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VERIFICATION AND VALIDATION OF FINITE ELEMENT MODELS FOR TRANSPORTATION PACKAGINGS

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ABSTRACT

Design, performance assessment, and certification of transportation packagings for high-level radioactive materials are based on testing and/or computer simulations, whereby the packagings are subjected to sequential tests involving 30-ft free drop, crush, puncture, 30-minute fire at 800°C, and water immersion, as prescribed in Title 10 Code of Federal Regulations Part 71.73. Finite element modeling has been used extensively for evaluating the structural performance of transportation packagings. Verification and validation of finite element modeling is crucial in building confidence and help establish the predictive accuracy of modeling. However, in the current practices of finite element modeling for transportation packagings, there are issues that could affect the credibility and usefulness of the modeling results. These issues are discussed in the following text, with proposed measures for improvement. This paper also recommends additional instrumentation for testing to enable comprehensive model validation.

INTRODUCTION

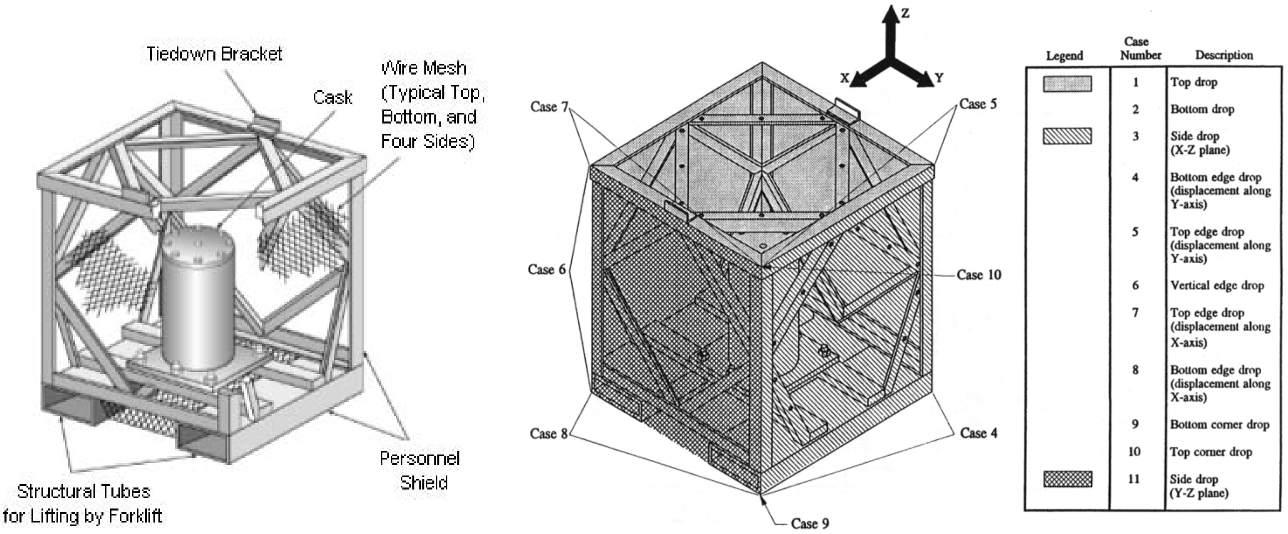
Transportation packagings of high-level radioactive materials certified to Title 10 of the Code of Federal Regulations Part 71 (10 CFR 71) must comply with the regulatory safety requirements concerning the effects on a packaging of the tests specified in § 71.71 ("Normal conditions of transport," NCT) and § 71.73 ("Hypothetical accident conditions," HAC). The packagings must be evaluated by subjecting a specimen or scale model to a specific test, or by another method of demonstration acceptable to the Commission, as appropriate for the particular feature being considered [1]. Methods of demonstration of compliance with the regulatory requirements may include 1) testing of prototypes or samples of the packaging, 2) reference to previous satisfactory demonstrations of a sufficiently similar nature, 3) testing with models of appropriate scale and calculation, or 4) reasoned argument, when the calculation procedures and parameters are generally agreed to be reliable or conservative. Finite element analysis computer codes, such as ABAQUS [2] is one of the Computational Modeling Softwares (CMS) widely used for determining structural performance of packaging designs. Nuclear Regulatory Commission (NRC) Interim Staff Guidance (ISG)-21 states that "*Any CMS application could be used for analyses of cask or package components; however, for any CMS used as the basis for demonstrating that the cask design satisfies regulatory requirements, adequate validation of that CMS must be demonstrated by the applicant.*"

Both verification and validation (V&V) of finite element modeling (FEM) are essential for building confidence and quantifying the predictive accuracy. In this paper, issues associated with the current V&V practices in finite element modeling for transportation packagings are discussed, as are the proposed measures for improvements. The paper also recommends additional instrumentation for testing, such as transient measurements of accelerations and strains, to provide data for a comprehensive model validation.

