This document was prepared in conjunction with work accomplished under Contract No. DE-AC09-96SR18500 with the U.S. Department of Energy.

WSRC-STI-2008-00210

Proceedings of ASME PVP2008
ASME Pressure Vessel & Piping Division Conference
July 27-31, 2008, Chicago, IL, USA

PVP2008-61009

Temperature Prediction in 3013 Containers in K-Area Material Storage (KAMS) Facility Using Regression Methods

Narendra K. Gupta
Savannah River National Laboratory, Aiken, SC 29808
nick.gupta@srnl.doe.gov

ABSTRACT

3013 containers are designed in accordance with the DOE-STD-3013-2004. These containers are qualified to store plutonium (Pu) bearing materials such as PuO_2 for 50 years. DOT shipping packages such as the 9975 are used to store the 3013 containers in the K-Area Material Storage (KAMS) facility at Savannah River Site (SRS). DOE-STD-3013-2004 requires that a comprehensive surveillance program be set up to ensure that the 3013 container design parameters are not violated during the long term storage. To ensure structural integrity of the 3013 containers, thermal analyses using finite element models were performed to predict the contents and component temperatures for different but well defined parameters such as storage ambient temperature, PuO_2 density, fill heights, weights, and thermal loading. Interpolation is normally used to calculate temperatures if the actual parameter values are different from the analyzed values. A statistical analysis technique using regression methods is proposed to develop simple polynomial relations to predict temperatures for the actual parameter values found in the containers. The analysis shows that regression analysis is a powerful tool to develop simple relations to assess component temperatures.

INTRODUCTION

The 3013 containers are designed in accordance with the DOE-STD-3013-2004 [1]. These containers are qualified to store plutonium (Pu) bearing materials for 50 years. DOT shipping packages such as 9975 are used to transport the 3013 containers from other U.S. Department of Energy (DOE) sites to the Savannah River Site (SRS) for long term storage until the Pu can be properly dispositioned. Additionally, these 9975 packages are used to store the 3013 containers in the KAMS facility. Separate analyses given in Reference 2, 3, 4, and 5 cover the safety basis for the off-normal no-flow and fire conditions in the storage areas. These analyses serve to provide non-accident condition, non-bounding, specific 3013 container temperatures for use in the surveillance activities.

This paper presents the thermal analyses for the Rocky Flats 3013 storage configurations to predict the relevant temperatures so that the structural integrity of these containers can be ensured. The primary intent of the paper is to present a statistically sound regression methodology to cover a wide range of contents' physical and thermal data such as density, decay heat, and fill height. The regression equations presented in this paper provide a very convenient method to calculate the necessary temperature data to ensure that the 3013 surveillance program can assess the integrity of the stored packages in the DOE complex. This paper documents the following:

- Temperatures profiles of the can surface temperatures at different points (T_1, T_2, and T_3) of the outer, inner and convenience cans as depicted in Figure 1. T_1 gives the temperature profile at top of the can, T_2 gives the temperature profile at middle of the can, and T_3 gives the temperature profile at the bottom of the can.
- Average gas temperature (T_G) within the 3013 inner and outer cans, and the convenience cans.

9975 PACKAGE

The 9975 package is designed to transport fissile materials across the Department of Energy (DOE) complex [6]. Although, the package is designed for transport, it is being used to store the fissile materials for long term storage at KAMS. It is the long term storage aspect that is being addressed in the surveillance program. The surveillance program addresses the long term integrity of the O-ring seals, the fiberboard physical condition and its thermal properties, and non-destructive/destructive examination of the 3013 vessels. The maximum allowed content decay-heat rate is 19 watts. Figure 3 shows the cutaway view of the 9975 package with the 3013 container.

The 9975 package is designed to meet the requirements of Code of Federal Regulations 10 CFR 71 [7] to ensure that the environment and public health are not adversely impacted during transport. However, the design requirements during normal and accident conditions for the long term storage are different from the normal and accident conditions during transport. The surveillance program is designed to ensure that the 9975 design envelope is not breached.

