Transportation Package Design Using Numerical Optimization*

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Introduction

The design of structures and engineering systems has always been an iterative process whose complexity was dependent upon the boundary conditions, constraints and available analytical tools. Transportation packaging design is no exception with structural, thermal and radiation shielding constraints based on regulatory hypothetical accident conditions. Transportation packaging design is often accomplished by a group of specialists, each designing a single component based on one or more simple criteria, pooling results with the group, evaluating the "pooled" design, and then reiterating the entire process until a satisfactory design is reached. The manual iterative methods used by the designer/analyst can be summarized in the following steps: design the part, analyze the part, interpret the analysis results, modify the part, and re-analyze the part. The inefficiency of this design practice and the frequently conservative result suggests the need for a more structured design methodology, which can simultaneously consider all of the design constraints.

Numerical optimization is a structured design methodology whose maturity in development has allowed it to become a primary design tool in many industries. These include automotive, aircraft, and aerospace, where the number of performance and safety constraints dictates state-of-the-art technologies and design tools. Numerical optimization, used as a design tool, is only a logical extension of increased use of advanced analytical tools and increased safety awareness by designers and the general public.

The purpose of this overview is twofold: first, to outline the theory and basic elements of numerical optimization; and second, to show how numerical optimization can be applied to the transportation packaging industry and used to increase efficiency and safety of radioactive and hazardous material transportation packages. A more extensive review of numerical optimization and its applications to radioactive material transportation package design was performed previously by the authors (Witkowski and Harding 1992). A proof-of-concept Type B package design is also presented as a simplified example of potential improvements achievable using numerical optimization in the design process.

Optimization Theory

Optimization is defined as the process, or methodology, of making something (such as a design, system, or decision) as fully perfect, functional, or effective as possible. In numerical optimization analyses, the requirements of an engineering design problem are mathematically formulated through the use of an objective function, design variables, and constraints. The objective function, or cost or merit function, is

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the function to be minimized/maximized, such as weight, volume, or cost, by variation of a set of design variables. Design variables are quantities that define a particular design, such as diameter, thickness, material strength, etc. Constraints are limitations on the performance or behavior of the system, such as stress or strain limitations, size restrictions, etc., and on the design objective specifically.

The general concept of gradient-based optimization techniques consists of

1) selecting initial values of the design variables
2) determining the active constraints
3) calculating a search direction based on the objective function and the active constraints
4) determining how far to go in the search direction (via one-dimensional search)
5) checking convergence and whether or not a local or global minimum has been found
6) iterating back to 2) if necessary

Gradient-based numerical optimization techniques differ from exhaustive search, random search, and other optimization techniques in that gradient-based techniques attempt to select the "best" search direction to minimize the objective function quickly. Inherently, gradient-based techniques require fewer function evaluations, which are frequently the most expensive and time-consuming aspect of structural design. Implicit in the use of gradient-based optimization techniques is having continuous design variables, objective and constraint functions, and continuous function derivatives.

The simplest minimization problems are those whose form is explicitly defined. The first derivative of the objective function with respect to the design variables can be set to zero and solved exactly. Unfortunately, most engineering problems of interest can not be expressed in this form. Typically, numerical approximation schemes, such as finite element and finite difference methods, must be used to provide function evaluations and derivative approximations. These values are used to select search directions and distances. One of the most common and simplest search schemes is based on the negative gradient of the objective function, often referred to as the steepest descent technique.

The method in which the search directions and distances are selected distinguishes different optimization schemes from one another. One pitfall of gradient-based optimization problems is that the analyst must insure that the achieved optimum is a global minimum and not just a local minimum. For most problems, nothing short of running the problem at several initial points in the design space and comparing optimal solutions can verify that the solution is a global minimum.

