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Validation of Computer Models for Nuclear Material Shipping Packages

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ABSTRACT

Computer models are abstractions of physical reality and are routinely used for solving practical engineering problems. These models are prepared using large complex computer codes that are widely used in the industry. Patran/Thermal is such a finite element computer code that is used for solving complex heat transfer problems in the industry. Finite element models of complex problems involve making assumptions and simplifications that depend upon the complexity of the problem and upon the judgment of the analysts. The assumptions involve mesh size, solution methods, convergence criteria, material properties, boundary conditions, etc. that could vary from analyst to analyst. All of these assumptions are, in fact, candidates for a purposeful and intended effort to systematically vary each in connection with the others to determine there relative importance or expected overall effect on the modeled outcome. These kinds of models derive from the methods of statistical science and are based on the principles of experimental designs. These, as all computer models, must be validated to make sure that the output from such an abstraction represents reality [1,2]. A new nuclear material packaging design, called 9977, which is undergoing a certification design review, is used to assess the capability of the Patran/Thermal computer model to simulate 9977 thermal response. The computer model for the 9977 package is validated by comparing its output with the test data collected from an actual thermal test performed on a full size 9977 package. Inferences are drawn by performing statistical analyses on the residuals (test data – model predictions).

INTRODUCTION

Computer modeling is an essential step in the design of new systems and components. Among many steps necessary in the modeling effort, verification and validation are two critical steps in making a useful computer model. Verification is the process of checking the structural details such as geometry, assumptions, boundary conditions, etc. of the model. This step is rather routine and it ensures the correct computer representation of your mathematical model. On the other hand, validation is the process of ensuring that the output of the model represents your physical process or the component. This step is a rather difficult element of the modeling and simulation effort. In fact before any modeling effort is undertaken, a serious thought should be given to how a resulting computer model will be validated. Once the validation step is successfully completed, simulations, which are running experiments on the validated model, can be carried out and its predictions implemented.

Validation of computer models is essentially a statistical process and it will be wise to involve a statistician on the design team. Except in very simple cases, rarely an initial computer model will produce results which will match the reality, your physical process. Since every design involves uncertainty and variability, statistical thinking will force the design team to think of the experimental design methods, number of tests to be performed, available manpower, costs, and schedule in planning the tests and the data collection process,. Statistical thinking can reduce the overall cost of the data collection effort and get useful data that can be effectively used in the validation step. Model validation is an iterative process and any replication should be done only after getting initial modeling results. Validation should complement any replication effort and subsequent model improvement. Savannah River National Laboratory (SRNL) radioactive material (RAM) package design team learned some important lessons from the 9977 package testing and plans to implement this statistical thinking in the Normal Conditions of Transport (NCT) and Hypothetical Accident Conditions (HAC) testing plan of future designs.

Computer models are widely used in the design of nuclear material packages. Since it is prohibitively expensive to test the nuclear material packages for all modes of failure, computer simulations help in assessing the safety margins in the design. Therefore, to gain confidence in the predictability of the computer models, validation of the computer models is an important step and is almost a must in the current regulatory review environment.

9977 RAM PACKAGE

The 9977 is general purpose fissile RAM package designed to transport fissile materials across the Department of Energy (DOE) complex. The important components are a 36-inch tall 35 gallon stainless steel drum, insulating and impact absorbing materials, and a stainless steel containment vessel. These components guard against leakage of toxic nuclear material, radiation leakage, and nuclear criticality during storage, Normal Conditions of Transport (NCT) and under Hypothetical Accident Conditions (HAC) during transport. Containment vessel has inner and outer O-rings to provide a leak tight system to prevent leakage. While polyurethane foam and Vermulite TR-19 provide impact absorbing and insulating capability to guard against physical damage and high temperatures to the containment vessel in an accident and subsequent possible fire during HAC. Figure 1 shows a schematic of the 9977 package. The testing data, modeling results, and the mechanical design details are documented in a Safety Analysis Report for Packaging (SARP) [3]. This RAM package design is currently under regulatory review for certification.