Thermal Operating Parameters

The safety analyses [2, 3, 4] for the storage facility give the maximum ambient temperature inside the storage area. The 9975 package with payload provides the thermal data for the contents. The thermal data include content density, decay heat, and fill height inside the convenience cans. Since the building ambient temperature varies somewhat during the year, and the thermal data could fall anywhere within certain limits, it was agreed to restrict the number of analyses just for the input data given in Table 1.

Table 1 - 3013 Contents Variables

Variable	Low	Mid	High
Fill Height (cm)	*	*	17.0
Oxide Bulk Density (g/cc)	1.0	3.0	5.0
Heat Generation (W/kg)	3.0	6.0	12.0
Total heat load (W)	5.0	10.0	19.0
Oxide Mass (g)	2000	3000	5000

* Calculate fill height based on oxide mass and bulk density, but never exceed a fill height of 17.0 cm or a maximum heat load of 19.0 watts.

Based on the above input data and the convenience can geometry, the fill heights and thermal loads given in Table 2 were derived for preparing the finite element models.

Table 2 – Fill Height of PuO_2

Density	Rocky Flats Configuration		
(g/cc)	Height (cm/inches)	Weight (kg)	Heat Load (watts)
1	17/6.693	1.592	4.777
3	13.62/5.364	3	10
5	13.62/5.364	5	19

Fill Gases

An important consideration in setting up the finite element thermal models was the consideration of fill gases. The primary fill gas composition in the 3013 containers is 75% helium and 25% air by volume. This gas composition meets the 'less than 5% oxygen' requirement in the DOE standard for the PuO_2 contents [1]. Thermal conductivity of the PuO_2 powder changes with the fill gases. A methodology that considers the PuO_2 powder porosity, its particle geometry, and fill gas thermal properties was used to calculate the effective thermal conductivity [8][1].

Thermal Models

A general heat transfer code MSC Patran/Thermal [9] was used to model the 9975 package during storage. This code was used to design the 9975 package for transport and the model originally was benchmarked with actual test data. The code is capable of modeling complex geometries and a wide variety of thermal boundary conditions. The code cannot model internal convection mode of heat transfer that requires the solution of Navier-Stokes fluid dynamics equations. The modeling experience with 9975 package shows that internal natural convection can be ignored. Convection and radiation boundary conditions were imposed on the outer drum surface of the drum surface.

Two different finite element models were created to model different fill heights, i.e., one for the 1g/cc powder and one for the 3 g/cc and 5 g/cc powders. Color representations of these two finite element models are shown in Figures 3 and 4. The finite element models of the 3013 containers with the 3 g/cc and 5 g/cc, 1 g/cc PuO_2 powder are shown in Figures 5 and 6. The internal heat generation rates, thermal conductivity of the PuO_2 powder were varied to simulate different thermal loading parameters. A total of 12 different thermal models were analyzed to cover the full range of loading conditions.

RESULTS

The temperature results are tabulated for locations T1, T2, and T3 and for the average gas temperature for each can. The results for the outer can are listed in Table 3, for the inner can in Table 4, and for the convenience can in Table 5.

Table 3 - Outer Can Temperatures

Table 3 – Outer Can Temperatures (cont'd)

Density (g/cc)	Watts (W)	Temp (ºF)	Location T1 (ºF)	Location T2 (ºF)	Location T3 (ºF)	Gas (ºF)
1	4.777	55	84.47	87.35	83.14	85.18
3	10	55	126.25	136.09	128.74	129.42
5	19	55	182.75	200.56	188.87	188.51
1	4.777	85	113.18	116.03	112.09	113.92
3	10	85	153.44	163.07	156.22	156.56
5	19	85	208.20	225.70	214.71	213.87
1	4.777	120	146.80	149.59	145.94	147.55
3	10	120	185.45	194.84	188.52	188.50
5	19	120	238.38	255.58	245.36	243.98
1	4.777	162	187.34	190.07	186.74	188.11
3	10	162	224.25	233.39	227.64	227.24
5	19	162	275.69	292.55	283.24	281.21