Structural Analysis and Optimization

Structural optimization involves coupling structural analysis (for function and constraint evaluations) and optimization routines. Often this is not a trivial chore with existing codes that have set interfaces and modes of operation. Use of in-house finite element analysis (FEA) codes is desirable since modifications can be easily made to access information that may be inaccessible in commercial codes at a particular point in a calculation. This may make interfacing between the FEA and optimization codes more efficient.

Initial research in the area of structural optimization was exclusively focused on determining the optimal set of sizing variables, such as plate thicknesses, bar cross-sectional areas, moments of inertia, and composite laminate angles. Sizing variable optimization does not change the shape of the structure, only its geometric properties. Therefore, the topology of finite element models do not require updating since only the internal stiffness properties change. Many problems cannot be properly analyzed only with sizing variable optimization. For example, if the stress concentration in a cask body due to a seal test port is analyzed, only shape optimization allows for modification of the hole's shape. Current research primarily deals with finding the optimal shape, or shape optimization. In shape optimization, geometries and surface contours are free to "flow", therefore, the finite element model must be periodically updated to incorporate changes in the geometry and element connectivity.

Since one of the goals of optimization is to automate the design process, automatic mesh generation is a necessity. Even with slight changes in the geometry, distortion of the element mesh can severely corrupt the model predictions. Adaptive generation techniques are being investigated at Sandia National Labs (SNL) to produce 2 and 3-dimensional quadrilateral and brick element meshes for complicated geometries which are automatically refined in high stress gradient areas to retain accuracy (Blacker, et al. 1990). An example of an automatically generated mesh, formed by translating and rotating 2-dimensional meshes, is shown in Figure 1 (Blacker, et al. 1991). Automated, adaptive mesh generation is a requisite technology for automated numerical shape optimization, which requires model updates as the shape evolves during the optimization process.

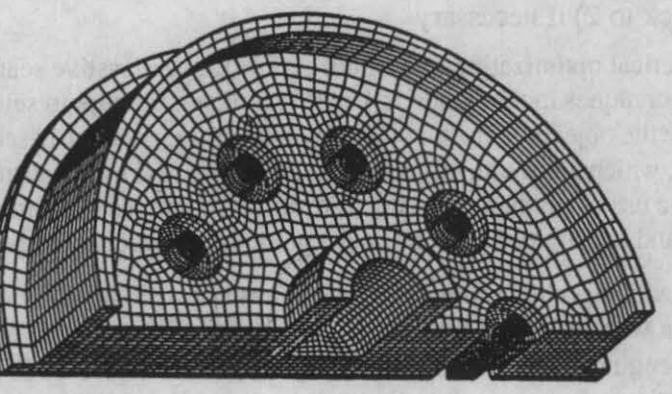

Figure 1. Three-dimensional mesh constructed by combining, translating and rotating two-dimensional meshes.

Current adaptive analysis research at SNL involves automatically re-meshing problems where the initial mesh becomes too distorted due to large deformations to complete a single analysis, such as occurs in the analysis of air transport packages. The algorithm takes the final deformed geometry before the analysis is halted, re-meshes the geometry, and restarts the analysis using the new meshed geometry. This capability allows large deformation calculations to run for much longer times.

After obtaining and/or developing the previously mentioned tools, i.e., an automatic mesher, structural and thermal analysis codes, and an optimization code, the actual numerical shape optimization process can be initiated. The initial and most important phase is to formulate the problem such that it is numerically tractable, yet still accurately represents the key characteristics that need to be modelled. If particular geometric regions are allowed to change, these areas must be represented using design variables. One approach to represent changing boundaries is to use polynomials to describe the boundaries and take the coefficients of the polynomials as the design variables. Only a small number of design variables are thus required to characterize the shape. Ideally, an accurate model using the smallest number of parameters and constraints should be posed to minimize the design space that the optimization routine must search.

The search algorithm involves individually perturbing each of the design variables by a small amount to see how the objective function value is affected. These data are referred to as sensitivity derivatives and are used to select new search directions. The calculation of these sensitivities requires many function evaluations and can be very costly, especially for detailed models with numerous design variables.

