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Sensitivity Analysis of the Thermal Response of 9975 Packaging Using Factorial Design Methods

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ABSTRACT

A method is presented for using the statistical design of experiment (2^k Factorial Design) technique in the sensitivity analysis of the thermal response (temperature) of the 9975 radioactive material packaging where multiple thermal properties of the impact absorbing and fire insulating material Celotex and certain boundary conditions are subject to uncertainty. 2^k Factorial Design method is very efficient in the use of available data and is capable of analyzing the impact of main variables (Factors) and their interactions on the component design. The 9975 design is based on detailed finite element (FE) analyses and extensive proof testing to meet the design requirements given in 10CFR71 [1]. However, the FE analyses use Celotex thermal properties that are based on published data and limited experiments. Celotex is an orthotropic material that is used in the home building industry. Its thermal properties are prone to variation due to manufacturing and fabrication processes, and due to long environmental exposure. This paper will evaluate the sensitivity of variations in thermal conductivity of the Celotex, convection coefficient at the drum surface, and drum emissivity (herein called Factors) on the thermal response of 9975 packaging under Normal Conditions of Transport (NCT)[1]. Application of this methodology will ascertain the robustness of the 9975 design and it can lead to more specific and useful understanding of the effects of various Factors on 9975 performance.

INTRODUCTION

The 9975 package is designed to meet the requirements of 10CFR71 to ensure that environment and public health are not adversely impacted during normal transport and accident conditions. The package is designed by detailed structural, thermal, criticality, and shielding analyses. However, this conventional design approach is deterministic assuming fixed material properties and boundary conditions. The design is, of course, tested for hypothetical accident conditions to ensure that it meets important basic requirements of environment, public health, and safety. Figure 1 shows the schematic of the 9975 package in vertical orientation. Only vertical orientation is analyzed in this paper. The package consists of an outer 35 gallon stainless steel drum, a primary containment vessel (CV) for the radioactive material (RM) containers, a secondary containment vessel for added protection to prevent leakage of RM, a lead shield, an air shield for the Celotex near the drum closure lid, and Celotex as the insulating and energy absorbing material for CV protection during accidental fire and impact conditions.

Federal regulations in 10CFR71 set the design requirements for the Normal Conditions of Transport (NCT) and Hypothetical Accident Conditions (HAC). Only NCT design requirements and the pertinent thermal analyses are addressed here. NCT requirements require consideration of solar heat flux in a 100°F environment. Therefore heat is exchanged with the environment through natural convection and radiation. Heat is lost to the environment through natural convection and radiation from the drum surface. Radiation conditions involve solar spectrum for the surface absorptance and infra red emittance at thermal radiation wavelengths. Although 10CFR70.71 permits 12 hour of sun followed by 12 hours of 'no sun' for NCT, only steady state analysis with constant solar flux is performed for conservative temperature estimates.

Although the package is designed assuming conservative deterministic models, uncertainty in some or all of the model parameters is rarely considered. These uncertainties can be broadly classified into three categories [2]: (1) uncertainty due to the natural heterogeneity of the material or boundary conditions which leads to a spatial variability of thermal conductivity (k), specific heat (Cp), density (ρ), convection heat transfer coefficient (h), or emissivity (ε); (2) uncertainty due to the limited availability of information about the properties; and (3) uncertainty due to experimental errors which consists of fixed errors (bias) and random (precision) errors. This paper addresses category 1 uncertainties due to the variance in k, Cp, ρ, h, and ε. For the NCT steady state analysis, only k, h, and ε are important. There is no experimental error (pure error) in this analysis since the package thermal response is calculated using deterministic computer codes which give exactly the same results for a defined set of factor values no matter how many times the computer code is run. There is, however, model bias since the exact mathematical model is not known.

Uncertainty is best handled by assigning probability distributions to the various parameters. However, enough experimental information is not available to specify appropriate probability distributions for k, Cp, ρ, h, and ε. Fortunately, for this application, the uncertainty is narrowed due to the high degree of confidence in the 9975 design which is demonstrated by the actual testing under regulatory conditions that have considerable conservatism built into the requirements. The approach followed

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[1] Hypothetical Accident Conditions (HAC) sensitivity analysis will be addressed in a later paper.

here is by performing sensitivity analyses using design of experiment (DOEx) or factorial design methods widely used in the chemical industry. The DOEx analyses will demonstrate the robustness of the design for expected variations in the random variables or factors. The main purpose of this analysis is to examine the robustness of the 9975 design considering the variability of these factors. No attempt is made to arrive at an optimal solution.