Table 4 – Inner Can Temperatures

Density (g/cc)	Watts (W)	Temp (ºF)	Location T1 (ºF)
1	4.777	55	84.98
3	10	55	127.32
5	19	55	184.67
1	4.777	85	113.68
3	10	85	154.49
5	19	85	210.10
1	4.777	120	147.29
3	10	120	186.48
5	19	120	240.24
1	4.777	162	187.82
3	10	162	225.26
5	19	162	277.52

---

[1] A recent investigation at LANL indicates that our estimate for the effective thermal conductivity of the PuO_2 powder may be too low.

Table 4 – Inner Can Temperatures (cont'd)

Location T2 (ºF)	Location T3 (ºF)	Gas (ºF)
87.92	84.80	86.24
137.30	133.06	131.45
202.74	196.19	192.25
116.57	113.68	114.95
164.24	160.36	158.58
227.82	221.76	217.59
150.12	147.45	148.55
195.97	192.46	190.50
257.65	252.13	247.67
190.57	188.15	189.07
234.48	231.38	229.22
294.56	289.68	284.88

Table 5 – Convenience Can Temperatures

Density (g/cc)	Watts (W)	Temp (ºF)	Location T1 (ºF)
1	4.777	55	86.91
3	10	55	130.50
5	19	55	190.23
1	4.777	85	115.57
3	10	85	157.60
5	19	85	215.53
1	4.777	120	149.12
3	10	120	189.51
5	19	120	245.55
1	4.777	162	189.59
3	10	162	228.19
5	19	162	282.69

Table 5 – Convenience Can Temperatures (cont'd)

Location T2 (ºF)	Location T3 (ºF)	Gas (ºF)
89.17	84.05	93.73
141.64	131.33	146.48
210.50	193.45	212.74
117.80	112.96	122.46
168.49	158.71	173.57
235.47	219.14	238.10
151.31	146.77	156.09
200.11	190.91	205.47
265.16	249.63	268.22
191.74	187.52	196.63
238.51	229.92	244.17
301.92	287.32	305.48

REGRESSION ANALYSIS

Estimating the 3013 component temperatures at parameter (density, heat load, and storage temperature) values other than listed in Table 2 is best accomplished by performing regression analysis on the various results. However, regression analysis is a statistical method and certain conditions must be satisfied for the regression equation to be a good predictor [10]. These conditions are:

1. The errors (residuals) have a zero mean.
2. The errors (residuals) have constant variance.
3. The errors (residuals) are uncorrelated, i.e. they are independent.
4. The errors (residuals) are normally distributed.

It is possible to evaluate all the conditions except condition 2. Condition 2 can be evaluated only if we have multiple responses at every independent variable. This is not possible because the responses (temperatures) are obtained by computational model rather than physical experiments. Therefore, there is no experimental error, only model error in the regression equation. Condition 3 is satisfied because each response is independent of any other response. Conditions 1 and 4 will be checked after the errors are computed. The requirement of normality is important to perform the hypothesis tests to estimate how well the model fits the data.

It should be noted that content density manifests itself in the form of fill height in the finite element model even though density is not important in the steady state heat transfer analysis. In addition, density and heat load are correlated but then there is no requirement that the predictors (density, heat load, and storage temperature) be independent.

A review of the temperature profiles at T1, T2, and T3 locations of the 3013 components shows that the temperature varies linearly with density and storage temperature. Therefore, a linear regression equation should be sufficient. The regression equation is of the form:

$$\begin{aligned} T &= \beta_0 + \beta_1 \text{ Density} + \beta_2 \text{ Heat Load} + \beta_3 \text{ Storage Temperature} + \varepsilon \\ &= \beta_0 + \beta_1 \text{ Density} + \beta_2 \text{ Watts} + \beta_3 \text{ Temp} + \varepsilon \end{aligned}$$

Where T is the temperature, ε is the error term, and the βs are the regression parameters that will be calculated from the computed data.