Therefore, approximate or reduced models are often used because they are less expensive to evaluate, assuming that a reliable approximate model can be developed.

The logic flow of the optimization process is shown in Figure 2. After the initial design has been defined,

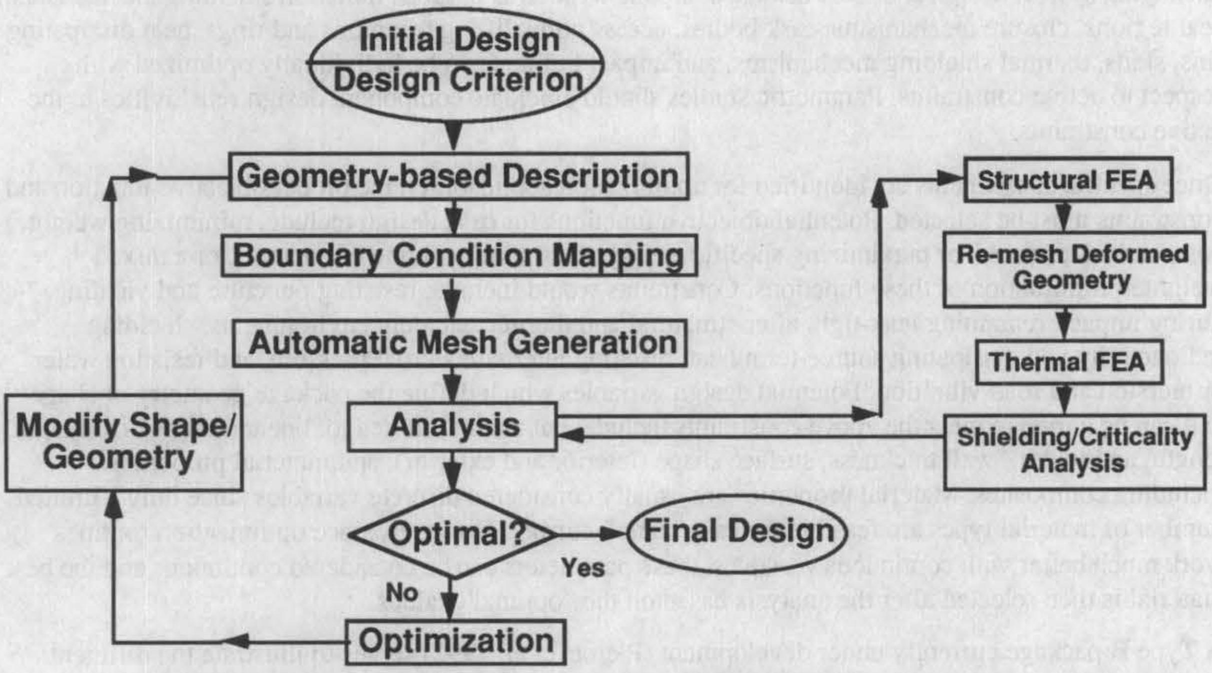

Figure 2. Flow chart for shape optimization analysis

constraints are evaluated to verify feasibility. Structural and thermal analyses, for example, would be required to determine whether containment constraints for radioactive material packagings were met after accident environments. If any of the constraints are violated or the objective function is not currently minimized, the optimization routine adjusts the design variables to find an improved solution. This involves calculating gradients and sensitivities of the objective function and constraints to the design variables. This information is used to select new search directions. Unfortunately, this step can be very costly since it involves several model, or constraint, evaluations and must be repeated whenever the design variables are changed. Note, that if a design variable is changed that affects the shape, a new finite element mesh must be generated to insure that an accurate model is available for further analysis. When a new set of "more-optimal" design variable values are determined the model must again be checked to see if the optimality tests are passed. This iterative loop is continued until the optimum is found, i.e., when the objective function value cannot be reduced any further and all of the constraints are satisfied.

