling methods are only presented as they seem relevant to the discussion. The intent of these calculations is to demonstrate methods and sensitivities, and not to produce defensible quantitative results. Thus, the full reproduction of the numerical algorithms, equations, and material property assumptions are omitted. Selected features of the model will be illustrated.

SIERRA permits different module interaction methods for coupled conjugate heat transport simulations. Selected methods for this study are illustrated graphically in Figure 1. Three different methods were employed to assess the fire scenario.

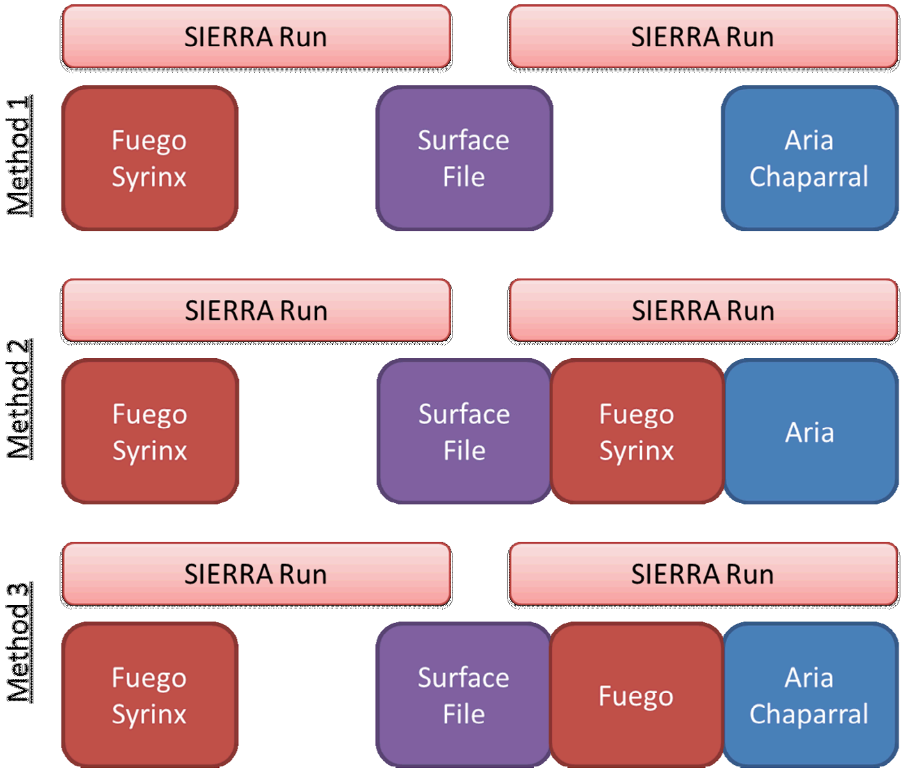
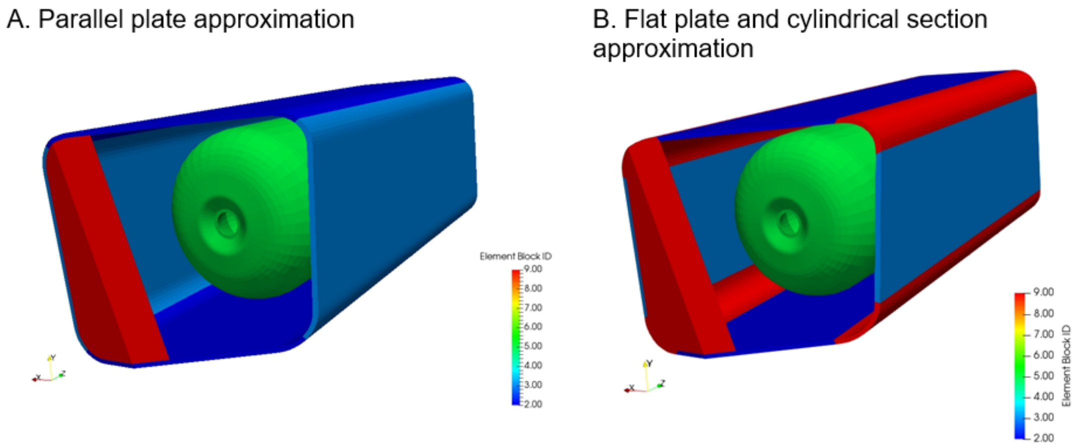


Figure 1. A graphical illustration of the three simulation methods employed for this set of calculations

Noticeably absent from this list is a monolithic SIERRA run that jointly solves the external flow, the shipping container heat transport and reactions, internal radiation and convection transport using a volume method, and heat transport in the booster. Such a calculation is enabled by the code, but is not in this case particularly practical for obtaining results because the joint solver method tends to augment the duration of the simulations by driving the time-step for all physics regions to a low and unsustainable value. This issue may be partially circumvented by sub-stepping.