FINITE ELEMENT MODELING FOR TRANSPORTATION PACKAGINGS

As specified in 10 CFR 71.73(c) (1), (2) and (3), respectively, free drop, crush and puncture tests of the specimen shall be performed in orientations for which maximum cumulative damage is expected. For example, the 30-ft free drop test should consider different drop orientations such as end drop, side drop, and center of gravity (CG)-over-corner drop that produces the highest g-load on the packaging components, as well as slapdown for which a slender packaging can produce a higher g-load in the secondary impact. The 30-ft free drop is followed by crush (only for light-weight packages, < 1,100 lb) and puncture tests to cause additional cumulative structural damage to the packaging. In addition, these structural tests should consider different loading and environmental combinations [3], such as temperatures, pressure, insolation and decay heat load. Taking all of these factors into consideration would involve many tests; judicious use of finite element modeling, therefore, is imperative in order to facilitate assessment of the safety performance of the packaging design.

Figure 1(a) shows a schematic of a Model 9516 Type B packaging for shipping up to 500-W Pu-238 heat source materials [4]. The containment vessel (CV) of the package is inside a cask with bolted lid, and the cask bottom is welded to a bottom plate, which is attached with six bolts to the two bottom beams of a bird-cage structure that serves as a personnel shield of the package. Figure 1(b) shows eleven (11) possible 30-ft free drop orientations in the table insert, and finite element analyses were performed [4] to help determine the worst drop orientation — the 30-ft bottom-down drop that produces the highest g-load and causes most damage to the CV. Therefore, only one 30-ft bottom-down drop test was performed, which was followed by a crush test without the personnel shield (conservative assumption) and a puncture test directly impacting the cask lid. This test sequence was considered to cause the most cumulative damage to the 9516 packaging, which was verified in an independent confirmatory evaluation.



Legend	Case Number	Description
▒	1	Top drop
	2	Bottom drop
▨	3	Side drop (X-Z plane)
	4	Bottom edge drop (displacement along Y-axis)
	5	Top edge drop (displacement along Y-axis)
	6	Vertical edge drop
	7	Top edge drop (displacement along X-axis)
	8	Bottom edge drop (displacement along X-axis)
	9	Bottom corner drop
	10	Top corner drop
▩	11	Side drop (Y-Z plane)

(a) **(b)**

Figure 1. Schematic of (a) Model 9516 Type B Packaging and (b) 30-ft Drop Orientations

Figure 2 shows two HAC tests for a model ES-3100 Type B drum-type packaging for shipment of highly enriched uranium or two DOE 3013 cans containing plutonium oxide [5]. The ES-3100 packaging consists of a strengthened 30-gallon drum with bolted lid and a CV inside the drum. The structural evaluation of the ES-3100 package was performed by a combination of testing and finite element analysis [5]. The test and analytical results show that the drum assembly maintained its structural integrity under HAC. During the packaging certification review, one of the major concerns was that the structural tests under HAC may not have represented the worst test sequence, causing the most cumulative damage to the packaging. Other concerns were that the shallow-angle slapdown drop and crush tests were conducted at ambient temperature, not at -40 ^{o}F, and the effects of the friction coefficient (μ) on the slapdown test were not determined. These concerns were addressed in the independent confirmatory evaluation by Han et al [6]. Figure 3 shows snapshots of (a) the 30-ft bottom-to-lid slapdown drop with a μ of 0.2, followed by (b) a side crush for which the crush plate was aimed at the lid-end of the package already damaged from the preceding slap-down drop. The finite-element analyses showed that the packaging design meets the regulatory requirements, and that a reduced temperature of -40 ^{o}F only resulted in slight increase of the calculated strain of the CV.