Application of Numerical Optimization to the Transportation Cask Design Problem

A new generation of multipurpose radioactive material packagings will likely be needed in the United States in the near future and numerical optimization, as a design tool, could play a key role in developing more efficient and robust transportation packagings. Both sizing and shape optimization have the potential to make significant contributions in the design of new cask components, to be used in containers for on- and off- site transport and storage of radioactive, hazardous, and mixed hazardous wastes from civilian power generating reactors and the weapons complex.

Unfortunately, optimization analyses can be time consuming and expensive, thus, the use of this technology for a particular design problem must be warranted. It must also be highlighted that most shape optimization problems presented in the literature lack the complexity of the full cask design problem. A cask component design problem may be more cost effective than trying to optimize an entire packaging system design at once. Package components such as baskets, radiation shielding mechanisms, seal regions, closure mechanisms, cask bodies, access ports, lifting trunnions and rings, heat dissipating fins, skids, thermal shielding mechanisms, and impact limiters can be individually optimized with respect to active constraints. Parametric studies should elucidate component design sensitivities to the active constraints.

Once specific components are identified for optimization applicability, the proper objective function and constraints must be selected. Potential objective functions for cask design include: minimizing weight, cost, cask size, stress, or maximizing specific energy absorption, volume of contents, or a mixed weighted formulation of these functions. Constraints would include: resisting puncture and yielding during impact, remaining leak-tight after structural and thermal accident environments, shielding radioactivity and dissipating source-term heat, resisting internal/external pressure, and resisting water immersion and road vibration. Potential design variables which define the package geometry or shape and can be varied to meet the above constraints include, but are not limited to: linear dimensions (height, length, and width), wall thickness, surface shape (interior and exterior), and material properties, including composites. Material properties are usually considered discrete variables since only a limited number of material types are feasible for cask manufacturing. However, since optimization routines work much better with continuous variables, these parameters can be considered continuous and the best material is then selected after the analysis based on the "optimal" values.

A Type B package currently under development (Pierce, et al. 1992) serves to illustrate the different steps involved in sizing and shape optimization analysis and how this tool could be used to improve the transportation cask design process. The current package design consists of nested cylindrical containment vessels with elastomeric seals inside a composite overpack of metallic wire mesh and thermal insulation cloth for protection in an accident environment. The outer diameter and length of the containment vessel are 15.2 cm (6.0 in.) and 52.5 cm (20.7 in.), respectively. The outer diameter and length of the overpack are 45.7 cm (18.0 in.) and 98.9 cm (38.9 in.), respectively. The overpack consists of approximately 77 kg (170 lbm) of composite wire mesh material.

Package weight, defined as the sum of individual composite layer weights, is chosen as the objective function to be minimized. To minimize the number of design variables and keep the problem simple, thicknesses of three separate layers are chosen as the three design variables for the numerical optimization problem. X_1 is designated as the inner radial thermal blanket thickness, X_2 the middle wire mesh composite radial thickness, and X_3 the outer thermal blanket radial thickness, as shown in the cutaway in Figure 3. Thicknesses of these layers in the longitudinal directions are assumed to remain in the original ratios of the outer containment vessel and overpack diameters to lengths. Constraints include: 1) a minimum inner radius of 7.94 cm for the inner thermal blanket layer to accommodate the fixed-design containment vessels; 2) a minimum wire mesh composite layer thickness of 10 cm, an approximation of the minimum thickness to provide sufficient cushioning in a dynamic crush accident environment; 3) an internal radiative decay heat load of no greater than 20 Watts; and 4) a maximum inner surface temperature of 505 K (450 °F) to avoid heat degradation in the elastomeric seals. Shielding constraints are deemed negligible for the proposed contents.

