TO: Bruce Mabrito
FROM: Asad Chowdhury
SUBJECT: Waiver of SDP for DRIFTVNT Version 1.0
DATE: July 29, 2002

A waiver of the software development plan (SDP) is requested as per section 5.4.1 of TOP-018. An SDP is not required when the software (i) development is low cost, less than 2-3 man-months of effort, (ii) has straightforward implementation, and (iii) has minimal schedule impact. The DRIFTVNT version 1.0 software satisfies all three requirements. In regard to requirement (i), less than 1 man-month of effort is estimated

SOFTWARE VALIDATION TEST PLAN FOR DRIFTVNT VERSION 1.0

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–02–012

Prepared by

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11-25-02
Date

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1.0 SCOPE OF THE VALIDATION

This software validation test plan is for DRIFTVNT Version 1.0 which is a stand-alone set of subroutines designed to be integrated into another software package. Initially, DRIFTVNT Version 1.0 will be callable from the MULTIFLO software; however, it may also be used stand-alone for future scoping calculations. This validation test will be performed over uniform wall conditions of temperature and pressure for one MULTIFLO time step. A single time step keeps wall conditions uniform and uniform wall conditions permit a direct comparison between test output and hand calculations. The results of these calculations will be compared to analytical results for validation.

2.0 REFERENCES

Painter, S., C. Manepally, and D.L. Hughson. "Evaluation of U.S. Department of Energy Thermohydrologic Data and Modeling Status Report." San Antonio, Texas: CNWRA. September 2001.

3.0 SOFTWARE AND HARDWARE ENVIRONMENT

Validation is to be performed on the SUN server known as Spock, which uses the Solaris 5.8 operating system. The commercial programs Mathematica 4.1, running on the Windows NT (version 4) machine BRAHMA, and MathReader 4, running on the Windows NT(version 4) machine PITOR, will be used for analytical comparisons. No special peripherals are required.

4.0 PREREQUISITES, ASSUMPTIONS AND CONSTRAINTS

Requires the MULTIFLO Software, Version 1.5.2 with file multi.dat edited such that one time step is executed.

5.0 TEST CASES

5.1 Verification of Wall Temperature and Vapor Pressure under Convective Heat Transfer

This test is performed to validate the air temperature and vapor pressure output from DRIFTVNT against an analytical model described in Appendix A. This test is run for a single time step with assumed uniform wall conditions in the emplacement drift. Uniform wall conditions permit a direct comparison between test output and hand calculations. The equations developed for analysis in Mathematica are presented in Appendix A.

5.1.1 *Test Input and Output*

Test input files and output files are on the accompanying disk labeled DRIFTVNT Validation Test Plan Version 1.0 and are described in the following table:

File Name	Description
analytical_convective.nb	Mathematica 4.1 analytical results (Air temperature and vapor pressure calculated values)
driftvnt.dat	Initialization and configuration parameters for the DRIFTVNT module. For this test, emissivity is set to 0 to eliminate the effects of radiation. (Radiative heat transfer is evaluated in test case 5.2.)
driftvnt.out	Output results for the DRIFTVNT module. Contains the output to be compared against the analytical model.
multi.bc	Boundary condition data
multi.con	Connection information
multi.dat	Run-time parameters for METRA
multi.dcm	Fracture and matrix parameters for the Dual Continuum Model (DCM)
multi.int	Initial pressure, temperature and saturation distribution
multi.phk	Porosity and permeability distribution
test1.out	Screen output

5.1.2 *Test Procedure*

The test procedure is as follows:

(1) Modify the file multi.dat file as follows:

(a) Set the first Time[y] value to 0.000001.
(b) Insert a "skip" after this line.
(c) After the last Time[y] value, insert a "noskip."

(2) Invoke METRA (Note: METRA is part of MULTIFLO). At the command prompt, type, "metra multi > test1.out &."

(3) Using the screen output, "test1.out," verify that the code runs to completion without error.

(4) Using the analytical results generated from Mathematica 4.1 (file analytical_convective.nb), verify the output results with the analytical results generated.

5.1.3 *Expected Results*

Calculated air temperature and vapor pressure values should be comparable to the analytical results from Mathematica 4.1. The calculated values should all fall within 5 percent of those values calculated from Mathematica 4.1.