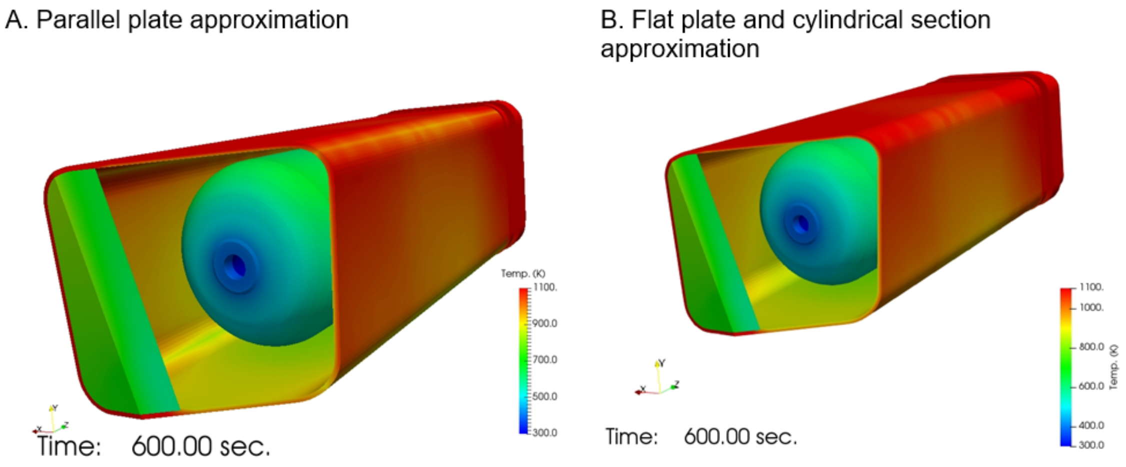
Segregated SIERRA simulations employ a surface mesh region to receive convection and radiation surface parameters from the Fuego CFD calculation. The surface mesh is read for the subsequent SIERRA run to apply boundary conditions predicted by the CFD. CFD calculations were generally too expensive to obtain results for the full 15 minutes of required exposure. For this model, the boundary conditions generally reached a steady condition (this will be illustrated in the results section), and the efficiency of the simulation is augmented by repeating the application of the steady-state conditions to obtain the full exposure time. Because the current models lack physics, including off-gassing of the composite binder and thermal deformations, this is not a particularly bad assumption. As models add fidelity of this nature, more fully-coupled calculations may be necessary.

Among the materials simulated for the canister and booster is a composite shell. This composite has the benefit of being lightweight, pliable, readily shaped, and strong. Composites also tend to be difficult to model thermally due to their significant dependence between thermal conductivity and lay-up direction. Fibers are normally more conductive than the binder, and transfer heat preferentially in the direction of the fibers. To accurately model this feature, a non-isotropic thermal conductivity tensor was developed to vary the conductivity, depending on the direction of transport. The composite model was originally performed assuming flat parallel plates, even though the corners of the container were rounded. The thermal predictions were obviously affected by this assumption, as a thermal seam was apparent at the junction where the model was the least accurate. The accuracy of the thermal model through the rounded segments was improved by segmenting the computational blocks differently, and applying a cylindrical coordinate system tensor to the corner elements. Mesh blocks for the composite flat plat and flat/cylindrical models are shown in Figure 2 (composite in blue). Figure 3 shows the thermal anomaly at the seam for the flat plate approximation, and the more continuous result obtained with the more complex and accurate model.


