Software Release Notice
Developed or Modified Software

1. Software Name: DTHERM	Software Version: 1.2.1
2. Software Function: Calculate Stress, Temperature, and Displacement for Waste Package	
3. Summary of Actions: ❑ New Software ✓ Update to Existing Software ❑ Software Retirement	
4. Software Development	
4a. Software Requirements Description (SRD) Date Approved: N/A 4b. Software Development Plan (SDP) Date Approved: N/A 4c. Software Change Report (SCR) Nos: 558 & 559 4d. User's Guide Approval Data N/A 4e. Enclosed: ❑ Copy of Program Title Block ❑ Sample Source Code Header Block	
Installation Performed by: Troy Maxwell	Date: 1/10/05
Remarks: None	
5. Software Installation	
5a. Computer Platform(s): PC 5b. Operating System(s): Windows 2000 5c. Programming Language(s): Mathcad 2000	
5d. Installation Testing: ✓ Passed Testing Performed on: Griffon Description of Testing Performed: DHTERM 1.2 was installed using Mathcad 2000	
5e. Archive Copy: ✓ Enclosed ❑ Not Available, Why:	
Installation Performed by: Troy Maxwell	Date: 1/10/05
Remarks: None	
6. Software Assessment	
6a. Acceptance Testing: ❑ Enclosed ✓ Documented in Scientific Notebook No. 689E ✓ Documented in SCRs (see above) 558 & 559	
6b. Validation Status: ✓ Full Validation ❑ Limited Validation Date of Validation: 2-1-2005 ❑ Not Validated, Explain:	
Software Developer: [signature]	Date: 3-3-05
Remarks:	
7. Approval	
Manager: AGhosh for AHC	Date March 4, 2005
Remarks:	
7. QA Verification	
SRN Number: 353	
Software Custodian [signature]	Date: 3/14/2005
Remarks:	

TOP-6-2 (12/2004)

SOFTWARE CHANGE REPORT (SCR)

1. SCR No.: 558	**2. Software Title and Version:** DTHERM Version 1.2	**3. Project No:** 20.06002.01.342

4. Affected Software Module(s), Description of Problem(s): DTHERM_2D.mcd

1. Output mislabeled.
2. 3D plots not working.
3. Code does not allow axial stress to vary in the radial direction.
4. Radial and Axial displacement displayed incorrectly. The displacement output provides the total length or total radius of the expanded waste package. The length and radius is added to the displacement.
5. Code only calculates contact temperatures even if there is a gap present.
6. Condition statement in wrong units which creates an error on certain versions of Mathcad.
7. Did not provide adequate comments within the software.
8. The temperature calculations did not have a base temperature and units were in Kelvin.

5. Change Requested by: Name: D. Gute Date: January 17, 2005	**6. Change Authorized by (Software Developer):** Name: T. Maxwell Date: January 17,2005

7. Description of Change(s) or Problem Resolution (***If changes not implemented, please justify***):

1. Applied correct label to output. Added temperature to output. Added axial stress to output. Changed stress units to MPa.
2. Removed 3D functionality of software.
3. Adjusted governing equations to allow axial stress to vary in the radial direction.
4. Adjusted radial and axial displacement output to provide the distance the waste package is displaced and not the expanded length or radius.
5. Modified code to calculate temperature for no contact cases. Previous code calculated temperatures as if the inner and outer barriers were in contact.
6. Modified condition statement to compare pressures instead of the force from contact.
7. Added assumptions and term definitions.
8. Temperature calculations were modified to allow for a reference temperature. Temperature input and output values are now in Celsius.

8. Implemented by: T. Maxwell	**Date:** January 20, 2005

9. Description of Acceptance Tests:

See attachment, "Description of Acceptance Tests."

10. Tested by: George Adams	**Date:** March 3, 2005

CNWRA Form TOP-5 (05/2000)

Attachment 1

Description of Acceptance Tests

The following table documents the acceptance testing conducted for this SCR:

	Pass	Fail	Description of Test
1	☑	☐	On the Output screen, the stress and temperature values are labeled correctly. The stresses are labeled with MPa units.
2	☑	☐	DTHERM now has only 2D functionality.
3	☑	☐	For any sample calculation, the axial stress varies in the radial direction.
4	☑	☐	The radial and axial displacement solutions display the displacement instead of displacement plus length.
5	☑	☐	The temperature output for the outer surface of the inner barrier and for the inner surface of the outer barrier shows a temperature drop between the surfaces when a gap exist.
6	☑	☐	The condition statement no longer compares Fstar to Pa, but now will compare radial and axial stress to a pressure value.
7	☑	☐	DTHERM now contains assumptions as well as definition of terms within the software.
8	☑	☐	Stress and displacement are now calculated from a reference temperature and the input and results have units of Celsius.