Engineering Design Requirements

The 9977 package is designed to meet the requirements of Code of Federal Regulations 10 CFR 71 [4] to ensure that the environment and public health are not adversely impacted during NCT and HAC. The requirements set limits for the fissile material quantity and set criteria for the structural, thermal, shielding, criticality, fabrication, and quality assurance requirements. **Only NCT requirements related to thermal performance of the package will be addressed in this paper.** Thermal performance is tied to the temperature limits of the system components.

Mathematical Model

The heat transfer governing equations for unsteady state system in axisymmetric cylindrical coordinates (r,z) are:

$$\frac{\partial^2(kT)}{\partial r^2}+\frac{1}{r}\frac{\partial(kT)}{\partial r}+\frac{\partial^2(kT)}{\partial z^2}+q'''=C_p\rho\frac{\partial T}{\partial t} \qquad (1)$$

Where q''' is the volumetric heat generation by the fissile material per unit time, *k is* the thermal conductivity of the various materials of construction in the r and z directions, and T(r, z, t) is the temperature. Thermal conductivity could vary with the material system coordinates and temperatures. The boundary conditions are the heat transfer coefficient (*h*), emissivity (ε), and solar heat flux (fixed and specified by 10 CFR 71) at the drum outer surface. *k, h,* ε and solar heat flux are the input parameters. The partial differential equation representing the transfer function of the system is nonlinear and is solved using finite element (FE) numerical techniques. This equation will be solved to get results at different times to compare the model results with the test.

The response variable T(r, z, t) is determined by computer software MSC/PTHERMAL [5]. This software solves the physics based heat transfer partial differential equation (1) and its solutions are deterministic in nature. The finite element details, model assumptions, material properties and initial/boundary conditions are described in detail in Reference 3. The model results for 30 thermocouple locations at 180 different times as input for this paper are summarized in an Excel file and are not reproduced here for brevity.

Statistical Design and Prototype Testing

As explained before, the validation of the computer model explained above is carried out by comparing the model output at various time steps with the test data at those times. The test performed is the environmental chamber test and it tries to mimic an important regulatory requirement, i.e. performance of a package in a 100°F environment with no solar exposure. Before the test is performed a very detailed computer model is prepared for the planned test using the Patran/Thermal software and the test parameters. The computer model is exercised for the test conditions and the analyst advises the test team about the optimum thermocouple ranges, their locations and the time steps for the data collection instrumentation. For the 9977 package, the planned test is schematically shown in Figure 2. The thermocouple locations are shown in Figure 3.

The package has a 19 Watts (9977 fissile material power output limit) heater installed in the containment vessel and an ambient 100°F controlled test chamber where the package temperatures are monitored for nearly 140 hours, the time required to reach steady state conditions. The temperatures are monitored every 20 seconds in the beginning and at larger time intervals later when the temperature increases are not as steep. The test procedure, the instrumentation, and the results are documented in Reference 3.

The principle intent of this approach to the testing the 9977 package prototype had less to do with identifying the factors or prior assumptions that would affect the prototype performance under stress, but more to do with validating that what the computer model predicted at a given thermocouple location within the package was equivalent to the actual temperature measured. The minimization of this difference between predicted and actual, or residual, was the focus of model and was reflected by the behavior of these residuals over time.

Computer Model

As explained above, prior to the test a computer model is prepared and the test team has pretty good idea what test results are to be expected. If there are differences in the tested package or the test conditions, these are implemented in the computer model. The computer model predicted the temperature T(r,z,t) for each of the 30 thermocouples implanted within the 9977 package (Fig. 3). Predicted temperatures were generated for selected time intervals, more frequently at the beginning of the package test as temperature was changing rapidly and less frequently later in the 140 hr test interval as temperature was nearing equilibrium. Model predicted temperatures were compared to measured temperatures and the pattern residual differences among thermocouples were used to assess the computer model validity.

When package testing was conducted, large residual differences (hereafter residuals) were found for some thermocouples and not others. It was suspected that the polyurethane foam thermal properties (k, ρ, Cp) modeled in the model were not accurate. Subsequently the tested package was disassembled and several foam samples were tested at the vendor facilities and at the SRNL material testing laboratories to determine the actual properties of the package foam. Not only it was found that the foam thermal properties were 10% to 15% higher than expected, but the foam inside the package was found to have one large void at the bottom of the package in its tested configuration. After the discrepancies were incorporated in the thermal computer model, the model results matched very well with the observed temperatures. An axisymmetric finite element computer model of the actual tested package is shown in Figure 4.