A. Parallel plate approximation

B. Flat plate and cylindrical section approximation

Figure 2. Two thermal block approximations for the composite portion of the transport container


A. Parallel plate approximation

B. Flat plate and cylindrical section approximation

Figure 3. Two thermal results illustrating the discontinuous result at the seam using the parallel plate method

A variety of meshes were employed for these simulations. Table 1 lists the meshes and gives some basic properties. Fluid meshes varied from 1.6 to 8.2 million nodes. The canister and booster mesh was 0.8 million nodes. The ‘calorimeter’ mesh was the mesh used to capture the fluid results for mapping to the thermal calculation. The representative object was a thermal mock; it was not allowed to heat up in response to the fire conditions imposed on it.

Table 1. A list of the meshes used in this study

Mesh	Code	Nodes	Nominal Size (m)
fluid fine	Fuego/Syrinx	8,202,852	0.05
fluid med	Fuego/Syrinx	3,151,882	0.075
fluid coarse	Fuego/Syrinx	1,663,116	0.10
calorimeter fine	Fuego-conduction	71,344	0.017
calorimeter med	Fuego-conduction	22,021	0.025
canister and booster	Aria	815,564	-
internal fluid coarse	Fuego/Syrinx	66,604	0.02
internal fluid med	Fuego/Syrinx	493,429	0.01

The container that is located 61 cm above the pool surface is 65.5 cm x 65.5 cm x 2.18 m. Further dimensions of the assembly are omitted, and potentially proprietary. Detailed resolution of the aft side of the assembly was omitted, due to complexity and uncertainty in the significance to the thermal race problem of thermal ignition of the propellant. Its contribution is assumed negligible.

A parametric study centered around the importance of mesh refinement, cavity radiation and convection modeling was postulated. The mesh refinement was primarily intended to demonstrate mesh convergence related to the fire calculation. The convection and radiation assumptions were tested to get a sense of the effect of two different modeling approaches for the cavity radiation. Table 2 details the simulations proposed for this study, along with a description of the modules for radiation and convection used. Chaparral is a view factor surface radiation transport method, and is the Aria method for solving radiation. Syrinx is a Discrete Ordinates participating media radiation solver, used in Fuego to simulate complex media radiation problems.

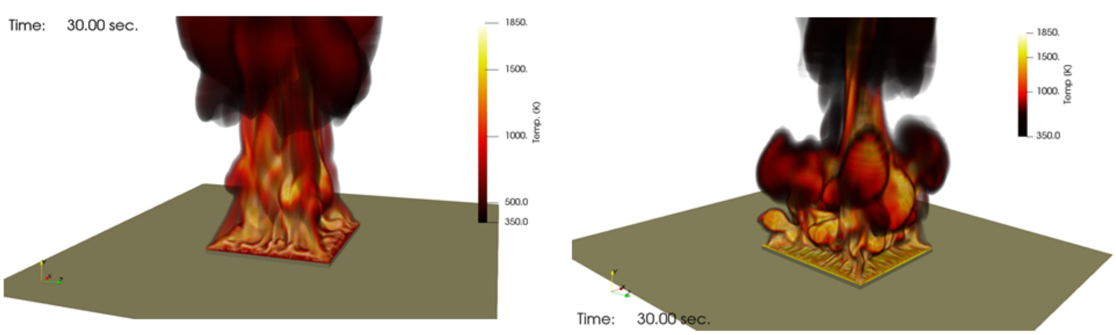
Table 2. A list of the Aria/Fuego jobs completed for this effort

Fire Mesh	Method	Radiation	Convection
coarse	1	Chaparral	Enclosure
medium	1	Chaparral	Enclosure
fine	1	Chaparral	Enclosure
coarse	3	Chaparral	Fuego
coarse	2	Syrinx	Fuego
medium	2	Syrinx	Fuego
fine	2	Syrinx	Fuego

RESULTS AND DISCUSSION

FIRE SIMULATIONS

The simulations included a transient start-up, followed by a relatively steady-state condition. The transient portion of the calculation was considered the first 30 seconds. After this point, the model was producing a relatively constant condition. The resolution resulted in significant observable differences in the formation of instabilities at the toe of the fire, as illustrated in Figure 4. The coarse mesh has noticeably fewer instabilities. The fine mesh also exhibits more complexity in the plume in the higher region.