Test Performed

1. Viewed DTHERM version 1.1 and version 1.2 and verified the output screen has been corrected.
2. Verify that DTHERM 1.2 has only 2D functionality and 3-D Plots.mcd, 3-D.mcd, and CONTENTS.mcd have been removed.
3. Using the "Test 1" input and the Model Parameters from Table 1, verified the axial stress varies in the radial direction by viewing the 2D plot for axial stress.
4. Viewed DTHERM version 1.1 and version 1.2 and verified the displacement output screen displays displacement instead of expanded length.
5. Using the "Test 1" input and the Model Parameters from Table 1, verified there is a temperature drop for no contact cases. Using "Test 2" input, verified that a temperature drop did not exist for contact cases.
6. Viewed condition statement with the DTHERM 1.2 code and verified the condition statement compares consistent units.
7. Viewed DTHERM 1.2 code and verified code now contains assumptions and term definitions.
8. Viewed DHTERM 1.2 code and verified stress and displacement were calculated based on a reference temperature using "Test 3". The test verifies the displacement output is the same for the same temperature differential $T_{ambient} - T_{ref}$.

Additional Test

Using the "Test 1" input and the Model Parameters from Table 1, change the Ambient Temperature to 25 C and the Waste Form Heat Decay Rate to 0.00. The output produces '0' for all stress and displacement which illustrates the boundary conditions are correctly calculated within the code.

Table 1 Model Parameters	
Model Parameter	**Parameter Value**
Boundary Conditions	
Waste Form Heat Decay Rate (kW)	11.8
Ambient Temperature (C)	250.0
Reference Temperature (C)	250.0
Ambient Pressure (Pa)	25.0
Initial Inner Barrier Internal Pressure (atm)	1.0
Inner Barrier Material Properties	
Inner Barrier Thermal Conductivity (W/mK)	25.44
Inner Barrier Thermal Expansion Coefficient (1/K)	$17.5\ (10^{-6})$
Inner Barrier Modulus of Elasticity (Pa)	$1.248\ (10^{11})$
Inner Barrier Poisson's Ratio	0.27
Outer Barrier Material Properties	
Outer Barrier Thermal Conductivity (W/mK)	21.63
Outer Barrier Thermal Expansion Coefficient (1/K)	$1.368\ (10^{-5})$
Outer Barrier Modulus of Elasticity (Pa)	$1.558\ (10^{11})$
Outer Barrier Poisson's Ratio	0.30
Waste Package Dimensions	
Inner Barrier, Inner Radius (mm)	712
Inner Barrier, Total Length (mm)	4876
Inner Barrier Thickness (mm)	50
Outer Barrier Thickness (mm)	20

	Radial Gap (mm)	Axial Gap (mm)	Output
Test 1	2.00	10.0	D
Test 2	0.25	10.0	D

Test 3	T_{ref}	$T_{ambient}$	$Q_{generated}$	P_{ii}
Input A	0	75	0	0
Input B	25	100	0	0
Input C	50	125	0	0

SOFTWARE CHANGE REPORT (SCR)

1. SCR No.: 559	**2. Software Title and Version:** DTHERM Version 1.2.1	**3. Project No:** 20.06002.01.342

4. Affected Software Module(s), Description of Problem(s): DTHERM.mcd

1. The code did not allow the user to input the internal initial pressure which was hard coded as 1atm.

5. Change Requested by: Name: D. Gute Date: February 11, 2005	**6. Change Authorized by (Software Developer):** Name: T. Maxwell Date: February 11, 2005

7. Description of Change(s) or Problem Resolution (*If changes not implemented, please justify*):

1. Added internal interior pressure to the user input prompt and modified the temperature iteration loop for no contact cases and interior pressure calculation for contact cases to reflect the user input.

8. Implemented by: T. Maxwell	**Date:** February 14, 2005

9. Description of Acceptance Tests:

	Pass	Fail	Description of Test
1	☑	☐	The internal interior pressure is provided as an input option and the temperature iteration loop for no contact cases and interior pressure calculation for contact cases reflect the user input. (Formally version 1.2 had internal pressure hard coded.)
2	☑	☐	Regression testing performed to validate results.

Test results are documented on Attachment 1.

10. Tested by: George Adams	**Date:** March 3, 2005

CNWRA Form TOP-5 (05/2000)

Attachment 1

Test Performed

1. a) Verified the internal interior pressure is provided as an input option and the temperature iteration loop for no contact cases reflect the user input. Using the input parameters from Table 1 and manually setting the initial internal pressure to 1000 atm, verified the intermediate values within the loop did not change from version 1.2 within the loop which is illustrated in Table 2.
   b) Verified the interior pressure calculation for contact cases was being used in the calculation instead of the previous hard coded 1 atm value.