A simplified one-dimensional axisymmetric (infinitely long cylinder) thermal model of the package is used to approximate the peak mid-plane inner surface temperature during the transient hypothetical fire accident condition. Previous two-dimensional P-Thermal (PDA Engineering 1991) transient conduction analyses indicated that peak inner temperatures occur at the mid-plane location. Emissivity/absorptivity

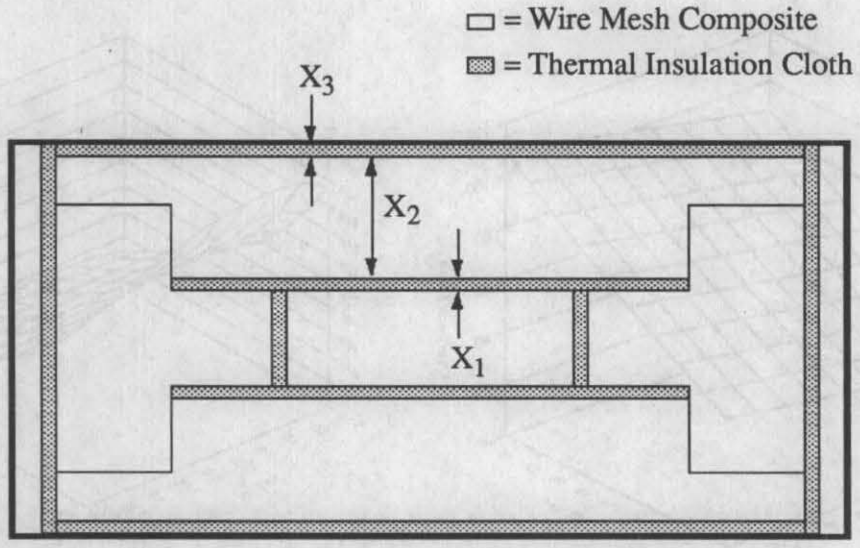

Figure 3 Cross section of wire mesh Type B example package with sizing design variables.

values of 0.9 and a convective heat transfer coefficient of 5 W/m^{2}K were assumed during the 30 minute 1075 K (1475 °F) fire and indefinite 311 K (100 °F) cool-down period. The model uses explicit finite difference methods to approximate the governing partial differential equation in cylindrical coordinates with 32 internal nodes. Temperature-variant material (thermal) properties are updated at each time step and peak internal surface temperatures are recorded over a three hour time period encompassing fire and cool-down periods. The time step was chosen as 0.03 seconds based upon numerical stability and accuracy criteria for the analysis technique.

Numerical optimization of the package design was accomplished in 27 iterations with ADS (Vanderplaats 1985), an optimization code using the Method of Feasible Directions for constrained minimization. The initial feasible design point was X_1=3 cm, X_2=20 cm, and X_3=5 cm. 106 function and constraint evaluations were performed automatically during the optimization process for gradient and search length calculations. The minimum package overpack weight (mass, actually) design, as determined by the numerical optimization code, was X_1=0.13 cm, X_2=12.7 cm, and X_3=0.13 cm, yielding an overpack mass of 49 kg, 36 percent less than the initial overpack mass of 77 kg. The three-dimensional plots of overpack mass and peak transient inner seal temperature as functions of X_2 and X_3 (with X_1 held constant at 0.13) shown in Figure 4 aid in visualizing the sensitivities of these parameters to the design variables and verify the optimal result. Although the overpack mass or weight can be reduced below the asterisked point in Figure 4, doing so increases the peak seal temperature thereby violating its maximum operating temperature constraint. Numerical verification that the optimal result is a global minimum was accomplished by starting at various feasible design points and arriving at the same minimum. Accuracy of the simplified model's inner surface or seal temperature at the optimum design point was verified using P-Thermal to solve a two-dimensional finite difference approximation of the same geometry and time dependent boundary conditions.