A. Coarse mesh

B. Medium mesh

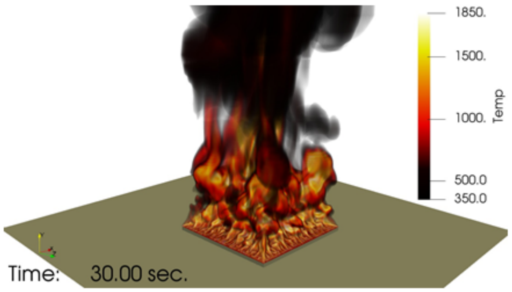

C. Fine mesh

Figure 4. Visualization of the fire using a volume rendering based on the predicted temperature

The nominal Fuego simulations included three mesh resolutions, for which results are desired to suggest mesh independence. Figure 5 shows key surface averaged metrics for the heat transport to the rocket booster. These plots suggest that the scenarios yield relatively similar environmental conditions on the container. On closer inspection, the fine scenario exhibits a lower dynamic range of incident radiative flux, and a lower mean. Tabulating the pseudo-steady variable results (30 second and beyond predictions) in Table 3 shows that the fine scenario resulted in moderately lower incident flux to the booster. This is of moderate concern. Numerical methods are desired to be convergent, although fire models are notoriously non-linear. In particular, the EDC (reaction) model includes some non-continuous assumptions that challenge convergence because of the difficulty integrating the functions of this nature in the domain.

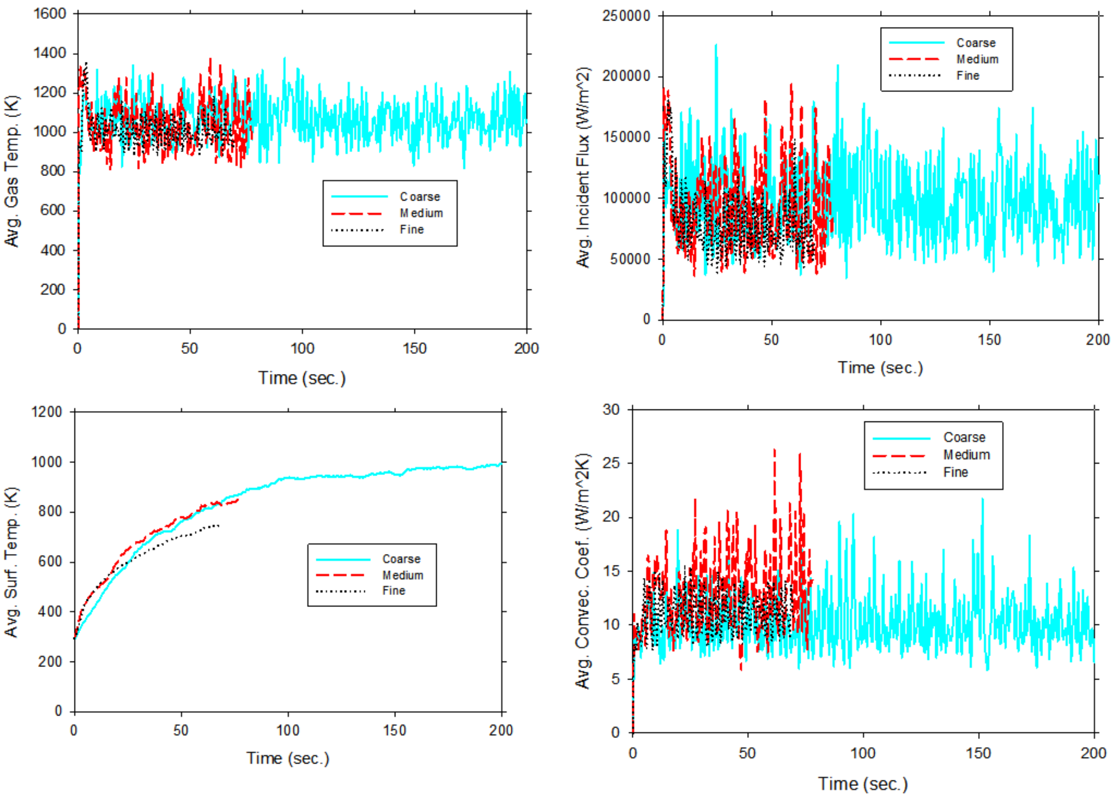
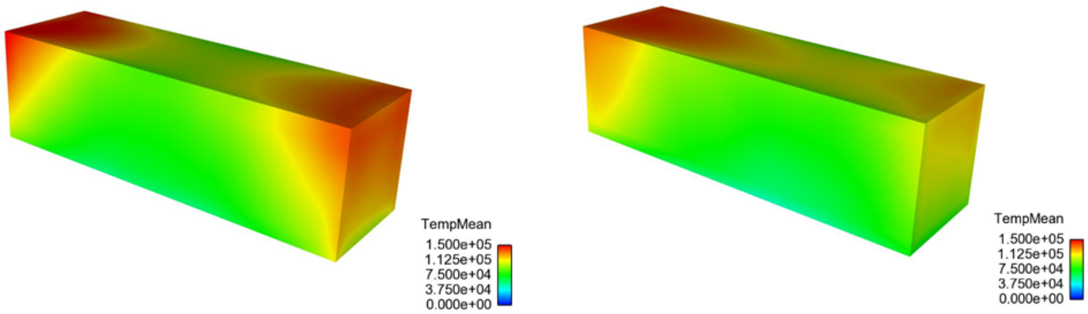