The factorial design method is best suited if the random variables are independent. The variable (or Factors) that impact the thermal response are thermal conductivity, specific heat, convection heat transfer coefficient, density, and emissivity. However, for the steady state conditions analyzed for the NCT, density and specific heat are not applicable and therefore, only thermal conductivity, heat transfer coefficient, and emissivity are considered for the sensitivity analysis.

The DOEx allows for identification of the factors to which the results are most sensitive. The identification of these factors can result in better control of their variability. This methodology is more efficient than a standard Monte Carlo technique which requires a large number of simulations. This methodology can also highlight the significant interaction of various factors than Monte Carlo schemes.

RESPONSE VARIABLES

The response variable is the temperature of Celotex, O-rings, and the contents. The 9975 design sets a maximum temperature limit for each of these components. Out of these three items, Celotex has been found to have the least safety margin. Therefore, only Celotex temperature will be analyzed in the sensitivity analysis here.

FACTORS EVALUATION

Thermal Properties Data

There is very limited amount of experimental data to estimate the variance of the thermal properties of Celotex type insulating and impact resistant materials. A quick search with keywords “stochastic heat transfer”, or “thermal conductivity variance”, or “statistical aspects of thermal conductivity of insulating materials” turned up very limited links and only one NIST [3] link to estimate the probability distributions of k. No data was found for estimating the specific heat variation.

Thermal conductivity and heat capacity are the two most important material properties in the study of heat transfer. A basic understanding of the microstructure of the fiberboard type material is necessary to postulate the variance of k and Cp. In solids, electrons and phonons (lattice structure vibrations) are the main energy carriers. In metals, electrons contribute the most to thermal properties while in insulators, where there is lack of free electrons, phonons are the main energy carriers. Since lattice vibration modes are directional, the continuum thermal conductivity of insulators is the result of cumulative effect of the lattice structures in that direction. Therefore, this type of behavior can be modeled by normal distribution.

Celotex thermal conductivity has been measured by Celotex Co. over a number of years (1933 to 1953). These values are documented in NIST database [3]. The values (Btu/°F-Hr-Ft) are reproduced in Table 1 for convenience.

Table 1 – Thermal Conductivity Values of Celotex

0.0573	0.0534	0.0524	0.0475
0.0574	0.0533	0.0572	0.0498
0.0574	0.0523	0.0528	0.0462
0.0573	0.0527	0.0563	0.0526
0.0541	0.0492	0.0471	0.0519
0.0604	0.0482	0.0502	0.0467
0.0534	0.0544	0.058	0.0594
0.0548	0.0496	0.0551	0.0594

It is found that normal distribution fits very well to this set of data. The Anderson-Darling normality test gives a p-value of 0.145. The normality plot is shown in Figure 2. The data gives a coefficient of variation (COV) of about 7.5%. For the factorial design levels, the upper and lower limits will be taken 2 standard deviations which will give about 15% variation from the mean. This will give about 95% coverage of the thermal conductivity values.

Celotex Thermal Conductivity for 9975 Package

The NIST database assumes Celotex as isotropic material since only one k value is given. For the 9975 use, ½” Celotex disks are glued together to fit around the containment vessel assembly. The inclusion of glue makes the Celotex somewhat orthotropic. Thermal properties of these Celotex disks have been determined by experiments by Jarrell [4], Lewallen [5], Sanchez [6], and Vormelker [7]. A comparison of k at different temperatures is given in Table 2 from these studies.

Table 2 – Celotex Thermal Conductivity Comparison

Temp	Sanchez/Jarrell		Vormelker		Difference	
°F	Normal	Parallel	Normal	Parallel	Normal	Parallel
77	0.03	0.07	0.034	0.060	12.97%	15.00%

The measurements by Jerrell [5] showed that the thermal conductivity was different normal to the cane fiber direction. The value was found to be higher in the cane fiber direction due to the glue between the ½” disks. The difference in the thermal conductivity in the two studies can be due to the heterogeneity of the Celotex from different batches. It is assumed that the variation in the thermal conductivity in the direction parallel to the fibers is same (15%) as in the normal direction.