The small differences in the observed temperatures and the model predictions will be analyzed in the statistical models in the following sections. It is expected that the statistical models will shed some lights on the differences and draw inferences which can be usefully implemented in future testing to get useful results cost effectively.

STATISTICAL ANALYSIS

In the simplest approach, computational model validation can be addressed for this problem by data display. This was accomplished by comparing the model (predicted) value for a given time slice subsequent to the beginning of the 9977 package test to its corresponding measurement (actual) value. Figure 5A presents both modeled (line) and measured values (data symbols) for the each of the pre-designated sampling points in the elapsed test time. These data correspond to a selection of 5 thermocouples (TC) placed in mid-axial positions within the 9977 package (TC0, TC7, TC12, TC18, and TC24, see Fig. 3). Note the increasing discrepancy between the modeled and measured values. By the end of the test at 140 hrs elapsed time, the model prediction for TC18 overestimates the measured value by 9.5%, while this discrepancy for TC24 is only about -0.24%. Figure 5B shows that for 3 of these 5 thermocouples (TC7, TC12, and TC18), the residual (= test data – model prediction) temperature was still increasing. These measurements suggest that this first computational model is not a valid representation of how inner can source material temperature is being conducted through the package.

Subsequently, it was discovered that the insulation in the bottom of 9977 package was not poured to a solid fill surrounding the inner can compartment. In other words, a void space was detected whereas the initial or first computational model assumed there was none. In addition, the thermal properties, i.e. *k*, and r were found to be higher than expected. These values were independently confirmed by the vendor and the labs at the Savannah River National Laboratory.

A second model was developed assuming and new predicted values were generated. Figure 6A presents both modeled (line) and measured values (data symbols) for each of the pre-designated sampling points in elapsed test time according to the revised or second model. Note the substantial improvement in the second model's ability to computationally predict the measured temperature. As in the first model, TC18 had the highest discrepancy between modeled and measured values. However, that discrepancy was been reduced to 5.3%, almost a 50% reduction in the computational residual. Furthermore, by 120 hrs of elapsed test time, the computational residual temperatures for all five thermocouples had stabilized and were no longer increasing.

Note that the sinusoidal behavior among TC24 computational residuals during the test (> 40 hrs) for either model (Figs. 5 and 6). This could not be due to the monotonically increasing function that underlies the computational model, but must be a function of the measured value. In fact, TC24 tracks the fluctuation in the actual external temperature (data not shown) to which he 9977 package was subjected during the test, i.e., test conditions were not actually constant as modeled. Figures 5B and 6B both show this sinusoidal behavior for TC24, and TC0 also suggesting that both are tracking the external test condition temperature. Note further that the oscillations are dampened for in TC0 compared to TC24. This is due to package surface proximity, in that the TC24 is nearest the package surface and is the least insulated from the external test condition temperature. Such thermocouple behavior, though worrisome at first, provided assurance in the measurement capability of these sensors.

Another unusual feature of the computational residual plots is that at some sampling points early in the elapsed test time, the computational model underestimated the measured temperature, but the sign of this residual reversed thereafter for the remainder of the test. In other words, some feature of the computational model did not allow the predicted temp to rise fast enough to track the corresponding measured value.

The results by the data display methods used above constitute a weight of evidence approach to model validation. For this particular model, data display is a useful first attempt at model validation particularly since the computational model is predicting values in elapsed time. Were the 9977 package test to be conducted under an experimental design wherein a set of factorial effects were being screened for impact on the measurement response, a more appropriate measure of model validation would be to compare a ratio of the mean squared error (MSE) of the computational model residuals for one model, to another, presumably, more accurate model. This ratio will provide a summary statistic and follow a Fisher's F-distribution. This summary statistic approach may be especially useful in comparing response surface designs, subsequent to screening for the main effects for computational model residuals.