(a) **(b)**

Figure 2. ES-3100 Package HAC Tests: a) Package Positioned at a 30-ft Height for Slapdown Drop, and b) Crush Plate Lifted to 30-ft Height for the Sequential Crush

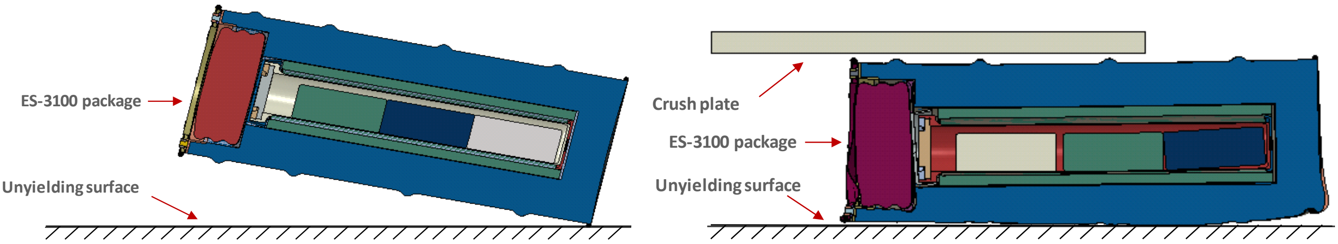


Figure 3. Finite Element Modeling of ES-3100 HAC Tests: a) 30-ft Bottom-to-Lid Slapdown Drop and b) Sequential Crush

MODEL VERIFICATION AND VALIDATION FOR TRANSPORTATION PACKAGINGS

Verification is the process of determining that a model implementation accurately represents the developer's conceptual description of the model and the solution to the model. Validation is the process of determining the degree to which a model is an accurate representation of the real world from the perspective of the intended use of the model. Model V&V, therefore, is the process that accumulates evidence of a model's correctness and accuracy for the physical event that the numerical model represents. The expected outcome of the model V&V process is the quantified level of agreement between model prediction and experimental data [7].

Model Verification

Model verification is the process of identifying and removing errors in the model by comparing the numerical solutions obtained from modeling to analytical or highly accurate benchmark solutions. The verification activities may be divided into code verification and solution verification.

The objective of code verification is to identify and eliminate programming and implementation errors within the software and to verify the correctness of the numerical algorithms that are implemented in the code. The purpose is to confirm that the code will work as intended. Code verification is the responsibility of both the code developers and the code users. The code developers should follow their software quality assurance (SQA) programs to ensure that the finite element code is reliable and robust and can produce repeatable calculation results. Code users should perform their own SQA by running all the relevant verification problems provided with the software (called "Verification Manual"). To the extent practical, code users should also verify the implementation of the numerical algorithms in the code. This verification activity may be accomplished by comparing solutions obtained from the code to problems with known analytical or highly accurate benchmark solutions.

Solution verification is performed after code verification. The solution verification is used to quantify errors introduced during utilization of a code for a particular simulation. Arguably, the most important solution verification activity is performing a grid or time convergence study to provide evidence that a sufficiently accurate solution has been computed. The solution verification quantifies the error of a numerical simulation by demonstration of convergence for the particular model under consideration.

The solution verification has three main aspects: 1) assuring the accuracy of input data, 2) estimating the numerical solution error, and 3) assuring the accuracy of output data for the problem of interest. Verification of input data is needed to ensure that the correct input files, grids, tabulated data, etc., are used. Similarly, verification of output data is needed to ensure that the code user takes the correct post-processing steps after the simulation is completed. Since numerical errors cannot be entirely removed, the solution verification test problems aim to quantify the numerical accuracy of the model. These test problems must be documented, accessible, repeatable, and capable of being referenced. The verification of output data ensures that the correct files have been used and appropriate post-processing steps have been taken.

One potential error that could be introduced into the input data for transportation packaging models comes from the material properties and the selection of material models used for simulation. A transportation packaging consists of components made from American Society of Mechanical Engineers (ASME) Code materials and non-Code materials. The Code materials are ferrous and non-ferrous metallic materials whose behaviors can be described by well-established metal plasticity models in the finite element codes. However, the material properties vary, and the ASME Code only gives the minimum strength values for each material specification. If the properties of the materials used for fabricating the packaging components are not available, the analyst may use the ASME Code data or data obtained from authoritative references. Non-Code materials are used in the transportation packagings as impact limiting and thermal insulating materials, such as wood, foam, honeycomb, clay, and concrete. The mechanical behavior of these materials is generally more complicated than that of metallic materials. Commercial finite element codes have constitutive models that are only suitable for certain non-Code materials. For other non-Code materials whose behaviors cannot be appropriately described by existing constitutive models, code users must develop their own material models.