Convection Heat Transfer Coefficient

The convective heat transfer coefficients are normally estimated from the published correlations where accuracy is limited typically to 20% confidence [2]. Therefore, the factor levels will be taken 20% above and below the mean values. The mean values for the 9975 design parameters [8] are given in Table 3.

Table 3 – Convection Heat Transfer Coefficients

Surface	Correlation[a]
Flat Lid of the drum	$0.22*(\Delta T)^{1/3}$
Curved surface	$0.19*(\Delta T)^{1/3}$

[a] ΔT = temperature difference between the model surface and the environment (°F)

Radiation Heat Transfer Data

Emissivity values for the drum surface can vary substantially due to the difference in surface finish, material variability, accumulation of dirt, etc. The drum specification calls for surface finish No. 2B in the ASTM Standard SA-480. This finish is described as “cold-rolled, bright finish”. In accordance with the Standard, the descaled stainless steel sheet gets a final light cold-rolled pass on polished rolls. 9975 Safety Analysis Report [8] lists the emittance for the three types of ‘as received’ stainless steel. These values at 400°K are given in Table 4.

Table 4 – Emittance for Surface Finish

Surface Condition	Emittance
Close to polished	0.124
Medium finish	0.21
Very dull surface	0.296

A value of 0.21 is used in the certified 9975 design. The lower and upper factor levels for the emittance will be taken as 0.124 and 0.296.

Factor Levels

There are three levels of treatments that are available for this design of experiment model. The three levels are mean, lower, and upper. In the experimental design, two level models are considered most useful for practical considerations. Therefore only lower and upper levels are considered here. If the temperature response surface is believed to have considerable curvature, additional levels will be included in the design. The lower and upper levels for the factors k, h, and ε or A, B, and C are calculated from the expected values and are given in Tables 5, 6, and 7.

Table 4 - Levels for Factor A (k)

Temperature	Lower	Upper	Direction[a]
70 to 300°F	0.0615	0.0831	radial
76	0.0264	0.0357	Axial
187	0.0289	0.0391	Axial
295	0.0306	0.0414	Axial
439	0.0323	0.0437	Axial
533	0.0247	0.0334	Axial

[a] Radial direction is parallel to the fibers

Table 5 - Levels for Factor B (h)

Surface	Upper	Lower
Horizontal Plate	$0.176*(\Delta T)^{1/3}$	$0.264*(\Delta T)^{1/3}$
Vertical Plate	$0.152*(\Delta T)^{1/3}$	$0.228*(\Delta T)^{1/3}$

Table 7 - Levels for Factor C (e)

Lower	Upper
0.124	0.296

MODEL

The 9975 package thermal analysis is a complex problem to solve. The package has heat generation, natural convection boundary conditions, radiation boundary conditions, heat flux, internal gaps, multiple materials, variable material properties, etc. The problem is normally solved deterministically using numerical methods for the best estimates, sometimes too conservatively, of these factors. However, the emphasis in this study is to explore the sensitivity of the thermal response to the observed variation of only certain factors. The sensitivity analysis is undertaken by fitting a metamodel to the results of factor values chosen by experimental design so that a closed form may be discerned. While this form will not be a perfect representation of the relationship between factor changes and package response (temperature T of certain components), an appropriate form facilitates both analysis and understanding. A relation between the response variable T and all the factors can be expressed as,

$$T_1 = f_1(X_1, X_2, ..., X_n)$$

A metamodel is a simplification of the model under study, which is deterministic and employs a subset of the factors

$$\overline{X} = \{Xj \mid j = 1,2,\ldots,m\}, \text{ where } m < n:$$

$$T_2 = f_2(X_1, X_2, ..., X_m) + \varepsilon_m$$

T_2 is the response of the metamodel and ε_m is the composition of the error of the effects of any excluded factors and the error of fitting the metamodel to the underlying relationship. The main issues in this simplified model are: (1) the choice of underlying functional form f_2, (2) the choice of factors and their levels, (3) the selection of response values to construct the model, and (4) validation of the model. The nature of f_2 is unknown and a simple formulation in x_1 (k), x_2 (h), and x_3 (ε) is assumed [9].

$$T = c_0 + c_1x_1 + c_2x_2 + c_3x_3 + c_{12}x_1x_2 + c_{13}x_1x_3 + c_{23}x_2x_3 + \varepsilon_m \quad (1)$$