In order to develop a summary statistic approach to our present time series computational model, there are several measurement issues that can be addressed, such as

- Measurement criteria - In other words, how much discrepancy between modeled and measured values is too much? How large of a computational residual is too large?
- Measurement independence - Measurements in time are correlated with one another. This correlation structure negates an important and assumed probability distribution property that current measurements do not depend on prior measurements.
- Measurement error - This is a function of the computational model prediction and the empirical model fit to the data

The fact that the "better" of the two models presented here (i.e., model 2) only reduces the model vs. measurement discrepancy, begs the question of what we should expect to observe. Would the only truly valid model be expected to track the measured temperature so well that we should observe only random variation about the model prediction curve? If this were the case, then the sum of the residuals should not differ significantly from zero. This is obviously not the case in this study. Moreover, such model behavior may not be practically achievable given several things

1. our state-of-the-science understanding for the heat transfer process
2. the actual vs. modeled thermal properties of the insulation material
3. the manufacturing conditions during package construction compared to the bench scale certified specifications
4. the spatial placement accuracy of the thermocouples within the package compared to the spatial coordinates of these sensors assumed in the model
5. the calibration error of the thermocouples themselves (several failed or provided obvious aberrant measurements during the test)

The computer code PATRAN/THERMAL is validated to within 1% accuracy of the theoretical solutions of the published or text book heat transfer analytical models. However, considering that the computer model is an incomplete representation of the actual physical model, any prediction within 5% of the test measurement is considered acceptable.

Future Statistical Research

One approach to preserving the assumption of measurement independence is by the method of temporal variograms [6]. Here, by a convention borrowed from mining or geostatistics [7], a sample of computational model residuals is constructed such that that intervening time interval (h) between measurements is sufficiently large to ensure that the correlation between any pair of measurements or selected points in time is negligible. These values can be transformed into standard normal deviates and statistically tested as having come from a standard normal probability distribution. Successive samples can also be constructed by selecting the first computational residual as 1 time-step unit beyond the first measurement of the previous sample and selecting others at h time-step units apart thereafter. Once 10 or more of such samples have been constructed, the Bootstrap method [8] to generate and empirical distribution of the sample means and obtain an upper and lower 95% confidence limits and test criteria for model validity. For such an approach to be useful of course, computational model biases and capabilities will have to meet rather stringent statistical conditions which may not be acceptable to engineering judgment. However, further research in this line of reasoning will at a minimum improve the understanding between statisticians and engineers regarding the formulation of the problem of computational model validity.

CONCLUSIONS

The analyses presented above show that the computer models can effectively represent physical reality if the models are properly validated. This includes adequate validation of the computer codes used to develop the computer models. Also, the verification of the computer models as regards to the geometry, material properties, and boundary conditions of the system at hand is equally important.

By means of a “weight of evidence” approach, we have portrayed these study data via statistical data display techniques to illustrate

1. the unacceptable disparity between modeled and measured values and
2. the subsequent improvement achieved in residual temperature reduction from a second computational model that accommodates the discovered void space in the 9977 package.

This “weight of evidence” approach to model validation by a time series review of computer model residuals can be improved. In addition to validation, future efforts and package prototype testing could incorporate the statistical principles of screening designs such as a fractional factorial design. Since there are many prior assumptions, many can be relaxed in the form of a high and low value for that assumption or effect and tested by computer model prediction for its importance relative to high and low values of other prior assumptions or main effects. In this way, we may vary systematically the modeling effort to verify our understanding of the physical science in the engineering design of the package and validate the modeling effort by demonstrating sufficiently small residuals among all experimental design points.

We conclude also that the engineering approach to model validation would require a specification of a maximum % difference in temperature residuals that would be considered acceptable within the context of computational model assumptions. Short of this, there is ample room to research a statistical basis for a YES or NO decision regarding computational model validation, which research the authors intend to pursue.