The regression equations will be developed for the locations T1, T2, and T3 shown in Figure 1 for the outer can, the inner can, and the convenience can. The equations will also be developed for the average gas temperature inside the 3013 cans. The regression analysis was performed using MINITAB [11].

Outer Can

The regression equations for the temperatures at locations T1, T2, and T3 of the outer can are as follows:

Temp (T1) = 8.36 + 9.67*Density + 3.84*Watts + 0.915*Temp
Temp (T2) = 7.75 + 12.2*Density + 4.15*Watts + 0.910*Temp
Temp (T3) = 4.46 + 11.7*Density + 3.83*Watts + 0.925*Temp
Temp (Gas) = 7.92 + 10.7*Density + 3.90*Watts + 0.914*Temp

<u>Test for Error Correlation</u>: The Lag1 scatter plot for errors in predicted temperatures at location T1 shows that the errors are not correlated. This is shown in Figure 7. The errors for the temperatures at locations T2 and T3 and gas are similarly uncorrelated.

<u>Test for Normality of Errors (Residuals)</u>: The plot for T1 shows that the errors are normally distributed. This is shown in Figure 8. The normality test for the residuals at locations T2 and T3 and gas is also satisfied. Table 6 shows that all the predictors (variables) are statistically significant.

Table 6 – Regression Equation Coefficients

Predictor	Coef	SE Coef	T	P
Constant	8.356	1.859	4.5	0.002
Density	9.669	2.186	4.42	0.002
Watts	3.841	0.6077	6.32	0
Temp	0.91539	0.01355	67.54	0

The coefficient of determination, $R^2 = 99.9\%$ shows that the equation fits the data very well.

Inner Can

The regression equations for the temperatures at locations T1, T2, and T3 of the inner can are as follows:

Temp (T1) = 8.47 + 9.74*Density + 3.92*Watts + 0.915*Temp
Temp (T2) = 7.91 + 12.3*Density + 4.23*Watts + 0.909*Temp
Temp (T3) = 5.10 + 12.6*Density + 3.93*Watts + 0.920*Temp
Temp (Gas) = 8.11 + 10.7*Density + 4.08*Watts + 0.914*Temp

Test for Error Correlation: The Lag1 scatter plot for errors in predicted temperatures at location T1 shows that the errors are not correlated. This is shown in Figure 9. The errors for the temperatures at locations T2 and T3 and gas are similarly uncorrelated.

Test for Normality of Errors (Residuals): The plot for T1 shows that the errors are normally distributed. This is shown in Figure 10. The normality test for the residuals at locations T2 and T3 and gas is also satisfied. The hypothesis test for the inner can also shows that all the variables are statistically significant.

Convenience Can

The regression equations for the temperatures at locations T1, T2, and T3 of the convenience can are as follows:

Temp (T1) = 9.35 + 9.58*Density + 4.21*Watts + 0.912*Temp
Temp (T2) = 7.66 + 13.5*Density + 4.34*Watts + 0.906*Temp
Temp (T3) = 4.64 + 12.2*Density + 3.91*Watts + 0.922*Temp
Temp (Gas) = 13.0 + 15.8*Density + 3.58*Watts + 0.914*Temp

Test for Error Correlation: The Lag1 scatter plot for errors in predicted temperatures at location T1 shows that the errors are not correlated. This is shown in Figure 11. The errors for the temperatures at locations T2 and T3 and gas are similarly uncorrelated.

Test for Normality of Errors (Residuals): The plot for T1 shows that the errors are normally distributed. This is shown in Figure 12. The normality test for the residuals at locations T2 and T3 and gas is also satisfied. The hypothesis test for the convenience can also shows that all the variables are statistically significant.