Where x_1, x_2, and x_3, collectively represented by column vector $\overline{X}$, are the coded values of k, h, and ε respectively as explained below. c’s are the parameters to be determined from the response data. ε_m represents the lack-of-fit error. The term $x_1x_2x_3$ involving interaction among all three factors is ignored since three factor interaction in a three factor analysis is normally negligible. This will become evident when the regression analysis is performed. The formulation in Eq. 1 is justified on the basis of Taylor series expansion of the function f_2 at the center point $\overline{X} = 0$. If the response surface T is differentiable in the region of interest and there are no sharp gradients, i.e., T does not have too much curvature, Eq. 1 can be a good representation in the region of interest. Only first partial derivatives and there linear combinations are assumed in the first attempt. In statistical analysis, Eq. 1 is a multiple linear regression model since only linear combinations of the parameters occur. The coded factor x_1, x_2, and x_3 are bounded by +1 and -1 and are related to the natural factor values by the following relations.

$$x_1 = \frac{k - (k_{low} + k_{high})/2}{(k_{high} - k_{low})/2} \qquad (2)$$

$$x_2 = \frac{h - (h_{low} + h_{high})/2}{(h_{high} - h_{low})/2} \qquad (3)$$

$$x_3 = \frac{e - (e_{low} + e_{high})/2}{(e_{high} - e_{low})/2} \qquad (4)$$

If lower factor level is designated as -1 then the upper level becomes +1. The mid level (mean) will be 0. For a two level model, a full 2^3

factorial design can be represented by the 8 run design matrix shown in Table 8. The design matrix is symbolically shown in Figure 3.

Table 8 – Design Matrix

Run	x_1	x_2	x_3	Response (T)
1 (-1)	-1	-1	-1	289.82
2 (a)	+1	-1	-1	284.68
3 (b)	-1	+1	-1	249.23
4 (ab)	+1	+1	-1	245.00
5 ©	-1	-1	+1	259.53
6 (ac)	+1	-1	+1	254.91
7 (bc)	-1	+1	+1	231.27
8 (abc)	+1	+1	+1	227.32

The response variable T in the Table above is determined for the 8 runs using computer software MSC/PTHERMAL [10]. This software solves the physics based heat transfer partial differential equations and is deterministic in nature.

RESULTS

An analysis of variance (ANOVA) is performed using the statistical software package MINITAB [11]. The estimate for the effects x_1, x_2, and x_3 for the model in Eq. 1 is shown in Table 9.

Table 9 – Estimate of Factor Effects

Factor	Effect	Coef. (c's)	SE Coef.	T	P
Constant		255.22	0.0285	8955.09	0
A	-4.48	-2.24	0.0285	-78.67	0.008
B	-34.03	-17.01	0.0285	-596.99	0.001
C	-23.93	-11.96	0.0285	-419.76	0.002
A*B	0.4	0.2	0.0285	6.94	0.091
A*C	0.2	0.1	0.0285	3.43	0.181
B*C	6.11	3.05	0.0285	107.11	0.006

The results show that the interactions AB and AC are insignificant at confidence level $\alpha = 5\%$. The coefficient c_{123} for the interaction A*B*C (not shown in Table 9) is -0.03 and is therefore negligible compared to other factors as expected. The estimated effects and ANOVA results after dropping these interactions are shown in Tables 10 and 11.

Table 10 – Estimated Effects for Significant Factors

Term	Effect	Coef	SE Coef	T	P
Constant		255.22	0.1284	1987.44	0.000
A	-4.48	-2.24	0.1284	-17.46	0.000
B	-34.03	-17.01	0.1284	-132.49	0.000
C	-23.93	-11.96	0.1284	-93.16	0.000
B*C	6.11	3.05	0.1284	23.77	0.000

Table 11 – ANOVA Results

Source	DF	Seq SS	MSE	F	P
Main Effects	3	3501.04	1167.01	9.0E+03	0.000
2-Way Interactions	1	74.54	74.54	565.03	0.000
Residual Error	3	0.40	0.13		
Total	7	3575.98			

$$\text{RMS error} = \sqrt{\frac{SS_E}{2^3}} = \sqrt{\frac{0.4}{8}} = 0.224$$

The error residuals are normally distributed as shown in Figure 4. The DOEx model based on Eq. 1 can now be formalized. The interactions x_1x_2 and x_1x_3 have been dropped.

$$T = 255.22 - 2.24x_1 - 17.01x_2 - 11.96x_3 + 3.05x_2x_3 \qquad (5)$$

R^2 for this model is 99.999%. This shows almost perfect representation of the data in the model. However, the R^2 value could be deceptive since the model is good only for the factorial points in Table 8. The model should be tested for its validity for other independent factor values which will exclude the factor values used for the model in Eq. 1. This is the validation phase and is described below.