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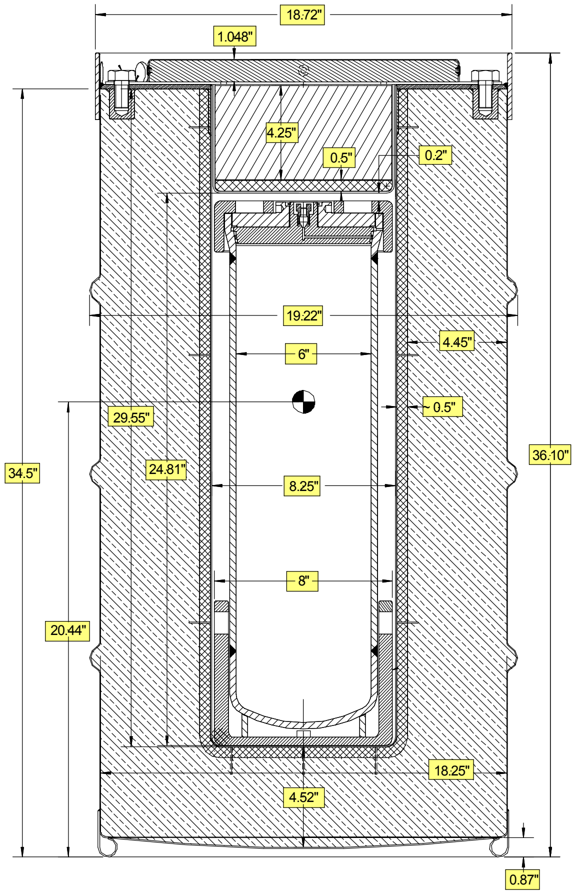