Figure 4 shows data from compression tests of Kaolite 1600, which is used in the ES-3100 transportation packaging as an impact limiting and thermal insulating material [5]. The compressive stress increases with compressive strain, and is a strong function of temperature. The behavior at high temperature (100 ^{o}F) is akin to crushable foams; therefore, a "crushable foam model" may be used for the Kaolite 1600 in the finite element analysis. However, Kaolite behaves differently from crushable foam under impact loading — Kaolite would fracture, crush, and powder, dissipating the impact force in many different directions without delamination along any specific plane [8]. Therefore, a user-defined constitutive model should be developed for impact analysis.

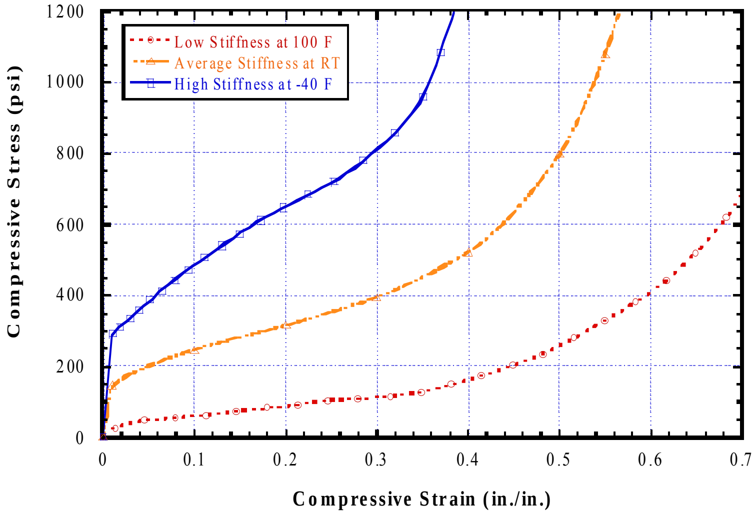


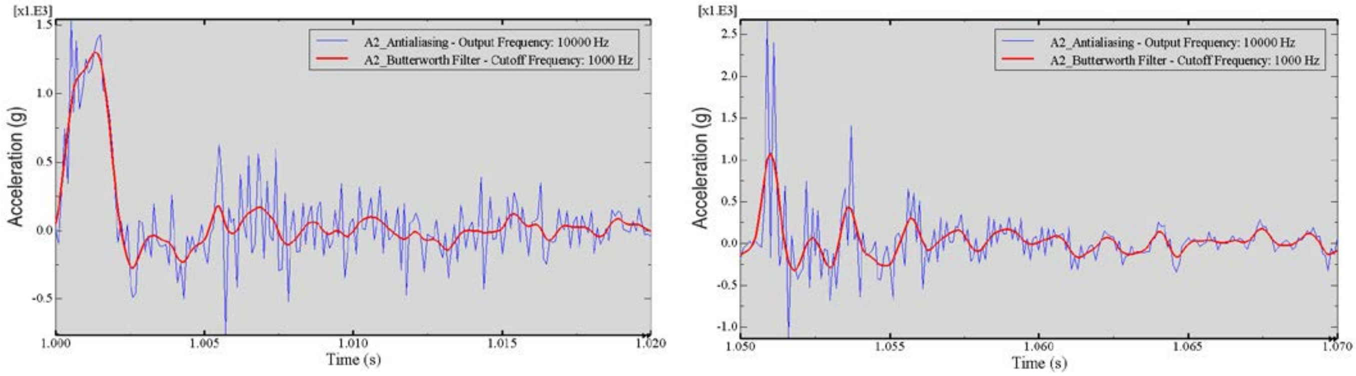
Figure 4. Compressive stress-strain curves of Kaolite 1600 at different temperatures

The main sources of numerical solution errors in computational simulation are round-off error, iterative convergence error, and discretization error. Round-off error is introduced due to the use of finite arithmetic on digital computers. Round-off error can be very important for accuracy for both ill-conditioned systems of equations and time-accurate simulations. The adverse effects of round-off error can be mitigated by using more significant digits in the computation, e.g., double precision of 64 bits instead of single precision of 32 bits. Iterative convergence error arises due to incomplete iterative convergence of a discrete system. Iterative methods are generally required for complex nonlinear systems of equations. The discretization error is the difference between a numerical solution and the exact solution to the continuum partial differential equations. Discretization error arises due to the mapping of partial differential equations to discretized equations. This process introduces discretization parameters such as the element size and the time step. The discretization error is often related to the truncation error due to Taylor-series expansion for linear problems. For nonlinear problems, the relationship is not straightforward.