VALIDATION OF LINEAR MODEL

Eight independent factor values are chosen to test the validity of the model in Eq. 5. These validation points are also shown on the hypercube in Figure 3. These factor values and RMS error calculations are given in Table 12. The actual values of the response variable were calculated using the software MSC PThermal [10].

Table 12* – Validation Factor Level Matrix

Run #	x_1	x_2	x_3	x_2x_3
1	-1	-1	0	0
2	1	-1	0	0
3	-1	1	0	0
4	1	1	0	0
5	0	-1	-1	1
6	0	-1	1	-1
7	0	1	-1	-1
8	0	1	1	1

* Table 12 is continued on the next page

Table 12 – cont'd

Predicted	Actual	Absolute Error	SS_E
274.47	273.04	1.430	2.0449
269.99	268.187	1.803	3.2508
240.45	239.556	0.894	0.7992
235.97	235.477	0.493	0.243
287.24	287.106	0.134	0.018
257.22	257.087	0.133	0.0177

247.12	246.995	0.125	0.0156
229.3	229.18	0.120	0.0144
	Average	0.6415	0.80045

$$\text{RMS error} = \sqrt{Average} = \sqrt{0.8005} = 0.8947$$

This error though small compared to the mean temperature of 255.22°F is still 4 times the RMS for the main model. Therefore, the model given in Eq. 5 is missing some additional terms that were neglected in the linear model. A new model is chosen that will include square terms also. This model is the well known central composite design or CCD with 15 factor values. The additional factor values are the hypercube face center points and the center of the hypercube. These points are also shown in Fig. 3. The model is given in Eq. 6.

$$T = c_0 + c_1x_1 + c_2x_2 + c_3x_3 + c_{11}(x_1)^2 + c_{22}(x_2)^2 + c_{33}(x_3)^2 + c_{12}x_1x_2 + c_{13}x_1x_3 + c_{23}x_2x_3 + \varepsilon_m \qquad (6)$$

The design matrix now consists of factor levels in Table 8, 6 face center points, and one center point. The additional 7 factor levels are shown in Table 13. Run numbers represent the experiment number. Run #15 is the center point.

Table 13 – Additional Factor Levels

Run #	x_1	x_2	x_3	x_2x_3
9	-1	0	0	0
10	1	0	0	0
11	0	-1	0	0
12	0	1	0	0
13	0	0	-1	0
14	0	0	1	0
15	0	0	0	0

A response surface analysis using MINITAB [11] software is performed. The estimated coefficients for the various effects in Eq. 6 are given in Table 14. The P value indicates that square terms are important for factors B and C. Only interaction BC is significant.

Table 14 – Response Surface Analysis Scoping Results

Term	Coef	P
Constant	251.81	0.000
A	-2.24	0.000
B	-16.92	0.000
C	-11.84	0.000
A*A	0.18	0.535
B*B	2.14	0.001
C*C	1.08	0.011
A*B	0.2	0.266
A*C	0.1	0.554
B*C	3.05	0.000

The error residuals are normally distributed as shown in Figure 4. The estimated effects and ANOVA results after dropping A*A, A*B and A*C terms are shown in Tables 15 and 16.

Table 15 – Estimated Effects

Term	Coef	SE Coef	T	P
Constant	251.87	0.2176	1157.407	0.000
A	-2.24	0.1357	-16.477	0.000
B	-16.92	0.1357	-124.68	0.000
C	-11.84	0.1357	-87.235	0.000
B*B	2.19	0.2565	8.536	0.000
C*C	1.14	0.2565	4.428	0.002
B*C	3.05	0.1517	20.119	0.000

Table 16 – ANOVA Results

Source	DF	Seq SS	Adj MS	F	P
Regression	6	4415.64	735.94	4.00E+03	0.000
Linear	3	4314.19	1438.06	8.00E+03	0.000
Square	2	26.91	13.45	73.05	0.000
Interaction	1	74.54	74.54	404.77	0.000
Residual	8	1.47	0.18		
Total	14	4417.11			

VALIDATION OF RESPONSE SURFACE MODEL

We will use the same Validation Factor Level Matrix given in Table 12 that was used in the linear model. The RMS calculation is given in Table 17.