5.2 Verification of Canister Temperature and Heat Load under Radiative Heat Transfer

This test is performed to validate the container temperature and heat load output from DRIFTVNT against an analytical model described in Appendix B. This test is run for a single time step with assumed uniform wall conditions and no convective heat transfer in the emplacement drift. The equations developed for analysis in Mathematica are presented in Appendix B.

5.2.1 *Test Input and Output*

Test input files and output files are on the accompanying disk labeled DRIFTVNT Validation Test Plan Version 1.0 and are described in the following table:

File Name	Description
analytical_radiative.nb	Mathematica 4.1 analytical results (Air temperature and vapor pressure calculated values)
driftvnt.dat	Initialization and configuration parameters for the DRIFTVNT module. For this test, the volumetric flowrate of air is set to 0 to eliminate the effects of convective heat transfer.
driftvnt.out	Output results for the DRIFTVNT module. Contains the output to be compared against the analytical model.
multi.bc	Boundary condition data
multi.con	Connection information
multi.dat	Run-time parameters for METRA
multi.dcm	Fracture and matrix parameters for the Dual Continuum Model (DCM)
multi.int	Initial pressure, temperature and saturation distribution
multi.phk	Porosity and permeability distribution
test2.out	Screen output

5.2.2 *Test Procedure*

The test procedure is as follows:

(1) Modify the file multi.dat file as follows:

(a) Set the first Time[y] value to 0.000001.
(b) Insert a "skip" after this line.
(c) After the last Time[y] value, insert a "noskip."

(2) Invoke METRA (Note: METRA is part of MULTIFLO). At the command prompt, type, "metra multi > test2.out &."

(3) Using the screen output, "test2.out," verify that the code runs to completion without error.

(4) Using the analytical results generated from Mathematica 4.1 (file analytical_radiative.nb), verify the output results with the analytical results generated.

5.2.3 *Expected Results*

Calculated container temperature and radiative heat load at the wall should be comparable to the analytical results from Mathematica 4.1. The calculated values should all fall within 5 percent of those values calculated from Mathematica 4.1.

6.0 NOTES

None.

APPENDIX A: CONVECTIVE HEAT TRANSFER ANALYTICAL SOLUTION (Painter, et. al., 2001)

The equations presented in this appendix are used to develop the analytical solution in Mathematica 4.1 for comparison to test results. The terms used in this appendix are included in the following table:

Parameter	Definition
β	Moisture transfer coefficient
Δ_n	Length of segment n
ρ	Density of drift air
C_p	Specific heat of drift air
h_c	Heat transfer coefficient for the container
h_w	Heat transfer coefficient between the drift wall and the flowing air
n	A single portion of the emplacement drift (or segment) in which the temperature of the canister and temperature at the wall are assumed constant
P	Barometric pressure
P_v	Partial vapor pressure in the flowing air
P_{vs}	Partial pressure of moisture saturated air at the wall temperature
Q	Volumetric flowrate of drift air
r_c	Container radius
r_w	Drift radius
S	Liquid saturation of the rock
$T_{a,n}$	Temperature of the drift air in segment n
$T_{c,n}$	Temperature of the container in segment n
$T_{w,n}$	Temperature at the drift wall in segment n
y	Vapor pressure along the drift wall
φ	Porosity

The air temperature in a segment, n, is given by the following equation:

$$T_{a.n} = \frac{\alpha_c T_{c,n-1} + \alpha_w T_{w,n-1}}{\alpha_c + \alpha_w}\left[1 - e^{-(\alpha_c+\alpha_w)\Delta_{n-1}}\right] + T_{a,n-1}\, e^{-(\alpha_c+\alpha_w)\Delta_{n-1}} \qquad \text{(A-1)}$$

The constants are defined as follows: $\alpha_c = \frac{2\pi r_c h_c}{Q\rho C_p}$ and $\alpha_w = \frac{2\pi r_w h_w}{Q\rho C_p}$.