Table 1. Model Parameters	
Model Parameter	**Parameter Value**
Boundary Conditions	
Waste Form Heat Decay Rate (kW)	0
Ambient Temperature (C)	25
Reference Temperature (C)	25
Ambient Pressure (Pa)	0
Initial Inner Barrier Internal Pressure (atm)	1000
Inner Barrier Material Properties	
Inner Barrier Thermal Conductivity (W/mK)	25.44
Inner Barrier Thermal Expansion Coefficient (1/K)	17.5 (10^{-6})
Inner Barrier Modulus of Elasticity (Pa)	1.248 (10^{11})
Inner Barrier Poisson's Ratio	0.27
Outer Barrier Material Properties	
Outer Barrier Thermal Conductivity (W/mK)	21.63
Outer Barrier Thermal Expansion Coefficient (1/K)	1.368 (10^{-5})
Outer Barrier Modulus of Elasticity (Pa)	1.558 (10^{11})
Outer Barrier Poisson's Ratio	0.30
Waste Package Dimensions	
Inner Barrier, Inner Radius (mm)	712
Inner Barrier, Total Length (mm)	4876
Inner Barrier Thickness (mm)	50
Outer Barrier Thickness (mm)	20
Radial and Axial Gaps	
Radial Gap (mm)	2
Axial Gap (mm)	10

Table 2. Test 1 Results				
Iterations	**a1il (v. 1.2)**	**a3il (v. 1.2)**	**a1il (v. 1.2.1)**	**a3il (v. 1.2.1)**
0	-0.00403	0.01317	-0.00403	0.01317
10	-0.00396	0.01297	-0.00396	0.01297

Regression Testing

2. The data from Table 6-1 and 6-2 for Case 1 A, from the Software Validation Plan and Report for DTHERM Version 1.2 were input and the percent difference was calculated. The results of the regression testing are shown the following table. In accordance with TOP 18 5.8.9, this is a minor change to the software, and testing was performed to show that results did not change from the previous validated results.

Table 3. Regression Test Results				
DTHERM 1.2				
Case 1A	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**
r_1	-0.175	-0.236	1.157	1.363
r_2	-0.006	2.608	3.831	3.395
r_3	-0.001	-0.608	-0.607	0.607
r_4	-0.001	0.598	0.599	0.600
DTHERM 1.2.1				
Case 1A	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**
r_1	-0.175	-0.236	1.157	1.363
r_2	-0.006	2.608	3.831	3.395
r_3	-0.001	-0.608	-0.607	0.607
r_4	-0.001	0.598	0.599	0.600
Percent Difference of DTHERM 1.2 and 1.2.1				
r_1	0.00%	0.00%	0.00%	0.00%
r_2	0.00%	0.00%	0.00%	0.00%
r_3	0.00%	0.00%	0.00%	0.00%
r_4	0.00%	0.00%	0.00%	0.00%

SOFTWARE VALIDATION PLAN AND REPORT FOR DTHERM VERSION 1.2

Prepared by

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Approved by:

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Element Manager
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February 1, 2005

Date

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TABLES

1 SCOPE OF THE VALIDATION

DTHERM is a software program that was developed using the MATHCAD 2000 Professional (Service Release 2a) programming environment. The DTHERM program is designed to approximate the waste package inner and outer barrier stresses that could occur as the result of the respective barrier materials having different thermal expansion properties. The theory and mathematical basis for DTHERM is identified in DTHERM (2002). To facilitate the assessment of the different waste package designs (which are needed to accommodate the different waste forms that will be disposed of at the potential geologic repository) subjected to varying environmental conditions (e.g., preclosure ventilation, igneous intrusion, accumulated rock fall, and so on), the program allows the user to define (i) the relevant mechanical properties of the waste package inner and outer barrier materials, (ii) the dimensions of the waste package inner and outer barriers, (iii) the externally applied temperatures and pressures, and (iv) the waste form decay heat rate. The results calculated by DTHERM are graphically represented by two-dimensional plots of the radial stress, axial stress, circumferential "hoop" stress, and von Mises stress as functions of the radii of the inner and outer barriers.

The DTHERM program was validated by comparing the expected results obtained from finite element analyses of the waste package structure with those obtained from DTHERM using two sets of consistent modeling parameters. The ABAQUS/Standard finite element program developed by Hibbitt, Karlsson & Sorenson, Inc., which is an approved supplier for the Southwest Research Institute, was used for the finite element modeling aspect of the DTHERM validation. There are four unique cases of differential thermal expansion that can occur between the inner and outer barriers of the waste package. Each of the four differential thermal expansion cases were validated for two different scenarios. The four differential thermal expansion cases equate to the following four contact interactions between the inner and outer barriers of the waste package: (Case 1) no radial or axial contact, (Case 2) radial contact only, (Case 3) axial contact only, and (Case 4) both radial and axial contact.

The closed-form solutions that are used within DTHERM to estimate the temperatures and stresses created by differential thermal expansion of the waste package Inner and outer barriers are derived and documented within the DTHERM MATHCAD source program itself. The derivations of the closed-form solutions are based on standard engineering theory documented in Kreith and Bohn (2000); Shames and Cozzarelli (1992); and Timoshenko and Goodier (1970).

2 REFERENCES

Grohmann, A.J. and D. Gute. "DTHERM." Version 1.1. San Antonio, Texas: CNWRA. 2002.