The optimal overpack design reduces overpack weight by over 35 percent from the original single composite layer design. Further reductions would be expected with a more accurate definition of the minimum wire mesh layer thickness for energy absorption. These results are meant only as an example of the potential weight savings to be gained since they were derived using relatively simple approximations of the actual design constraints. Also, if cost were the objective function to be

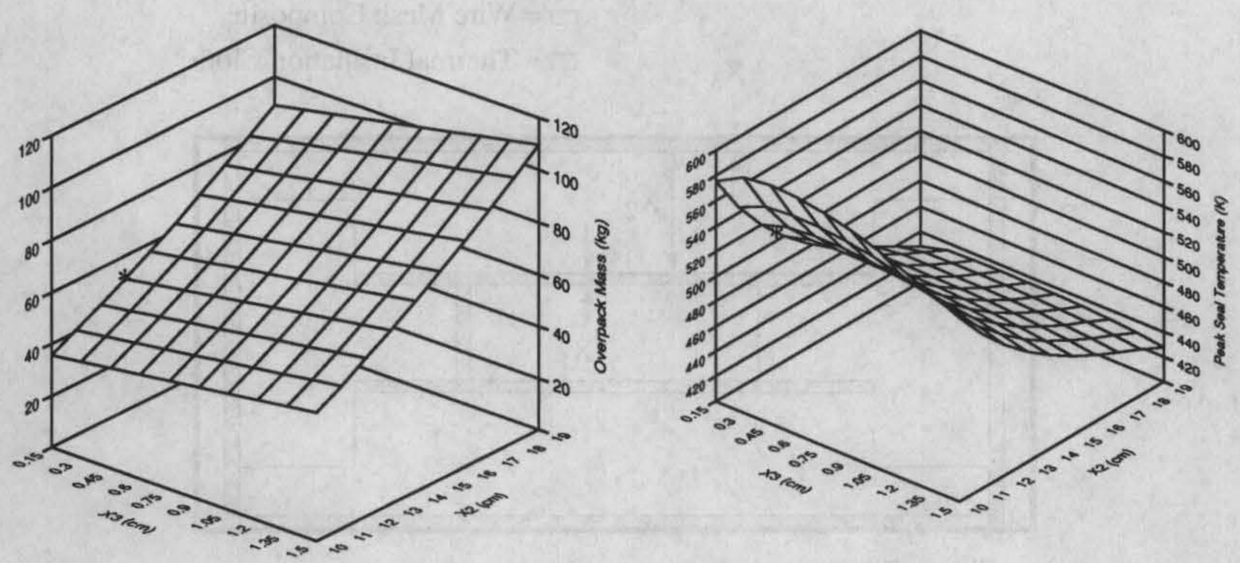

Figure 4 Package overpack mass and peak seal temperature as functions of design variables X_2 and X_3. The optimal design is X_1=0.13 cm, X_2=12.7 cm, X_3=0.13 cm, and is denoted by an asterisk (*).

minimized, the optimal result would likely be much closer to the original Type B package design without the thermal insulating cloth layers since these are relatively expensive on a per weight basis compared to the wire mesh composite material. However, the significant reduction in package weight without violation of the constraints suggests that improved transportation packaging designs are achievable through the use of numerical optimization.

Summary

Numerical optimization has proven to be successful in obtaining optimal designs in a more efficient and structured manner in many industries. Optimization of sizing variables is already a widely used design tool and even though shape optimization is still an active research topic, significant successes have been shown for many structural design problems. Coupled structural, thermal, and radiation design constraints make numerical optimization highly amenable to the efficient solution of the cask design problem. Current state-of-the-art technology at Sandia National Labs in the areas of structural mechanics, thermal mechanics, numerical analysis, adaptive finite element analysis, automatic mesh generation, and transportation cask design can enhance current industry-standard cask design and analysis techniques through numerical optimization. The complexity of transportation cask design problem with its numerous coupled constraints, however, cannot be over-emphasized. The automation of this design problem through numerical optimization requires integration of finite element analyses for thermal and structural evaluations, as well as codes for shielding and criticality. Numerous transportation-related constraints for system operations such as remote handling can be added as well. Development of this "black box" numerical design optimization tool has the potential to provide greater uniformity and cost effectiveness in package design through advanced, integrated analytical techniques.

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