The analytical solution for this test plan assumes a single segment (n=1). Therefore, the air temperature in the first segment is given by the following equation:

$$T_{a,1} = \frac{\alpha_c T_{c,0} + \alpha_w T_{w,0}}{\alpha_c + \alpha_w}\left[1 - e^{-(\alpha_c+\alpha_w)\Delta 0}\right] + T_{a,0}\, e^{-(\alpha_c+\alpha_w)\Delta 0} \qquad \text{(A-2)}$$

The analytical solution for this test plan assumes a constant emplacement drift wall temperature. The equation for the vapor pressure along the drift wall for constant wall temperature has the solution:

$$y(x) = \frac{y_s}{1 + PLOG\left[\gamma e^{\gamma - \eta y_s^2 x}\right]} \qquad \text{(A-3)}$$

Here, $y_s = 1 - \frac{P_{vs}}{P}$, and $\eta = \frac{2\pi r_w W\beta}{0.622\rho Q}$, $W = \varphi S$, $\gamma = \frac{y_s - y_0}{y_0}$, $y_0 = y(0)$, and

$PLOG(z)$ is the product log function defined implicitly as the solution, w , to the equation $z = w\exp[w]$.

Reference:

Painter, S., C. Manepally, and D.L. Hughson. "Evaluation of U.S. Department of Energy Thermohydrologic Data and Modeling Status Report." San Antonio, Texas: CNWRA. September 2001.

APPENDIX B: RADIATIVE HEAT TRANSFER ANALYTICAL SOLUTION (Painter, et. al., 2001)

The equations presented in this appendix are used to develop the analytical solution in Mathematica 4.1 for comparison to test results. The terms used in this appendix are included in the following table:

Parameter	Definition
$<T_c^4(x)>$	Container temperature as viewed from a point, x, on the wall (apparent container temperature)
$<T_w^4(x)>$	Wall temperature as viewed from a point, x, on the wall (apparent wall temperature)
Δ_i	Length of a segment, i
σ	The product of the Stefan-Boltzmann constant and the surface emissivity
n	A single portion of the emplacement drift (or segment) in which the temperature of the wall is assumed constant
$P_R^W(x)$	Radiative power delivered to the wall at a point, x, on the wall
r_c	Container radius
r_w	Drift radius
T_{ci}^4	Container temperature in a segment, i
T_{wi}^4	Wall temperature in a segment, i

The temperature of the container as viewed from a point, x, on the wall is given by the following equation: (The <>'s denote apparent container temperature.)

$$\left\langle T_c^4(x)\right\rangle = \frac{1}{\gamma(x)}\sum_{i=1}^{2n} T_{ci}^4 F_{c\to w}^i \tag{B-1}$$

The temperature of the wall as viewed from a point, x, on the wall is given by the following equation: (The <>'s denote apparent wall temperature.)

$$\left\langle T_w^4(x)\right\rangle = \sum_{i=0}^{2n} T_{wi}^4 F_{c\to w}^i(x) \tag{B-2}$$

The analytical solution for this test plan assumes a single segment (n=1). Therefore the temperature of the container as viewed from a point, x, on the wall in segment 1 is given by the following equation:

$$\left\langle T_c^4(x)\right\rangle = \frac{1}{\gamma(x)}\sum_{i=1}^{2} T_{ci}^4 F_{c\to w}^i \tag{B-3}$$

The temperature of the wall as viewed from a point, x, on the wall in segment 1 is given by the following equation:

$$\left\langle T_w^4(x)\right\rangle = \sum_{i=0}^{2} T_{wi}^4 F_{c\to w}^i(x) \tag{B-4}$$

where,

$$F_{c\to w}^i = G(x, x_i + \Delta_i) - G(x, x_i - \Delta_i) \tag{B-5}$$

$$\gamma(x) = 1 - G(x, 0) \tag{B-6}$$

and

$$G(x, x') = \frac{1}{\pi}\left[\frac{r_w(x - x')}{r_w^2 + (x' - x)^2} + \tan^{-1}\left(\frac{x' - x}{r_w}\right)\right] \tag{B-7}$$

The heat load delivered to the wall as viewed from a point, x, on the wall is then obtained from the following equation:

$$P_R^w(x) = 2\pi r_c \sigma \gamma(x)\left[\left\langle T_c^4(x)\right\rangle - T_w^4(x)\right] \tag{B-8}$$

Reference:

Painter, S., C. Manepally, and D.L. Hughson. "Evaluation of U.S. Department of Energy Thermohydrologic Data and Modeling Status Report." San Antonio, Texas: CNWRA. September 2001.