Kreith and Bohn. *Principles of Heat Transfer.* 6th Edition. New York, New York: Harper & Row Publishers. 2000.

Shames and Cozzarelli. *Elastic and Inelastic Stress Analysis.* Englewood Cliffs, New Jersey: Prentice-Hall, Inc. 1992.

Timoshenko, and Goodier. *Theory of Elasticity.* 3rd Edition. New York, New York: McGraw-Hill Book Company. 1970.

3 ENVIRONMENT

3.1 Software

- ABAQUS/Standard, UNIX compatible operating system
- Mathsoft MATHCAD 2000 Professional or Premium for Windows or any later version of MATHCAD

3.2 Hardware

- Sun 1420R Server (Solaris 8 operating system)
- PC with Pentium–133 or higher (Windows 95, 98, 2000 or NT 4.0 or higher operating system)

4 PREREQUISITES

The individual chosen to implement the software validation test plan should be knowledgeable in the use of MATHCAD and ABAQUS/Standard.

5 ASSUMPTIONS AND CONSTRAINTS

No assumptions and constraints required to implement the software validation test plan.

6 TEST CASES

6.1 Validation Test Parameters

Table 6-1 conveys the different combinations of radial and axial gaps that were used in the construction of the Finite Element Model (FEM). These combinations of radial and axial gaps result in the four contact cases between the waste package inner and outer barriers that were described in Section 1.0 as predicted by the DTHERM code for the fixed set of boundary conditions, geometrical dimensions, and material properties delineated in Table 6-2. As a result, Case 1 corresponds to no radial or axial contact, Case 2 is radial contact only, Case 3 is axial contact only, and Case 4 is both radial and axial contact. These four possible contact interactions were replicated by inputting the radial and axial gap parameters from Table 6-1 into the finite element model. Therefore, for the purpose of this validation exercise, the results of any FEM that has Case 1 gap parameters for input will be labeled Case 1. The four cases were implemented with two sets of gap parameters that modeled the waste package with no external pressure, 'A', and with external pressure, 'B'. The acceptance criteria for this validation test require the DTHERM results to be within 10 percent fo the FEM results.

Table 6-1. Radial and Axial Model Gaps Between the Waste Package Inner and Outer Barriers for the Four Cases Validated

	Case 1	Case 2	Case 3	Case 4
A-Radial Gap (mm)	2.00	0.25	2.00	0.25
A-Axial Gap (mm)	10.0	10.0	4.00	4.00
B-Radial Gap (mm)	6.00	1.00	6.00	1.00
B-Axial Gap (mm)	15.0	15.0	6.00	6.00

Table 6-2. Fixed Validation Model Parameters

Model Parameter	Parameter Value
Boundary Conditions	
Waste Form Heat Decay Rate (kW)	11.8
A-Ambient Temperature (C)	250.0
A-Ambient Pressure (Pa)	0.0
B-Ambient Temperature (C)	200.0
B-Ambient Pressure (Pa)	$7.0\ (10^{6})$
Initial Inner Barrier Internal Pressure (Pa)	$1.013\ (10^{5})$
Inner Barrier Material Properties	
Inner Barrier Thermal Conductivity (W/ m•K)	25.4
Inner Barrier Thermal Expansion Coefficient (1/K)	$17.5\ (10^{-6})$
Inner Barrier Modulus of Elasticity (Pa)	$124.8\ (10^{9})$
Inner Barrier Poisson's Ratio	0.27
Outer Barrier Material Properties	
Outer Barrier Thermal Conductivity (W/ m•K)	21.6
Outer Barrier Thermal Expansion Coefficient (1/K)	$13.7\ (10^{-6})$
Outer Barrier Modulus of Elasticity (Pa)	$155.8\ (10^{9})$
Outer Barrier Poisson's Ratio	0.30

Table 6-2. Fixed Validation Model Parameters (continued)	
Waste Package Dimensions	
Inner Barrier, Inner Radius (m)	0.712
Inner Barrier Total Length (m)	4.876
Inner Barrier Thickness (m)	0.050
Outer Barrier Thickness (m)	0.020
Outer Barrier, Inner Radius*	—
Outer Barrier, Total Length*	—
*Calculated using Inner Barrier dimensions and prescribed axial and radial gaps.	

6.2 Validation Test Procedure

The FEM cross-section was constructed with two-dimensional, four node continuum, axisymmetric elements for the Inner and outer barrier walls. The FEM was constrained axially at the waste package midpoint. Because the closed form solution in DTHERM neglects any bending effects, the inner and outer barrier lids were modeled as two node rigid body elements. The rigid body elements employ the top center nodes of the inner and outer barriers as their respective reference nodes. Hence, the potential axial forces generated between the inner and outer barriers caused by axial thermal expansion are governed by the movements of the rigid body elements.

The parameters from Tables 6-1 and 6-2 were input into DTHERM and the FEM and the results were compared based on the four contact scenarios discussed in Section 6.1.