CONCLUSIONS

1. Regression equations are developed to help in calculating temperatures for the storage conditions where the can PuO_2 weight, content heat load, and storage ambient temperatures are different from the values analyzed using the finite element models.
2. The regression analysis shows that a lot of tabular data can be reduced in the form of simple algebraic equations that are easy to use. However, it is necessary that simple statistical tests on the residuals be performed to ensure the validity of the equations.
3. Care should be exercised if PuO_2 has significant amount of impurities because the correlation between the PuO_2 decay heat and its density will be violated.

ACKNOWLEDGMENT

This paper was prepared in connection with work done under Contract No. DE-AC09-96SR18500 with the Department of Energy. By acceptance of this paper, the publisher and/or the recipient acknowledges the U.S. Government's rights to retain a nonexclusive, royalty-free license in and to any copyright covering this paper, along with the right to reproduce and to authorize others to reproduce all or part of the copyrighted paper.

DISCLAIMER

REFERENCES

1. DOE Standard Stabilization, Packaging, and Storage of Plutonium Bearing Materials, DOE-STD-3013-2004, April 2004.
2. Steady State Thermal Analysis of KAMS for No Flow Conditions (U), S-CLC-K-00203, Rev. 0, June 2004.
3. Thermal Analysis of Fires KAMS for No Flow Conditions (U), S-CLC-K-00204, Rev. 1, December 2005.
4. Integrated Thermal Analysis of the 9975 and SAFKEG Shipping Packages for KAMS for Phase 6 (U), S-CLC-K-00194, Rev. 1, May 2005.
5. K-area Materials Storage Facility Documented Safety Analysis, CN5A, WSRC-SA-2002-00005, Rev. 1, July 2006.
6. Model 9975 B(M)F-96, Safety Analysis Report for Packaging (U), WSRC-SA-2002-00008, Revision 1, Westinghouse Savannah River Company, Savannah River Site, Aiken, SC, January 2007.
7. Packaging and Transportation of Radioactive Material, Code of Federal Regulations, Title 10, Part 71, Washington, DC (January 2006).
8. Lam, P. S., Effective Thermal Conductivity of PuO2 Powder, SRT-MTS-96-2000, WSRC, January 1996.
9. MSC.PATRAN THERMAL 2003 r2, Online Manual, MSC Software Company, Santa Ana, California.
10. Introduction to Linear Regression Analysis, D. C. Montgomery and E. A. Peck, 2nd Edition, John Wiley & Sons, 1992.
11. MINITAB Statistical Software, Release 13, MINITAB Inc., www.minitab.com.

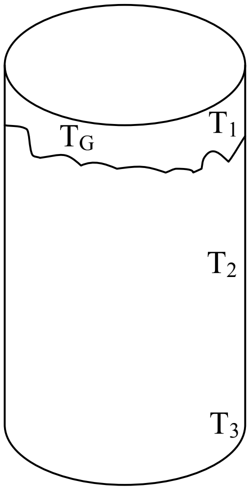

Figure 1 - Temperature profile locations for the 3013 cans (outer, inner, and convenience cans)

