SIMULATIONS OF MAGMA-WASTE PACKAGE INTERACTIONS USING COMPUTATIONAL FLUID DYNAMICS

Prepared for

U.S. Nuclear Regulatory Commission
Contract NRC–02–07–006

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September 2008

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ACKNOWLEDGMENTS

This report was prepared to document work performed by the Center for Nuclear Waste Regulatory Analyses (CNWRA) and its contractors for the U.S. Nuclear Regulatory Commission (NRC) under Contract Nos. NRC–02–02–012 (fiscal year 2007) and NRC–02–07–006 (fiscal year 2008). The activities reported here were performed on behalf of the NRC Office of Nuclear Material Safety and Safeguards, Division of High-Level Waste Repository Safety. The report is an independent product of the CNWRA and does not necessarily reflect the views or regulatory position of NRC.

The authors thank S. Painter for technical review, G. Wittmeyer for programmatic review, and L. Mulverhill for editorial review of this report. The authors also appreciate S. Odam for providing word processing support in the preparation of this document.

QUALITY OF DATA ANALYSIS AND CODE DEVELOPMENT

DATA: All CNWRA-generated original data contained in this report meet quality assurance requirements described in the Geosciences and Engineering Division Quality Assurance Manual. Sources of other data should be consulted for determining the level of quality of those data. The work presented in this report is documented in Scientific Notebook 801E.

ANALYSES AND CODES: The general purpose computational fluid dynamics simulation code FLUENT® Version 6.3 was used to generate results for this report and is controlled in accordance with the CNWRA software quality assurance procedure Technical Operating Procedure (TOP)–018, Development and Control of Scientific and Engineering Software.

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Fluent, Inc. “FLUENT User Manual Version 6.2.16.” Lebanon, New Hampshire: Fluent, Inc. 2006.

1 INTRODUCTION

1.1 Background

The proposed location for the potential high-level nuclear waste repository at Yucca Mountain, Nevada, is in a small volume basaltic volcanic field in the western Great Basin. Based on the recent volcanic history of that field and region, if a future event were to occur, it would begin with basaltic magma ascending through dikes one to several meters in width. With continued ascent, a conduit up to tens of meters in diameter might develop along the strike of the dike that reaches the surface, and eruptive activity, which includes effusion of lava flows and Strombolian—violent Strombolian eruptions, might ensue and construct a monogenetic, basaltic scoria cone. Discussion of the nature and style of past eruptions of basaltic volcanoes in the Yucca Mountain region is provided in U.S. Nuclear Regulatory Commission (NRC) (2005, 1999).

Because the probability that future igneous activity could disrupt the repository and transport radionuclides to the surface is greater than 1 in 10,000 in 10,000 years [frequency exceeds 10^{-8}/yr (Bechtel SAIC Company, LLC, 2004a)], volcanic hazard assessment has been studied as is required by regulations at 10 CFR Part 63.114(d). A range of models and data have been considered during the development of performance assessments conducted by the U.S. Department of Energy (DOE), and the NRC. A key component when abstracting these types of events is to understand how rising basaltic magma will interact with subsurface repository structures, such as tunnels, waste packages, and drip shields.

The unique configuration of the repository and the lack of direct physical evidence of the consequences should magma intersect open drifts introduces uncertainties in risk assessments. Current design plans describe open horizontal drifts approximately 5.0 m [16.4 ft] in diameter and up to 1,000 m [3,280 ft] long that are 200–300 m [657–985 ft] below the ground surface, and cylindrical waste packages are to be placed lengthwise in the drifts (Bechtel SAIC Company, LLC, 2004b, 2003; Danko and Bahrami, 2002; Ibarra, et al., 2006). Depending on the location of the developing dike, the ascending magma has the potential to intersect and intrude into the underground drifts in the repository and interact with the waste packages and other engineered barrier components.