Figure 5. Fuego predicted average boundary conditions

Table 3. Mean values of pseudo-steady variables on the exterior of the container

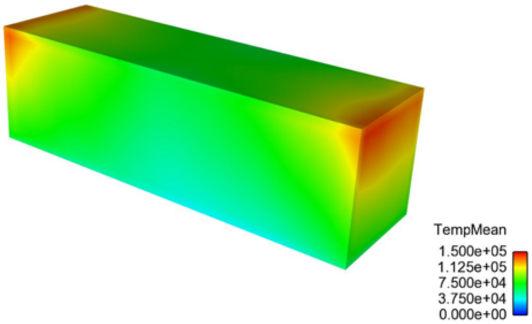
Mesh	**Convection Coefficient**	**Incident Flux**	**Gas Temperature**
Unit	$W/(m^2K)$	W/m^2	*K*
coarse	10.05	95,415	1062
medium	13.22	91,349	1036
fine	10.98	73,635	997

The scenario had been modeled previously with much coarser meshes. The coarse and medium results gave the appearance of convergence, but the fine mesh results suggest the results are not fully converged. Because this exercise was a demonstration exercise, a full exploration of this finding is not completed. Figure 6 shows mean temperature results for the 'calorimeter' mesh. These were averaged for the duration of the simulation from 30 seconds until the end of the Fuego simulation (see Figure 5 for time duration information). The coarse results appear symmetric, much as expected. The medium results are not symmetric. This suggests that there may have been a need for further averaging and longer Fuego simulations. The fine mesh results are more symmetric, but suggest generally lower temperatures. This indicates that the fire generally burned further away from the object in the model predictions for the fine case. The object was not in the most severe location, according to the model. When pool fires burn, there is a fuel-rich region that is roughly conical in shape above the pool surface. The top edges of the container appear hotter, and were better located for a more severe accident scenario.



A. Coarse mesh

B. Medium mesh



C. Fine mesh

Figure 6. The temporal mean incident flux (W/m^2) from three Fuego predictions

THERMAL RESPONSE SIMULATIONS

The thermal response simulations included Aria for simulating the run-away time of the propellant. An Arrhenius reaction rate was assumed for the propellant, with a highly exothermic reaction for the material. A dual-criteria condition suggested termination time. When the temperature of any location within the propellant reached 600 K (327°C) or the rate of change of the propellant reached 30 °C/sec, the propellant was assumed to be in run-away conditions.

Results from the test matrix are shown in Table 4. The effect of the fine Fuego fire mesh (resolution) was the most pronounced effect in these simulations. These scenarios experienced propellant run-away around 2 minutes later than the coarse and medium mesh results, which were more similar in run-away time (within the same minute). The effect of the cavity heat transport methodology (method 1 compared to method 2) was relatively minor by comparison, resulting in a variation of around 10-60 seconds. The effect of the radiation model alone (not including the convection approximation) can be inferred from the method 3 result compared to comparable method 2 result. This has a substantial effect for the coarse case, the only case where method 3 was used. Chaparral is thought to be a better true representation of the physics for this scenario as defined, because Syrinx was run with a discrete ordinates method and a quadrature of 4. A significant ray effect would be expected. Syrinx would be expected to be more accurate if there were soot present (believed to be the case in the physical system), but the models for this are not being employed presently. This curious result suggests that the similarity in run-away times between method 1 and 3 results may be the product of a compensatory result. Replacing Chaparral with Syrinx causes an increase in the run-away time, with the enclosure convection assumption presumably inducing a comparable decrease in time to run-away to make the method 1 and 3 agree.