Model Validation

The goal of model validation is to build confidence in the predictive capability by comparing the results of the computer simulation with experimental data. The key process in model validation is the assessment of the accuracy of computational modeling results by comparison with the data.

Figure 5 (a) shows the calculated acceleration histories of the bottom-down drop of the 9516 packaging [see Figure 1(a)], at a cut-off sampling frequency of 10,000 Hz with anti-aliasing, and a post-processing filter frequency of 1,000 Hz, respectively. The calculated peak acceleration [9] of 1,306 g compares reasonably well with the measured value of 1,084 g [4]. . However, the calculated peak acceleration of 1,020 g [see Figure 5(b)] during the top-down puncture drop is considerably differently from the measured acceleration of 1,799 g and 700 g. No explanation was provided [4] for the large discrepancy between the two measured values by the accelerometers, which were mounted at the same location on the package.



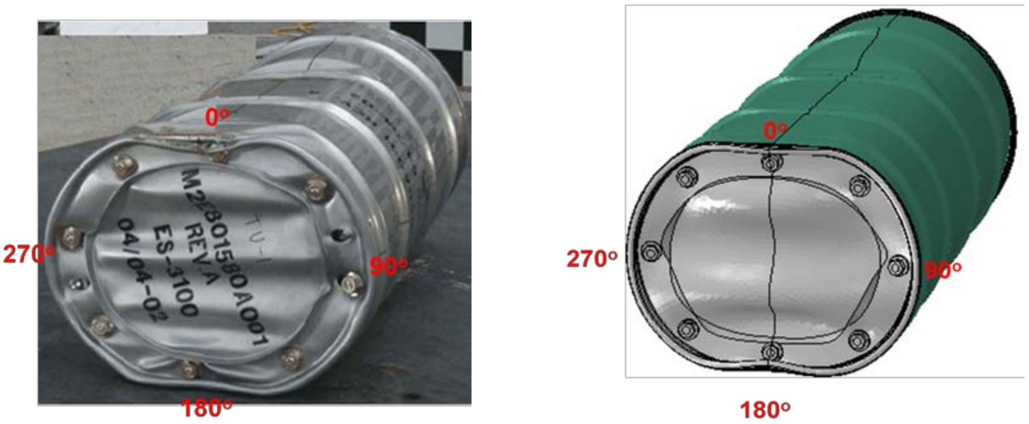
(a) **(b)**

Figure 5. Calculated acceleration history for 9516 packaging during a) 30-ft bottom-down drop with peak acceleration of 1,306 g, and (b) top-down puncture with peak acceleration of 1,020 g.

Figure 6(a) shows a deformed ES-3100 test specimen following the 30-ft slapdown drop and a crush test. The package deformation was measured at different locations, which provided data for model validation. The finite element modeling results, as shown in Table 1 and Figure 6(b) in deformed shape, are in good agreement with the data. Whereas the finite element modeling also computed the deceleration of the CV, the tensile and bending loads in the drum bolts, and strains in the CV and its lid closure during and after the dynamic tests, no data are available from the tests for model validation.

Table 1. Calculated vs. measured deformation in ES-3100 after 30-ft drop and crush tests

Axial measurement location	0 to 180°		90 to 270°	
	Test (in.)	Analysis (in.)	Test (in.)	Analysis (in.)
Top false wire	15.63	15.27	20.63	20.34
Top rolling hoop	16	15.79	20.44	20.42
CG & top rolling hoop	16.25	16.10	20.25	20.28
CG rolling hoop	16.5	16.47	19.88	20.03
Bottom rolling hoop	18.25	18.29	19.5	19.58
Bottom false wire	17.81	17.8	19.25	19.35



(a) **(b)**

Figure 6. (a) Deformation of ES-3100 package following the 30-ft slapdown test and (b) calculated deformation by finite element modeling

The authors of the paper [10] described the instrumentation plan and measurement planes for drop tests of a half-scale cask model CASTOR® HAW/TB2. Several drop tests were performed on the half-scale model, which was instrumented on 21 measurement planes with 23 piezoresistive accelerometers, 5 temperature sensors, and 135 strain gauges distributed in the cask interior and exterior. The extensive instrumentation provided separate and yet correlated sets of data on acceleration, strain and deformation that could be used for a more comprehensive model validation.