Table 17 – Validation Results

Predicted	Actual	Absolute Error	SS_E
273.22	273.04	0.180	0.0324
268.74	268.187	0.553	0.3058
239.38	239.556	0.176	0.031
234.9	235.477	0.577	0.3329
287.01	287.106	0.096	0.0092
257.23	257.087	0.143	0.0204
247.07	246.995	0.075	0.0056
229.49	229.18	0.310	0.0961
	Average	0.26375	0.1042

$$\text{RMS error} = \sqrt{Average} = \sqrt{0.1042} = 0.3228$$

The RMS in the new model is significantly less than in the linear model. The regression model in the natural variable form is easily calculated by substituting x_1, x_2, and x_3 from equations 2, 3, and 4 in Eq. 6.

The 95% confidence interval (CI) for the mean temperature can now be established. The CI is given by:

$$\begin{aligned}\text{Response mean} \pm t_{8,0.025}\text{SE} &= 251.18 \pm 2.306*0.218 \\ &= 251.18 \pm 0.50 \;\; = (250.68, 251.68),\end{aligned}$$

where $t_{8,0.025}$ is the Student t-distribution value at $\alpha = 0.05$ for 8 degrees of freedom, and SE is the standard error for the main model in Table 16.

This result shows that at 95% confidence level, the upper limit of the maximum Celotex temperature is 251.60°F. This is well below the 280°F limit recommended by Lewallen [4] and 300°F limit in the 9975 SARP [8] for the Celotex. This analysis shows that the 9975 design is robust to the expected variation in the Celotex thermal conductivity, convection heat transfer coefficient, and the emissivity of the drum outer surface.

CONCLUSIONS

1. The 9975 design is robust. The analysis demonstrates that the 9975 design is quite insensitive to the variability in the thermal conductivity of Celotex, convection heat transfer coefficient, and the emissivity of the drum surface.
2. Celotex thermal conductivity variability in the commercial grade Celotex will not impact the thermal response of the 9975 design. A similar variability in the in-plane thermal conductivity due to the Celotex disc bonding agent will not impact the design.
3. It is found that the convection heat transfer coefficient variation affects more than other factors. However, even a large variation of ±20% from the mean values used in the baseline analyses will not adversely impact the thermal integrity of the 9975 design. This is important because a good estimate of h is difficult in the transport conditions where more than one package is transported at any given time.

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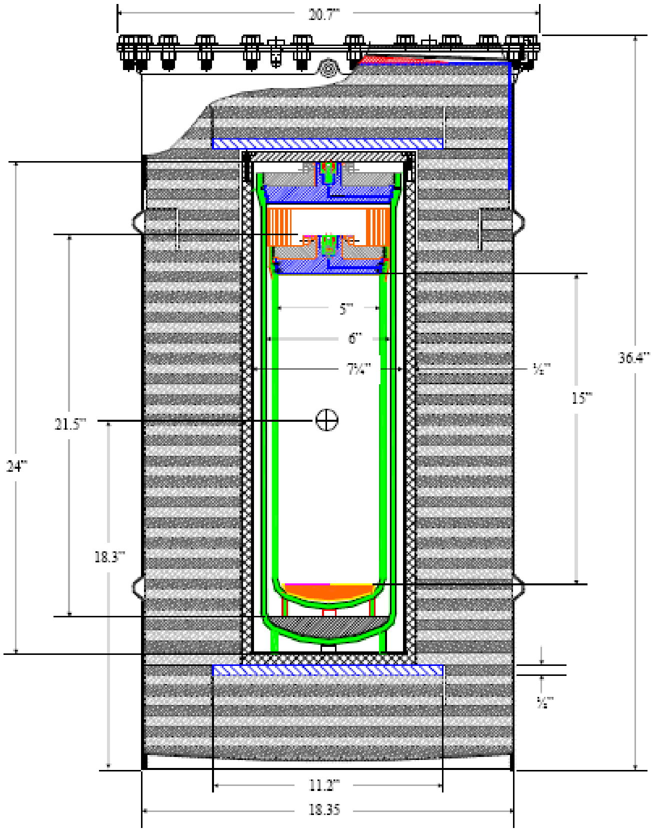