Focusing on the last column of Table 4, there is about a 70ºC spread in the run-away enclosure average temperature. The fine Fuego simulation meshes generally resulted in lower average run-away enclosure temperatures. This seems consistent with the generally longer times required for thermal run-away.

Table 4. Termination time and average enclosure temperature at run-away time for all the cases thermal

Fire Mesh	Method	Rad.	Conv.	Run-away Time *(s)*	Avg. Enclosure Temp. *(K)*
coarse	1	Chap.	Encl.	672	774
medium	1	Chap.	Encl.	696	772
fine	1	Chap.	Encl.	813	739
coarse	3	Chap.	Fuego	814	791
coarse	2	Syr.	Fuego	687	755
medium	2	Syr.	Fuego	730	757
fine	2	Syr.	Fuego	868	726

GENERAL DISCUSSION

The intended outcome of the parametric variations was an understanding of some model sensitivities for this scenario. It is generally a good idea to vary model parameters, rather than rely on a single result to produce prediction results. This exercise suggests a fairly large effect of model variations on the outcome of the simulation. Had the fine calculation not been run, we might have concluded that mesh convergence had been achieved. Having the fine results casts doubt on this result. It is very difficult to ascertain from these calculations what exactly the reason is for this issue. Fire calculations such as these use models that are not necessarily scale convergent. Examples of physical models employed in this effort that fit this description are:

- the EDC reaction model, which uses sub-grid approximations for mixing to rate-limit the reactions (Magnussen and Hjertager, 1977; Magnussen, 1981) [5,6]
- the turbulence model that is RANS based, but uses a time scale filtering (Tieszen et al., 2005) [7]
- convection and wall treatments that employ law of the wall

The scale dependencies could be factors that contribute to this. Increased resolution results in continually varying results. Fuego simulation results have been processed for mean incident flux, which is informative. Figure 4 shows the mean incident flux. The coarse and medium cases have higher means, and the conical colder zone beneath the package appears slightly larger. Medium mesh results are surprisingly asymmetric, whereas the other two cases are less so. This suggests the potential need for a longer mean for a true representative value.

A further review of the Fuego fire calculations post-simulation suggests that the variation of length-scales and time-scales were not consistent (not quite as would normally be desirable). Normally, one would linearly vary the time scale with the length scale resolved ($\Delta x/\Delta t$=constant). The decision was made not to enforce this strictly (to keep a regular rational number time-step) and the medium and fine scenarios were run with identical time-steps. Also, the temporal filter would normally be kept to between 2-4 times the time-step. This was mistakenly not adjusted for the medium and fine cases, resulting in a filter of 8 times the time-step. This is not thought to be a major issue, but changing this parameter can result in variability in the results, and fits the category of a scale dependency. This could not be re-run and remedied readily, as the fire simulation jobs took about a month of computing time on between 250-1000 CPUs (over the course of several months).

As a final check of the quality of the results, the residuals were examined for clues as to the convergence. These calculations were simulated with a cut-off number of non-linear solver iterations, meaning the results are generally not fully converged (to numeric precision) at each time iteration. A sampling of a couple of the variables (x-momentum and enthalpy at the final time) indicates fine Fuego mesh results generally had lower residuals, suggesting that these results best reproduce the model functions. Lacking other information, the fine simulation results would be best to consider as the highest quality solutions for that reason and for the reason of higher resolution. Whether the fine results best match the data is not uniquely a function of resolution, as there are numerous modeling assumptions in these complex models.

One feature of this modeling method is important to note here in the discussion. The Aria mesh had a sizable hole in the steel fore-plate on the canister. A corresponding hole was modeled in the Fuego region as an 'open' boundary with the requirement that 'flow must exit domain'. This prevents advection of the boundary values, which are ambient scalars for the calculation. This is not a particularly good assumption, as the container was immersed in a fire. Any other scalar assumptions would also be bad. Even though advection is not allowed across the open boundary, it will allow the boundary conditions (temperature) to diffuse across the interface. This results in some unexpected low temperatures near that region in the method 2 and 3 results, which can be seen in the predicted gas temperatures illustrated in Figure 7. If quantitative accuracy is important, the method for modeling this region should be either improved or at least parametrically evaluated for its significance in future efforts. It is anticipated that the assumed open boundary condition is driving longer run-away times and resulting in slower heating of the booster than would otherwise occur. A deliberate decision should be made on how to proceed with this model feature in the future, as it appears to have at least a moderate quantitative effect on the problem.