6.3 Validation Test Results

The estimated stresses calculated within DTHERM for the waste package Inner and outer barriers that are created by the differential thermal expansion effect are valid for the polar cross-section located at the waste package mid-length. The specific stress results that are used to validate the calculated DTHERM values are the radial, axial, hoop, and Von Mises stresses. The same FEM cross-section was used to validate the temperature and displacement results as well. All FEM results are recorded at the integration points. The coordinates of the integration points were input into DTHERM to produce comparable results. The integration point coordinates correspond to the following locations: inside of the inner barrier (r_1), outside of the inner barrier (r_2), inside of the outer barrier (r_3), and outside of the outer barrier (r_4). For cases that involve radial contact, the average gap contact pressure will be used for the FEM results while DTHERM will use the radius that defines the gap and not the integration point coordinate. This will be applied to Cases 2 and 4 at r_2 and r_3 for the radial stress.

6.3.1 Case 1 Validation Test Results

Tables 6-3 thru 6-6 are the validation test results for Case 1.

Table 6-3. Stress and Temperature Results of DTHERM A and FEM A for Case 1

Case 1	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
DTHERM A					
r_1	-0.175	-0.236	1.157	1.363	260.02
r_2	-0.006	2.608	3.831	3.395	259.02
r_3	-0.001	-0.608	-0.607	0.607	250.45
r_4	-0.001	0.598	0.599	0.600	250.00
FEM A					
Case 1	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.171	-0.203	1.180	1.367	261.15
r_2	-0.010	2.567	3.782	3.354	260.15
r_3	0.015	-0.640	-0.676	0.674	250.65
r_4	-0.002	0.588	0.527	0.562	250.05
Percent Difference of DTHERM A and FEM A					
r_1	*	*	1.97%	0.31%	0.43%
r_2	*	1.59%	1.30%	1.24%	0.43%
r_3	*	*	*	*	0.08%
r_4	*	*	*	*	0.02%

*The calculated differences are inconsequential for stresses 1.0 MPa or less

Table 6-4. Displacement Results of DTHERM A and FEM A for Case 1			
Radial Displacement (mm)			
Case 1	DTHERM A	FEM A	Percent Difference
Inner Barrier (r_1)	2.940	2.951	0.38%
Inner Barrier (r_2)	3.136	3.157	0.67%
Outer Barrier (r_3)	2.357	2.359	0.08%
Outer Barrier (r_4)	2.412	2.421	0.36%
Axial Displacement (mm)			
Inner Barrier	10.016	10.069	0.53%
Outer Barrier	7.527	7.574	0.62%

Table 6-5. Stress and Temperature Results of DTHERM B and FEM B for Case 1					
DTHERM B					
Case 1	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.177	-0.225	1.180	1.382	264.87
r_2	-0.006	2.619	3.853	3.413	263.87
r_3	-0.400	-140.279	-279.551	241.752	200.44
r_4	-6.630	-139.076	-272.119	229.920	200.00
FEM B					
Case 1	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.174	-0.186	1.221	1.401	268.05
r_2	-0.012	2.583	3.825	3.391	267.05
r_3	-0.887	-139.320	-279.120	240.960	200.65
r_4	-6.155	-138.080	-272.670	230.810	199.95
Percent Difference of DTHERM B and FEM B					
r_1	*	*	3.33%	1.33%	1.19%
r_2	*	1.41%	0.73%	0.64%	1.19%
r_3	*	0.69%	0.15%	0.33%	0.10%
r_4	7.72%	0.72%	0.20%	0.39%	0.03%
*The calculated differences are inconsequential for stresses 1.0 MPa or less					

Table 6-6. Displacement Results of DTHERM B and FEM B for Case 1			
Radial Displacement (mm)			
Case 1	DTHERM B	FEM B	Percent Difference
Inner Barrier (r_1)	3.000	3.038	1.23%
Inner Barrier (r_2)	3.200	3.249	1.52%
Outer Barrier (r_3)	0.674	0.673	0.11%
Outer Barrier (r_4)	0.730	0.737	0.93%
Axial Displacement (mm)			
Inner Barrier	10.223	10.365	1.37%
Outer Barrier	4.985	5.030	0.89%

Tables 6-3 and 6-6 illustrate the DTHERM stresses greater than 1.0 MPa, temperature, and displacement results are acceptable for Case 1. The stresses for both DTHERM A and FEM A at r_3 and r_4 are below 1.0 MPa and are considered to be inconsequential. However the axial stress at r_2, hoop stress, and Von Mises stress for r_1 and r_2 are above 1.0 MPa are within the 10 percent acceptance criteria. The radial stress for Scenario A is well below 1.0 MPa while Scenario B exhibits significant stress at r_4 from the ambient pressure. The radial stress at r_1, r_2, and r_3 and axial stress at r_1 for both DTHERM B and FEM B are below 1.0 MPa and are considered to be inconsequential. However the axial stress at r_2, r_3, and r_4, hoop stress, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. The ambient pressure has a significant effect on the stress of the outer barrier for Scenario B. This illustrates the impact the large exterior pressure has on the waste package as opposed to effect of differential thermal expansion when there is no exterior pressure or contact which the results show in Scenario A. The temperatures and displacements are within 10 percent difference for both Scenarios.