Current models of disruptive intrusive igneous events developed by the DOE suggest that the drifts will be filled rapidly by high temperature magma that will disturb the waste packages and lead to waste release (Bechtel SAIC Company, LLC, 2005; Sandia National Laboratories, 2007a). Some of these models considered multiphase flow of fragmented magma into an open drift immediately after intersection, followed by rapid filling of the drift. Other models considered effusive flow of hot basaltic magma inside the drift neglecting gravity. Additionally, in the last few years, a series of papers (Dartevelle and Valentine, 2005; Lejeune, et al., 2002; Menand and Phillips, 2007a,b; Menand, et al., 2007; Philips, et al., 2008; Woods, et al., 2002) focusing on various aspects of dike-drift interactions have collectively shown that a drift intersected by ascending basaltic magma will quickly fill with magma and concluded that the physical conditions such as the velocity of the magma and the static and dynamic pressure inside the drift will affect the integrity of the waste packages. These papers describe multiphase flow in a dike-drift configuration and experiments examining circulation patterns established in a drift after intersection under steady-state conditions.

In the case of an extrusive igneous event, DOE models assume only the contents in the waste packages directly intersected by a conduit is released and transported to the surface by ascending magma (Sandia National Laboratories, 2007a,b). Scenarios in which ascending magma jags along a drift, resulting in an offset conduit [e.g., dog-leg scenario presented in Woods, et al. (2002)], are dismissed as unlikely. Also, in Sandia National Laboratories (2007a), they treat magma as a single, incompressible phase, and determine that in the repository, it would be largely stagnant once all drifts are filled. Thus, their models do not include alternative eruption scenarios (e.g., a secondary conduit forms and horizontal flow develops down a drift), which might provide a mechanism to transport the contents of an increased number of waste packages directly to the surface.

In this report, Center for Nuclear Waste Regulatory Analyses (CNWRA) has developed computational models to evaluate uncertainties and assumptions associated with DOE models that may affect the igneous scenario model abstraction. This analysis explores whether alternate eruptive scenarios make any difference in the consequence. These CNWRA computational models build upon recent laboratory experiments and theoretical models by Phillips, et al. (2008) by adding realism in terms of scaling and by more accurately examining thermal effects.

1.2 Purpose and Scope

This summary report documents the important technical aspects and results of computational analyses designed to investigate the flow of magma into a horizontal subsurface tunnel including obstacles after intersection during initial ascent. These models are not designed to simulate the conditions of initial intersection or investigate possible changes to the properties of the leading/first magma to arrive at the drift, but rather the conditions after intersection as the drift is effusively invaded and filled with magma. CNWRA staff conducted these numerical simulations to gain a better understanding of and to develop critical technical insights into the behavior of the system and the associated risk-significant processes. Results presented here support the evaluation of the radiological dose consequences of potential igneous activity, including the alternative eruption scenarios described in NRC (2005) and Woods, et al. (2005). To analyze the flow and thermal fields in a drift, the work was restricted to two-dimensional numerical simulations under conditions of either transient or steady-state effusive flow of a single-phase magma. Differences in the predicted flow and thermal fields between preliminary simulations using two- and three-dimensions were insignificant, and three-dimensional simulations resulted in a large computational grid. Based on the two-dimensional simulations, all salient features can be captured in the simulation at a considerable reduction in computational burden. FLUENT® (Fluent, Inc., 2006), a computational fluid dynamics software package, was used to carry out these investigations.