In addition to showing the effect of the approximation made for the hole in the fore-plate, Figure 7 illustrates the value of assuming an internal cavity for convection. The mean cavity temperature approximation would imply a constant average convection temperature around the cavity. Compare this to the complexity and variability in the convection (gas) temperatures predicted by the fluid model. Cavity temperatures vary by around 400ºC, with the potential for significant effect on the heat transfer inside the cavity, depending on local surface temperatures. The green/yellow features on the bottom of the container internal surface appear to be thermal drafts, and are probably physical or at least physically representative.

A main objective of this effort was to produce calculations that enable models to be used for assessing complex systems in complex environments. This exercise demonstrates some of the challenges with this scenario. Having an existing model should facilitate work of this nature in the future, and these models can be used for parametric studies in lieu of expensive testing, once they have undergone appropriate validation for the scenarios of interest.

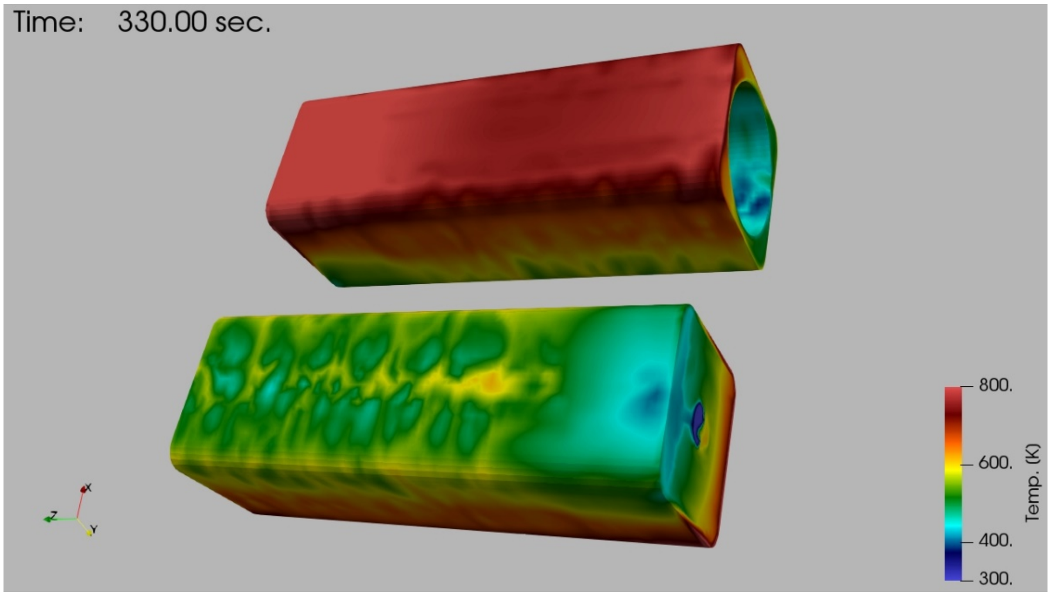


Figure 7. Example cavity gas temperatures (fine mesh at 5.5 minutes), viewed from two sides, primarily from the top in the top image, bottom in the bottom image

SUMMARY AND CONCLUSIONS

A simulation exercise was performed to model the thermal run-away of a rocket motor in a shipping container engulfed in a pool fire. This scenario is inspired by a test characteristic of safety tests for shipping approval. The present models for the thermal run-away are geometrically complex, and leverage the code-coupling capabilities of the SIERRA architecture to perform run-away simulation. The fire model did not demonstrate mesh convergence, and further attention is needed to better understand this behavior. The effect of the convection and radiation model for the cavity had a nearly equal magnitude of effect to the mesh resolution on the time at thermal run-away. Models such as these are complex, but can be useful to obtain insight into the behavior of systems in environments. Further work is needed to demonstrate the models to be quantitatively accurate.

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