6.3.2 Case 2 Validation Test Results

Tables 6-7 thru 6-10 are the validation test results for Case 2.

Table 6-7. Stress and Temperature Results of DTHERM A and FEM A for Case 2					
DTHERM A					
Case 2	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.210	-0.258	-22.977	22.743	251.44
r_2	-1.531*	2.593	-18.829	19.694	250.45
r_3	-1.531*	-0.615	58.434	59.470	250.45
r_4	-0.078	0.605	58.283	58.023	250.00

Table 6-7. Stress and Temperature Results of DTHERM A and FEM A for Case 2 (continued)					
FEM A					
Case 2	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.222	-0.475	-23.210	22.866	252.05
r_2	-1.536*	2.649	-19.063	20.081	251.05
r_3	-1.536*	-0.861	58.796	59.971	250.65
r_4	-0.239	0.905	59.003	58.683	250.05
Percent Difference of DTHERM A and FEM A					
r_1	†	†	1.00%	0.54%	0.24%
r_2	0.35%	2.13%	1.23%	1.93%	0.24%
r_3	0.35%	†	0.62%	0.84%	0.08%
r_4	†	†	1.22%	1.12%	0.02%

*Average contact pressure for radial contact
†The calculated differences are inconsequential for stresses 1.0 MPa or less

Table 6-8. Displacement Results of DTHERM A and FEM A for Case 2			
Radial Displacement (mm)			
Case 2	**DTHERM A**	**FEM A**	**Percent Difference**
Inner Barrier (r_1)	2.695	2.698	0.12%
Inner Barrier (r_2)	2.886	2.899	0.43%
Outer Barrier (r_3)	2.643	2.649	0.21%
Outer Barrier (r_4)	2.696	2.708	0.44%
Axial Displacement (mm)			
Inner Barrier	9.778	9.809	0.31%
Outer Barrier	7.256	7.300	0.60%

Table 6-9. Stress and Temperature Results of DTHERM B and FEM B for Case 2					
DTHERM B					
Case 2	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.216	-0.369	-37.673	37.381	201.44
r_2	-2.450*	2.479	-32.634	32.944	200.45
r_3	-2.450*	-139.408	-183.231	163.087	200.45
r_4	-6.760	-138.197	-177.971	155.195	200.00
FEM B					
Case 2	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.241	-0.738	-37.980	37.498	202.05
r_2	-2.458*	2.617	-32.880	33.485	201.05
r_3	-2.458*	-139.790	-182.400	162.100	200.65
r_4	-6.531	-137.710	-177.530	154.980	199.95
	Percent Difference of DTHERM B and FEM B				
r_1	†	†	0.81%	0.31%	0.30%
r_2	0.32%	5.26%	0.75%	1.62%	0.30%
r_3	0.32%	0.27%	0.46%	0.61%	0.10%
r_4	3.50%	0.35%	0.25%	0.14%	0.03%

*Average contact pressure for radial contact
†The calculated differences are inconsequential for stresses 1.0 MPa or less

Table 6-10. Displacement Results of DTHERM B and FEM B for Case 2			
Radial Displacement (mm)			
Case 2	DTHERM B	FEM B	Percent Difference
Inner Barrier (r_1)	1.987	1.991	0.21%
Inner Barrier (r_2)	2.137	2.149	0.57%
Outer Barrier (r_3)	1.144	1.149	0.45%
Outer Barrier (r_4)	1.197	1.209	0.98%

Table 6-10. Displacement Results of DTHERM B and FEM B for Case 2 (continued)			
Axial Displacement (mm)			
Inner Barrier	7.720	7.752	0.41%
Outer Barrier	4.556	4.582	0.57%

Tables 6-7 and 6-10 illustrate the DTHERM stresses greater than 1.0 MPa, temperature, and displacement results are acceptable for Case 2. The Radial stress for both DTHERM A and FEM A at r_1 and r_4 and the axial stress at r_1, r_3, and r_4, are below 1.0 MPa and are considered to be inconsequential. However the radial stress at r_2 and r_3, axial stress at r_2, hoop stress, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. The radial stress at r_1 and axial stress at r_1 for both DTHERM B and FEM B are below 1.0 MPa and are considered to be inconsequential. However the radial and axial stress at r_2, r_3, and r_4, hoop stress, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. The stress generated from the ambient pressure in Scenario B is much larger than the stress generated from contact caused by thermal expansion in Scenario A. This is most evident in the hoop stress when comparing the two scenarios. The temperatures and displacements are within 10 percent difference for both scenarios.

6.3.3 Case 3 Validation Test Results

Tables 6-11 and 6-14 are the validation test results for Case 3.