Typical data acquisition for dynamic testing of transportation packagings includes the use of accelerometers, strain gauges, high-speed photography, and post-test visual examination and measurement of the deformed packagings, and occasionally destructive examination. Modal testing is another method for testing transportation packagings subject to vibration, whereby the natural (modal) frequencies, modal masses, damping ratios, and mode shapes of the packagings are determined. A modal test usually consists of an acquisition phase and an analysis phase. The complete process is often referred to as a “modal analysis” or “experimental modal analysis.” Modal testing of an object is often conducted by impact hammer and/or shaker table, i.e., a vibration tester. In both cases, energy is supplied to the test object with known frequency content. Where structural resonances occur there will be an amplification of the response, which is clearly seen in the response spectra. Using the response spectra and force spectra, a transfer function can be determined. The transfer function (or frequency response function) is often curve fitted to estimate the modal parameters. Natural frequencies, mode shapes, and impedance data of the object thus obtained can be used to validate finite element modeling. A shaker table test of a mockup used fuel assembly is being considered by Sandia National Laboratories, as part of the DOE Used Fuel Disposition Campaign on Research and Development.

A validated finite element model should have the ability to represent the dynamic response of the structure to a specific accuracy and within a required frequency range [11]. Finite element models can be validated against data from dynamic tests, which are common practice in the civil, aerospace, and automobile industries. Modal testing is non-destructive, relatively simple, and can be performed on a prototype or production piece. Finite-element modeling and modal testing can thus be effectively coupled for verifying the dynamic structural performance of transportation packaging design, and the process can be iterated, if deemed necessary.

CONCLUSION

Finite element modeling is a cost- and time-effective tool for assessing the safety performance of transportation packagings of radioactive materials, while model V&V are essential for building confidence in the predictive accuracy of the modeling. General concepts and process in conducting a successful model V&V, as well as specific examples on transportation packagings, are presented in the paper. Issues associated with the current V&V practices for finite element modeling of transportation packagings are also discussed with suggested measures for improvement.

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REFERENCES

1. Title 10 Code of Federal Regulations, Part 71, “Packaging and transportation of radioactive material,” Nuclear Regulatory Commission, 2012.
2. Dassault Systems, ABAQUS 6.11 User’s Manual, 2011.
3. Nuclear Regulatory Commission Regulatory Guide 7.8, “Load Combinations for the Structural Analysis of Shipping Casks for Radioactive Material,” Revision 1, March 1989.
4. “Safety Analysis Report for Packaging for the 9516 package,” Rev. a, EnergySolutions Federal Services, Inc., June 2008.
5. “Safety Analysis Report for Packaging Model ES-3100 package with bulk HEU contents,” Rev. 0, Babcock & Wilcox Technical Services Y-12, LLC, August 2010.
6. Z.H. Han, Vikram N. Shah, and Yung Y. Liu, “Finite element analysis of drum-type shipping packages under hypothetical accident conditions,” PVP2012-78707, Proceedings of the ASME 2012 Pressure Vessels and Piping Conference, Toronto, Ontario, Canada, July 15–19, 2012.
7. William L. Oberkampf, and Timothy G. Trucano, “Verification and validation benchmarks,” Nuclear Engineering and Design, Volume 238, Number 3, pp. 716-743, 2008.
8. Gerald A. Byington, et al., United States Patent 6299950 B1, “Fireproof impact limiter aggregate packaging inside shipping containers,” September, 1997.
9. Z.H. Han, V.N. Shah, and Y.Y. Liu, “Dynamic Structural Analysis of the 9516 Transport Package,” ASME 2010 Pressure Vessel & Piping Conference, Bellevue, Washington, July 18-22, 2010.
10. A. Musolff, T. Quercetti, K. Müller, B. Droste, and S. Komann, “Drop test program with the half-scale model CASTOR® HAW/TB2,” Packaging, Transport, Storage and Security of Radioactive Material, Volume 22, Number 3, pp. 154-160, 2011.
11. Agilent Technologies, “The fundamentals of modal testing,” Application Note 243 – 3, May 1986.