Figure 1 – Schematic of the 9977 Package

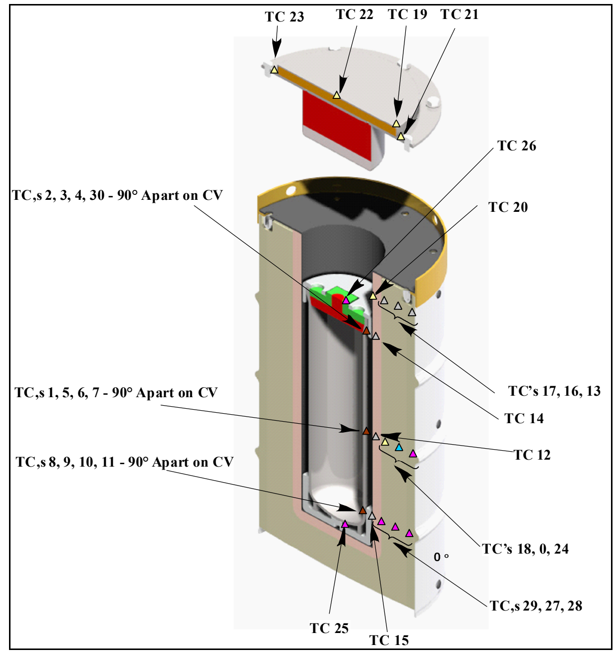

Figure 3 – Thermocouple Locations

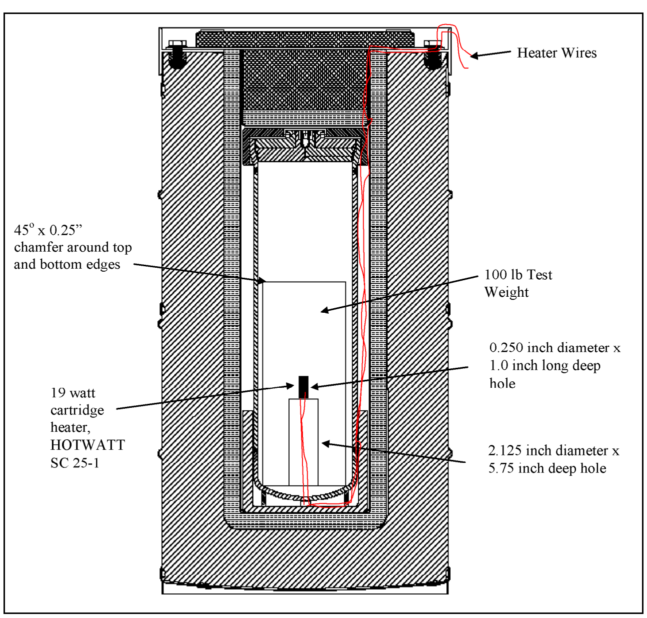

Figure 2 – Schematic of 9977 Environmental Chamber Test

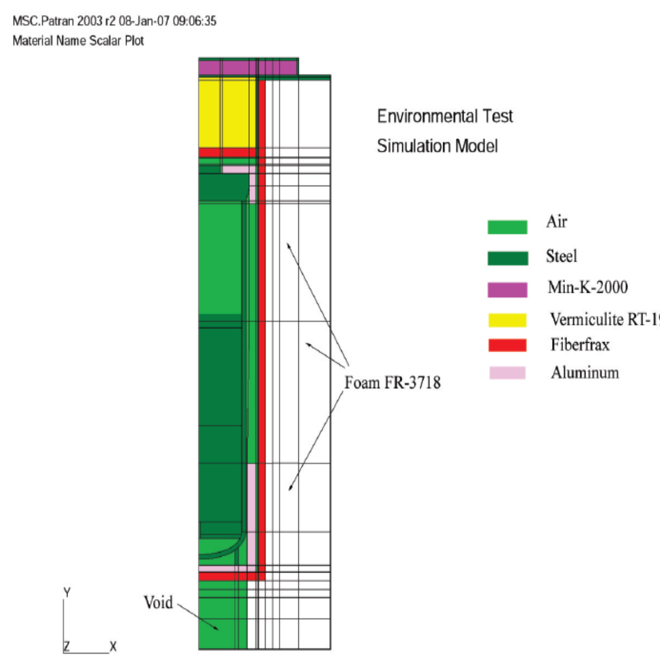

Figure 4 – 9977 Package Components

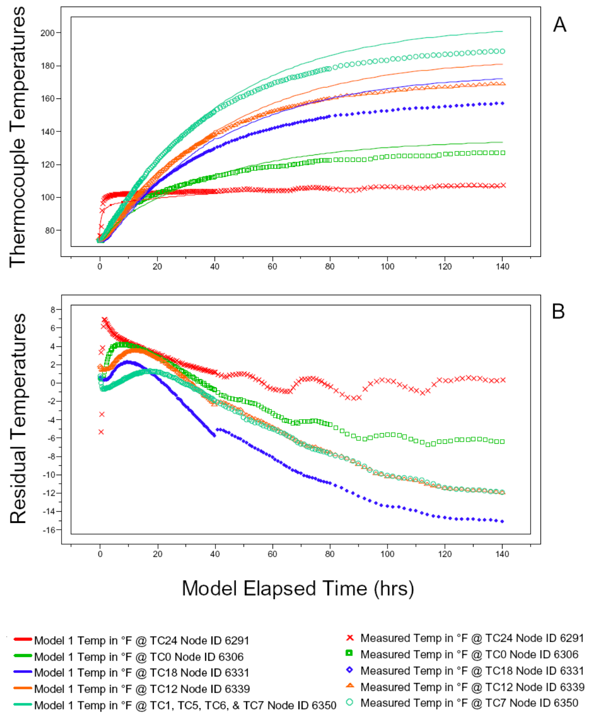

Figure 5A & 5B – Defective Model and Test data Comparison

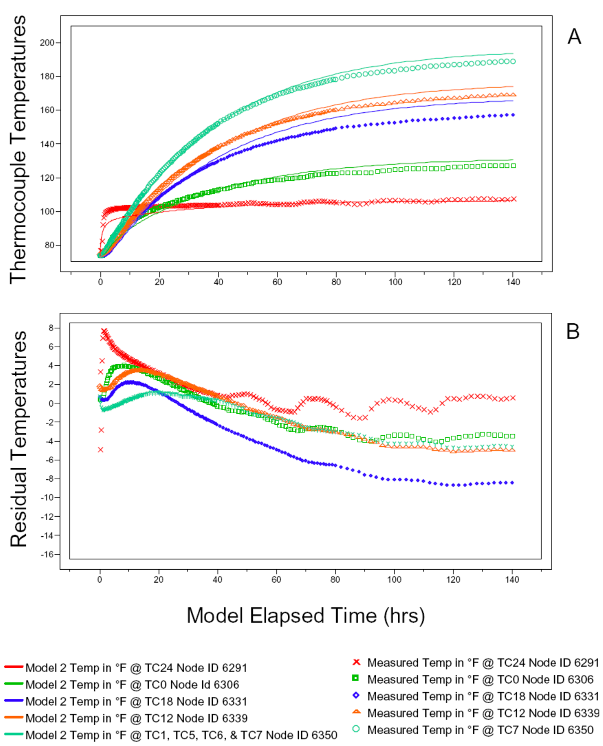

Figure 6A & 6B – Corrected Model and Test data Comparison