Table 6-11. Stress and Temperature Results of DTHERM A and FEM A for Case 3					
DTHERM A					
Case 3	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.175	-9.016	1.156	9.576	260.02
r_2	-0.006	-6.171	3.832	8.741	259.03
r_3	-0.001	20.291	-0.608	20.602	250.45
r_4	-0.001	21.498	0.600	21.205	250.00
FEM A					
Case 3	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.171	-8.688	1.180	9.267	260.85
r_2	-0.010	-5.918	3.781	8.466	259.85
r_3	0.015	19.558	-0.675	19.898	250.65

Table 6-11. Stress and Temperature Results of DTHERM A and FEM A for Case 3 (continued)					
FEM A					
Case 3	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_4	-0.002	20.786	0.527	20.529	250.05
Percent Difference of DTHERM A and FEM A					
r_1	*	3.78%	2.03%	3.34%	0.32%
r_2	*	4.28%	1.34%	3.25%	0.32%
r_3	*	3.75%	*	3.45%	0.08%
r_4	*	3.43%	*	3.29%	0.02%
*The calculated differences are inconsequential for stresses 1.0 MPa or less					

Table 6-12. Percent Difference of DTHERM A and FEM A for Case 3			
Radial Displacement (mm)			
Case 3	**DTHERM A**	**FEM A**	**Percent Difference**
Inner Barrier (r_1)	2.953	2.961	0.26%
Inner Barrier (r_2)	3.150	3.167	0.55%
Outer Barrier (r_3)	2.327	2.329	0.09%
Outer Barrier (r_4)	2.381	2.390	0.38%
	Axial Displacement (mm)		
Inner Barrier	9.845	9.893	0.48%
Outer Barrier	7.845	7.892	0.59%

Table 6-13. Stress and Temperature Results of DTHERM B and FEM B for Case 3					
DTHERM B					
Case 3	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.177	-39.939	1.179	40.457	264.91
r_2	-0.006	-37.093	3.855	39.160	263.92
r_3	-0.400	-46.229	-279.552	259.293	200.44
r_4	-6.630	-45.025	-272.118	248.525	200.00
FEM B					
Case 3	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.174	-39.445	1.221	39.986	265.65
r_2	-0.012	-36.676	3.825	38.725	264.65
r_3	-0.888	-46.342	-279.120	258.520	200.65
r_4	-6.155	-45.109	-272.670	249.330	199.95
	Percent Difference of DTHERM B and FEM B				
r_1	*	1.25%	3.40%	1.18%	0.28%
r_2	*	1.14%	0.78%	1.12%	0.28%
r_3	*	0.24%	0.15%	0.30%	0.10%
r_4	7.72%	0.19%	0.20%	0.32%	0.03%
*The calculated differences are inconsequential for stresses 1.0 MPa or less					

Table 6-14. Percent Difference of DTHERM B and FEM B for Case 3			
Radial Displacement (mm)			
Case 3	**DTHERM B**	**FEM B**	**Percent Difference**
Inner Barrier (r_1)	3.062	3.068	0.20%
Inner Barrier (r_2)	3.266	3.282	0.49%
Outer Barrier (r_3)	0.535	0.536	0.15%
Outer Barrier (r_4)	0.588	0.596	1.31%

Table 6-14. Percent Difference of DTHERM B and FEM B for Case 3 (continued)			
	Axial Displacement (mm)		
Inner Barrier	9.449	9.496	0.50%
Outer Barrier	6.449	6.492	0.67%

Tables 6-11 and 6-14 illustrate the DTHERM stresses greater than 1.0 MPa, temperature, and displacement results are acceptable for Case 1. The radial stress and hoop stress at r_3 and r_4 for both DTHERM A and FEM A are below 1.0 MPa and are considered to be inconsequential. However the axial stress, hoop stress at r_1 and r_2, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. The radial stress for Scenario A is well below 1.0 MPa while Scenario B exhibits significant stress at r_4 from the ambient pressure. The radial stress at r_1, r_2, and r_3 for both DTHERM B and FEM B are below 1.0 MPa and are considered to be inconsequential. However the radial stress at r_4, axial stress, hoop stress, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. The ambient pressure has a significant effect on the stress of the outer barrier for Scenario B. This illustrates the impact the large exterior pressure has on the waste package as opposed to effect of differential thermal expansion when there is no exterior pressure which is shown in Scenario A. Similar to the radial contact in Case 2, the axial contact stress in Scenario A is significantly less when compared to the hoop stress in Scenario B. The temperatures and displacements are within 10 percent difference for both scenarios.

6.3.4 Case 4 Validation Test Results

Tables 6-15 and 6-18 are the validation test results for Case 3.