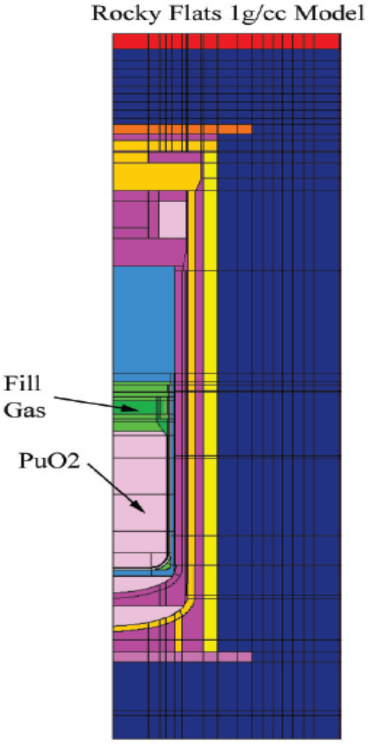

Figure 3 – Rocky Flats 1g/cc Model

Figure 2 – 9975 Cutaway View with 3013

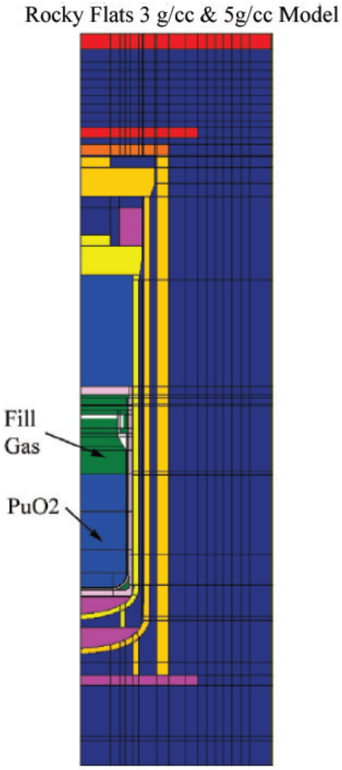

Figure 4 – Rocky Flats 3g/cc and 5g/cc Model

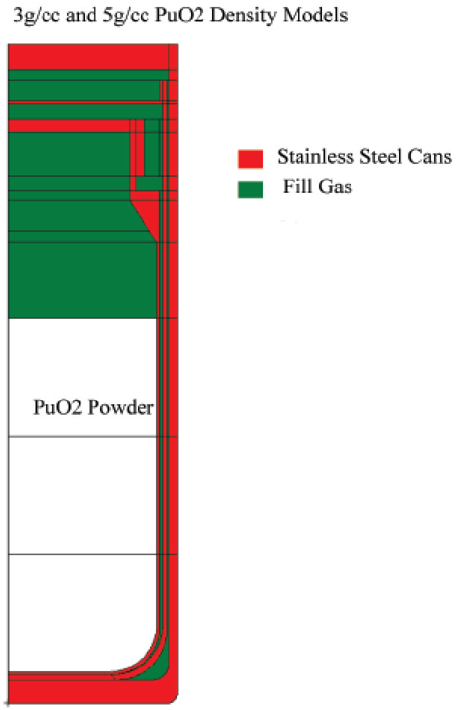

Figure 5 – 3013 Container Model for 3g/cc and 5g/cc PuO_2

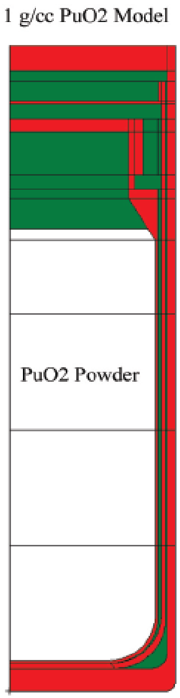

Figure 6 – 3013 Container Model for 1g/cc PuO_2

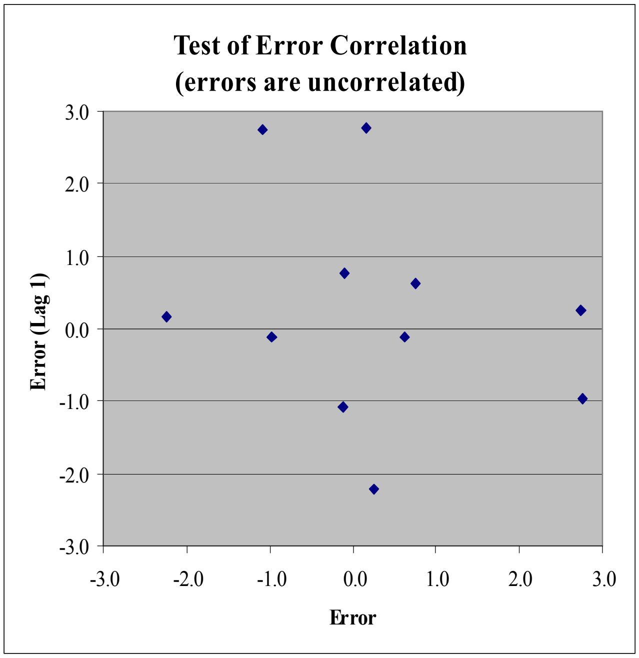

Figure 7 – Test for Residual Correlation
(Outer Can)