Figure 1 – 9975 Package Schematic

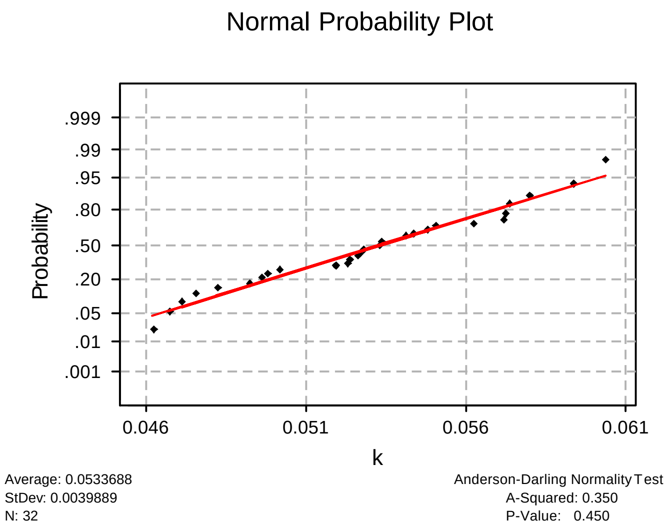

Figure 2 – Normality Plot of the Thermal Conductivity Data

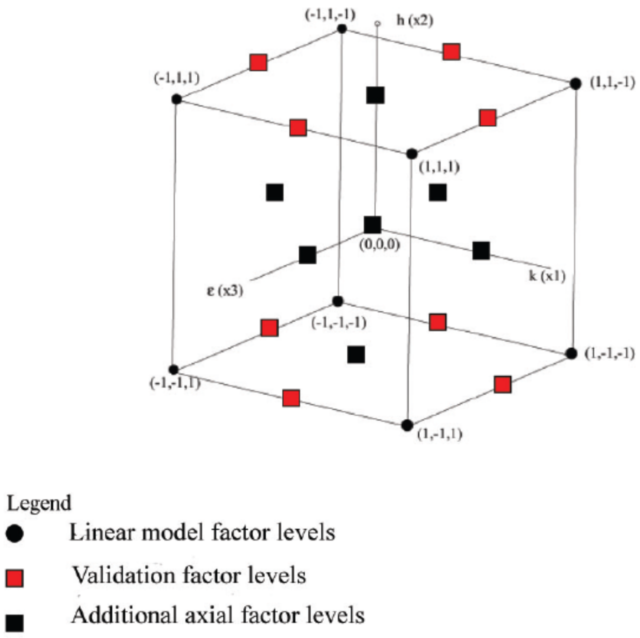

Figure 3 – Factor Levels Hypercube

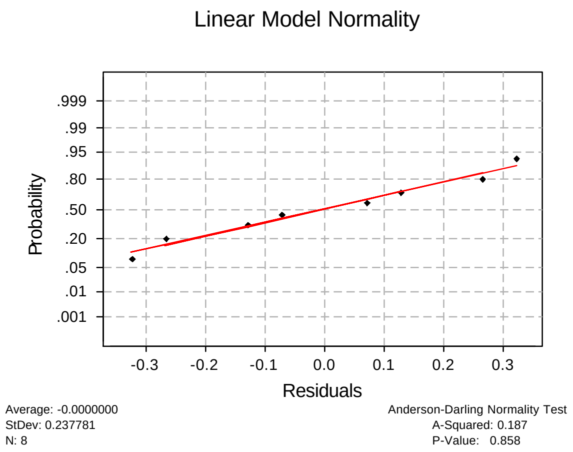

Figure 4 – Normality Plot for the Linear Model

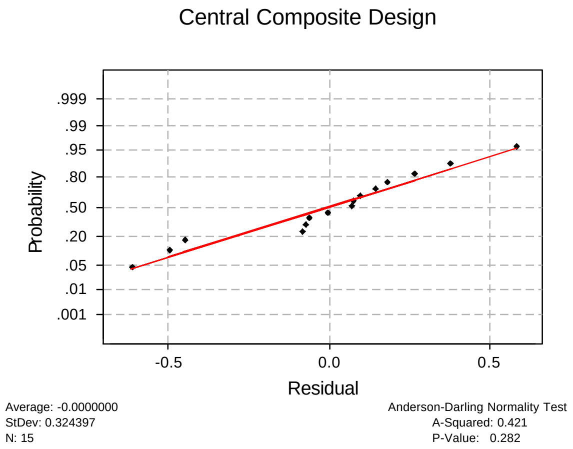

Figure 5 – Normality Plot for the CCD Residuals