Table 6-15. Stress and Temperature Results of DTHERM A and FEM A for Case 4					
DTHERM A					
Case 4	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.214	-10.442	-25.937	22.432	251.45
r_2	-1.719*	-7.587	-21.606	17.719	250.45
r_3	-1.719*	23.677	65.687	58.890	250.45
r_4	-0.088	24.898	65.369	57.214	250.00
FEM A					
Case 4	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_1	-0.228	-10.218	-26.028	22.536	252.05
r_2	-1.715*	-7.047	-21.699	18.213	251.05

Table 6-15. Stress and Temperature Results of DTHERM A and FEM A for Case 4 (continued)					
FEM A					
Case 4	**Radial (MPa)**	**Axial (MPa)**	**Hoop (MPa)**	**Mises (MPa)**	**Temperature (C)**
r_3	-1.715*	22.287	65.698	59.134	250.65
r_4	-0.266	24.114	65.791	57.863	250.05
	Percent Difference of DTHERM A and FEM A				
r_1	†	2.19%	0.35%	0.46%	0.24%
r_2	0.22%	7.66%	0.43%	2.71%	0.24%
r_3	0.22%	6.24%	0.02%	0.41%	0.08%
r_4	†	3.25%	0.64%	1.12%	0.02%

*Average contact pressure for radial contact
†The calculated differences are inconsequential for stresses 1.0 MPa or less

Table 6-16. Percent Difference of DTHERM A and FEM A for Case 4			
Radial Displacement (mm)			
Case 4	**DTHERM A**	**FEM A**	**Percent Difference**
Inner Barrier (r_1)	2.694	2.697	0.11%
Inner Barrier (r_2)	2.886	2.899	0.44%
Outer Barrier (r_3)	2.643	2.649	0.22%
Outer Barrier (r_4)	2.695	2.707	0.44%
Axial Displacement (mm)			
Inner Barrier	9.594	9.634	0.41%
Outer Barrier	7.594	7.633	0.51%

Table 6-17. Stress and Temperature Results of DTHERM B and FEM B for Case 4

DTHERM B					
Case 4	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.217	-3.675	-38.635	36.811	201.45
r_2	-2.511*	-0.822	-33.533	31.921	200.45
r_3	-2.511*	-131.536	-180.878	159.278	200.45
r_4	-6.763	-130.322	-175.670	151.415	200.00
FEM B					
Case 4	Radial (MPa)	Axial (MPa)	Hoop (MPa)	Mises (MPa)	Temperature (C)
r_1	-0.243	-3.988	-38.919	36.952	202.05
r_2	-2.518*	-0.617	-33.758	32.516	201.05
r_3	-2.518*	-132.080	-180.100	158.340	200.65
r_4	-6.540	-129.980	-175.260	151.260	199.95
Percent Difference of DTHERM B and FEM B					
r_1	†	7.85%	0.73%	0.38%	0.30%
r_2	0.28%	†	0.67%	1.83%	0.30%
r_3	0.28%	0.41%	0.43%	0.59%	0.10%
r_4	3.41%	0.26%	0.23%	0.10%	0.03%

*Average contact pressure for radial contact
†The calculated differences are inconsequential for stresses 1.0 MPa or less

Table 6-18. Percent Difference of DTHERM B and FEM B for Case 4

Radial Displacement (mm)			
Case 4	DTHERM B	FEM B	Percent Difference
Inner Barrier (r_1)	1.987	1.991	0.19%
Inner Barrier (r_2)	2.137	2.149	0.57%
Outer Barrier (r_3)	1.144	1.149	0.45%
Outer Barrier (r_4)	1.197	1.209	0.95%

Table 6-18. Percent Difference of DTHERM B and FEM B for Case 4 (continued)			
	Axial Displacement (mm)		
Inner Barrier	7.660	7.693	0.43%
Outer Barrier	4.660	4.693	0.70%

Tables 6-15 and 6-18 illustrate the DTHERM stresses greater than 1.0 MPa, temperature, and displacement results are acceptable for Case 4. The radial stress for both DTHERM A and FEM A at r_1 and r_4 are below 1.0 MPa and are considered to be inconsequential. However the radial stress at r_2 and r_3, axial stress, hoop stress, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. The radial stress at r_1 and axial stress at r_2 for both DTHERM B and FEM B are below 1.0 MPa and are considered to be inconsequential. However the radial stress at and r_2, r_3, and r_4, axial stress at r_1, r_3, and r_4, hoop stress, and Von Mises stress are above 1.0 MPa are within the 10 percent acceptance criteria. As shown in the previous cases, the stress generated from the ambient pressure in Scenario B is much larger than the stress generated from contact caused by thermal expansion in Scenario A. The temperatures and displacements are within 10 percent difference for both scenarios.

6.3.5 Validation Test Results Conclusion

The results from this validation indicate the stresses, displacements, and temperatures calculated by DTHERM are within the 10 percent acceptance criteria for all four cases. The stresses calculated in DTHERM are validated when their magnitude is above 1.0 MPa. Scenario A exhibited the accuracy of DTHERM to predict the stress caused by thermal expansion while Scenario B displayed DTHERM's capability to accurately predict large stresses caused by ambient pressure. DTHERM successfully predicted each of the four contact cases for both scenarios.