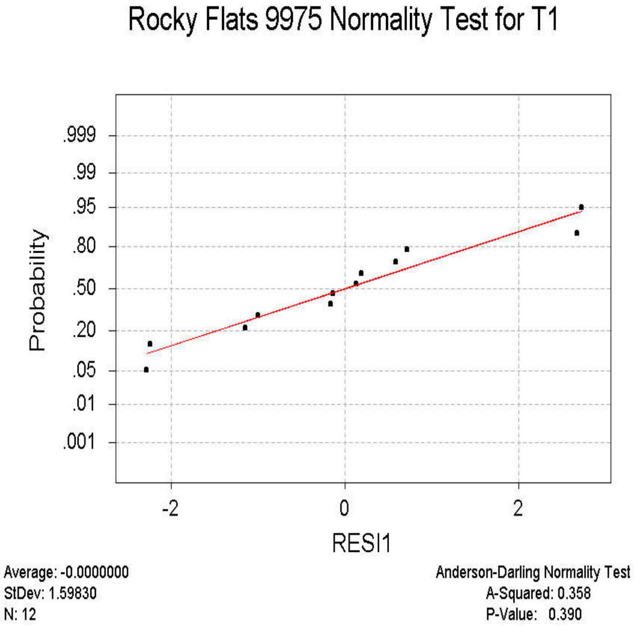

Figure 8 – Normality Test for Errors at Location T1
(Outer Can)

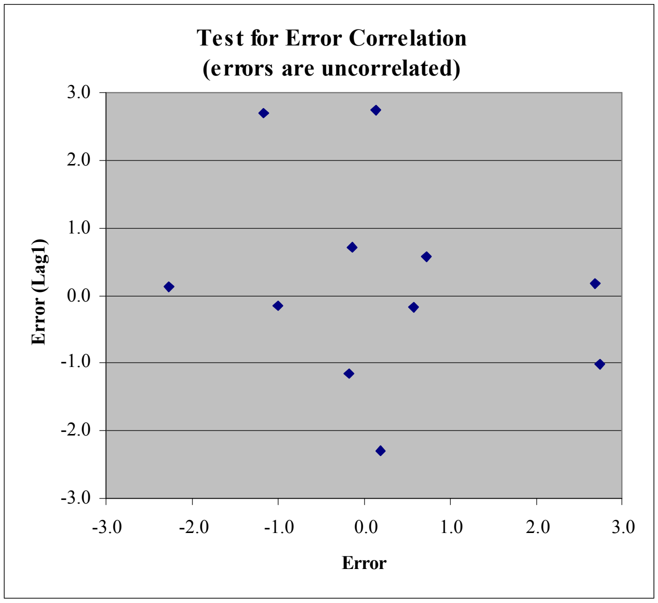

Figure 9 – Test for Residual Correlation
(Inner Can)