SOFTWARE REQUIREMENTS DESCRIPTION FOR THE COMPUTER CODE DRIFTVNT VERSION 1.0

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–97–009

Prepared by

George Adams
Scott Painter

Center for Nuclear Waste Regulatory Analyses
San Antonio, Texas

July 2002

ABSTRACT

This Software Requirements Description is intended to document the requirements for the computer code DRIFTVNT V1.0. DRIFTVNT is a set of subroutines that are invoked by another software package. Initially, DRIFTVNT will be integrated into MULTIFLO; however, it may be integrated into other software packages as well. For this reason, DRIFTVNT is maintained separately from MULTIFLO. DRIFTVNT is used to model the thermal radiation across an open emplacement drift as well as the effects of forced or natural ventilation in an emplacement drift. It is intended to function with a user-definable grid geometry.

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LIST OF FIGURES

ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) for the U.S. Nuclear Regulatory Commission (NRC) under Contract No. NRC–02–97–009. The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of Waste Management. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of the NRC.

QUALITY OF DATA, ANALYSES, AND CODE DEVELOPMENT

DATA AND ANALYSES: Neither data nor analyses are reported in this document. This document describes the requirements for DRIFTVNT.

CODE DEVELOPMENT: Codes will be developed in accordance with the procedures described in the CNWRA Technical Operating Procedure, TOP-018, which implements the guidance contained in the CNWRA Quality Assurance Manual.

1 INTRODUCTION

This Software Requirements Description document identifies the software requirements for implementing the In-Drift Thermal Radiation and Forced Ventilation Model (Painter, et al., 2001). It includes descriptions for the source code module level breakdown, control flow, and configuration. This software could be used in the high-level waste repository license application review process for Yucca Mountain, Nevada.

DRIFTVNT is a set of subroutines that are invoked by another software package. Initially, DRIFTVNT will be callable from the MULTIFLO software; however, it may also be used standalone for future scoping calculations. For this reason, DRIFTVNT is maintained separately from MULTIFLO. DRIFTVNT is used to model the thermal radiation across an open emplacement drift as well as the effects of forced or natural ventilation in an emplacement drift.

2 SOFTWARE REQUIREMENTS FOR DRIFTVNT, VERSION 1.0

This Software Requirement Description identifies the interface and functionality that is required to implement the In-Drift Thermal Radiation and Forced Ventilation Model. The technical basis for this model has already been described (Painter, et al., 2001) and is included as Appendix A.

2.1 Software Function

DRIFTVNT implements the model of thermal radiation and forced ventilation within the emplacement drift. This code accounts for the thermal radiation from the waste package to the drift wall, forced air ventilation, cooling of the waste package and the drift wall due to convective heat transport from the waste package and drift wall to the ventilation air, and drying of the drift wall by the ventilation air.

Model parameters are user configurable. The user specifies the number of slices through the emplacement drift and the number of boundary cells per slice for one-half of the drift wall. It is assumed that all slices have the same number of boundary cells at the drift wall, that the temperature at the drift wall is constant throughout the slice for a given time step, and the slice is symmetric about the vertical axis with respect to geometry and environmental conditions. In addition, it is assumed that a slice through the emplacement drift can be modeled as an unstructured grid.

2.2 Computational Approach

This section covers the interface requirements, software and hardware requirements, and module layout/data flow. This software does not require a user interface, has no graphics requirements, and does not require pre- or post-processing.

2.2.1 Interface Requirements

DRIFTVNT interfaces to the calling software through an interface module, IDRIFT. IDRIFT receives an array of cells in which each cell has an associated volume, temperature, pressure, and initial heat source flux. For DRIFTVNT, only the cells at the drift wall (boundary cells) are relevant. Therefore, IDRIFT, processes the information from received cells and extracts the required information from those at the wall of the emplacement drift. IDRIFT creates a volume-averaged set of data for each slice and passes this information to module DRIFT. DRIFT then process all the slices in the emplacement drift and returns heat and moisture flux from each of these slices. IDRIFT then takes this returned heat and moisture flux, transforms it into a heat and moisture flux for each of the boundary cells, and passes these fluxes back to the caller.

The interface module, IDRIFT, determines which cells are boundary cells through the use of a data file, driftvnt.dat, and through the use of input parameters from the caller. The data file specifies the number of slices and the number of boundary cells per slice, N, for one-half of the drift wall. In addition, IDRIFT receives an array of heat source locations from the caller. The code is structured such that the first N heat source locations map to slice 1, the next N heat source locations map to slice 2, and so on.

2.2.2 Data Flow and Module Layout

The module layout is shown in Figure 2-1. DRIFTVNT has three components: (1) an associated module DRIFT, (2) an interface IDRIFT, and (3) a data input file driftvnt.dat. The caller, which may for example be MULTIFLO, passes cell specific information (e.g. cell volume, cell temperature, and cell pressure) to the interface and receives cell specific information back from the interface (e.g., heat and moisture flux). The interface transforms the cell by cell information from the caller into slice by slice information for module DRIFT. Module DRIFT processes and returns heat and moisture flux. The heat and moisture flux is then transformed by the interface into cell by cell information and returned to the caller.

In order to accomplish this cell to slice conversion, the interface makes use of a data file. This data file, driftvnt.dat, provides configuration parameters to the interface specific to the emplacement drift geometry. For example, the data file contains the number of slices and the number of cells per slice. In addition, this file contains, initialization parameters such as tunnel radius, initial power from a waste package, and heat and moisture transfer coefficients. These initialization parameters are passed to module DRIFT for use in its heat and moisture transfer calculations.

2.2.3 Hardware and Software Requirements

The target platforms are a Windows PC based system running Windows NT 4.0 and a SUN Solaris 5.8 machine. The programming language is FORTRAN 77.

2.2.4 Software Validation

This software will be released as version 1.0. Version 1.0 will be validated in accordance with the Software Validation Test Plan for the Computer Code DRIFTVNT, Version 1.0 by December 13, 2002.

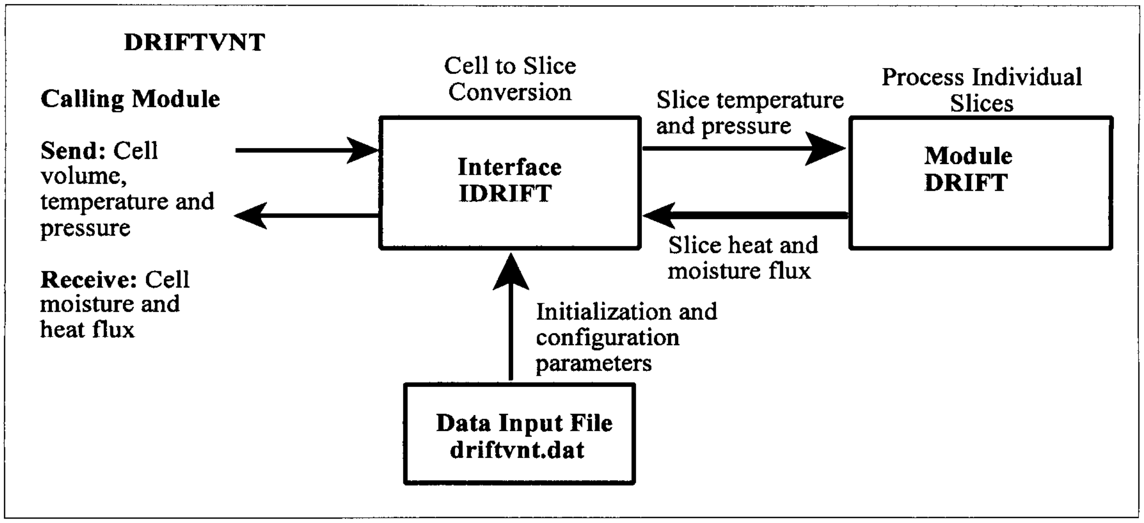

Figure 2-1. Data Flow Module Layout

3 REFERENCES

Painter, S., C. Manepally, and D.L. Hughson. "Evaluation of U.S. Department of Energy Thermohydrologic Data and Modeling Status Report." San Antonio, Texas: CNWRA. September 2001. (Included in Appendix A)