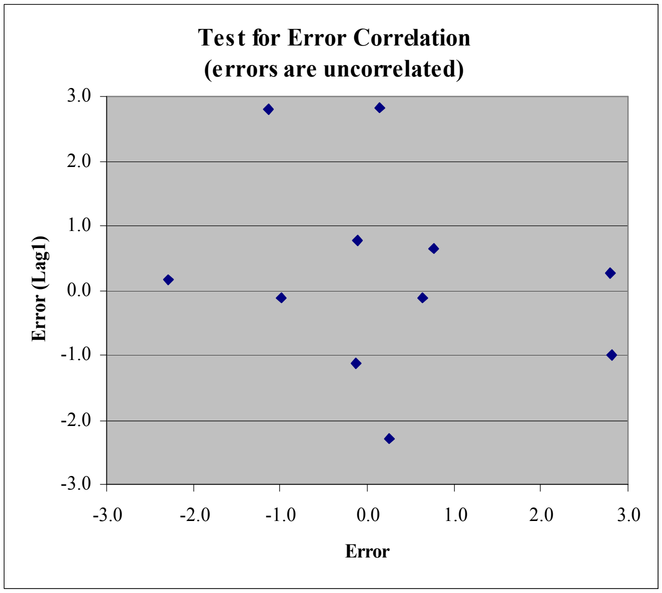

Figure 11 – Test for Residual Correlation
(Convenience Can)

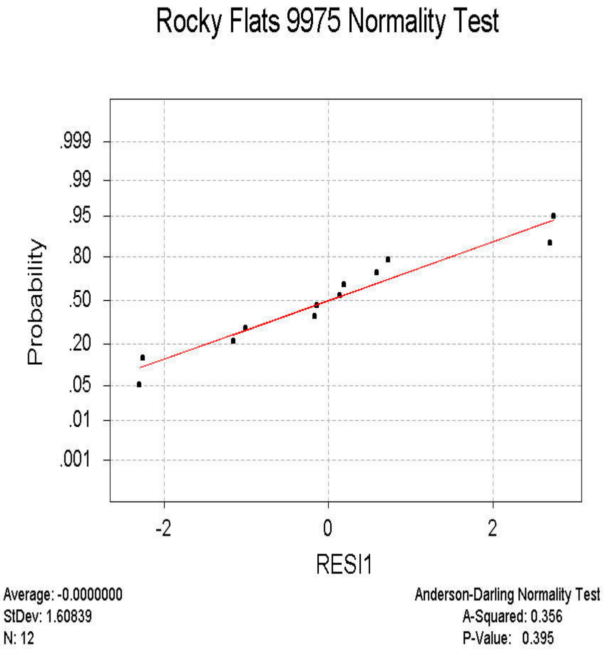

Figure 10 – Normality Test for Errors at Location T1
(Inner Can)

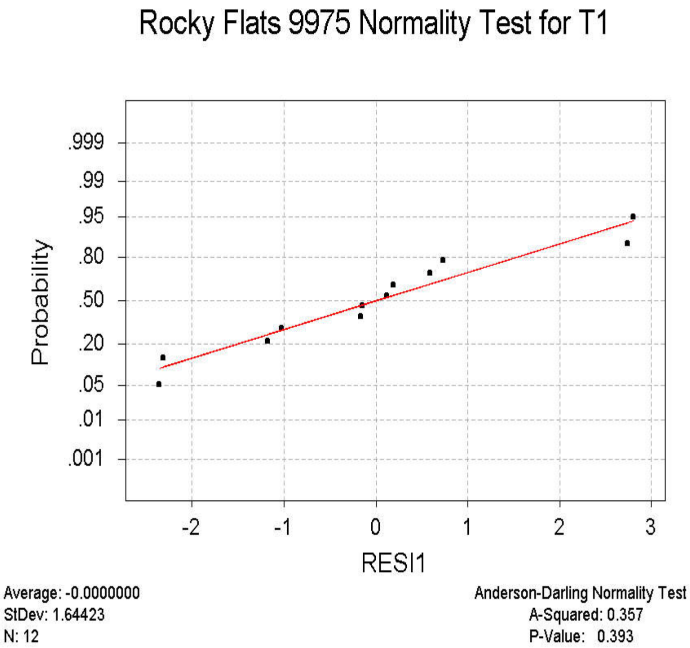

Figure 12 – Normality Test for Errors at Location T1
(Convenience Can)