2 METHODOLOGY

2.1 Model Geometry

As noted earlier, the configuration modeled in this study was restricted to two-dimensions. As seen in Figure 2-1, a 600 m × 6 m [1,968.50 ft × 19.68 ft] horizontal drift is intersected at its mid-point by a vertical 500 m × 8 m [1,640.42 ft × 26.25 ft] dike, which extends 300 m [984.25 ft] above the drift. Dike width was chosen based on the mean dike width used in the igneous scenario models included in the Total System Performance Assessment developed by the DOE (Sandia National Laboratories, 2007b). According to the proposed design of the repository (Bechtel SAIC Company, LLC, 2003), the waste canisters, about 5 m [16.4 ft] long and between 1.75 m [5.74 ft] and 2.11 m [6.922 ft] in diameter, will be placed lengthwise in the drifts separated by 0.1 m [0.328 ft]. In these simulations, however, separate waste packages were not considered. Instead, to enhance numerical stability of the solution, the waste packages were represented by two large, solid obstacles, one on both sides of the intersected drift and each 290 m [951.443 ft] long. Considering the length of one waste package is approximately 5 m [16.4042 ft], a length of 290 m [951.443 ft] represents approximately 58 waste packages. No inverts or drip shields were included in the model information. The geometric dimensions of the drift and the waste packages were based on materials available in open literature (Bechtel SAIC Company, LLC, 2004b, 2003; Danko and Bahrami, 2002; Ibarra, et al., 2006; Sandia National Laboratories, 2007b). The geometry of the configuration and the computational domain is provided in Table 2-1.

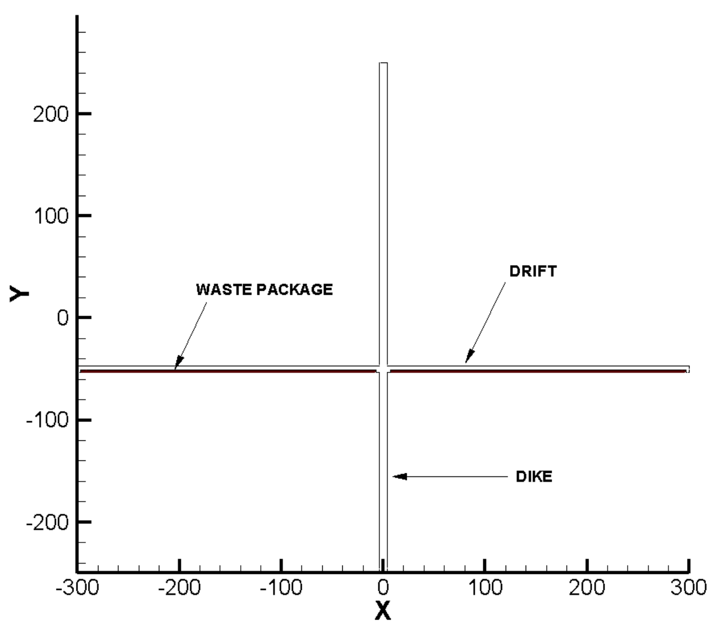


Figure 2-1. Schematic of the Modeled Dike-Drift Configuration; Length Is in Meters

Table 2-1. Model Construct Values	
Construct	**Value**
Drift Length	600 m (1,970 ft)
Drift Height	6 m (20 ft)
Dike Length	500 m (1,640 ft)
Dike Width	8 m (26 ft)
Extension of Dike Above Drift	300 m (980 ft)
Waste Package Total Length	290 m (950 ft)
Waste Package Diameter	1.8 m (5.9 ft)

2.2 Computational Grid and Boundary Conditions

The two-dimensional uniform computational grid used in these simulations consisted of 21,186 hexahedral cells (Figure 2-2). Table 2-2 provides the details of the grid dimensions for each geometric construct. No clustering of the grid was employed near the wall regions. A velocity boundary condition was applied at the dike bottom inlet with velocities ranging between 1–3 m/s [3.3–9.8 ft/s], a pressure outlet boundary condition was applied at the dike top outlet with the pressure specified as atmospheric, and a no-slip boundary condition was applied at the walls. All walls were treated as isothermal, and the drift rock wall temperature was specified at a constant 300 K [80.33 °F] (simulations reveal that no appreciable change occurred in the rock wall temperature in the time-span considered). Waste package temperature was specified as 350 K [170.33 °F] with a heat generation rate per unit volume of 232.78 W/m^3. The pressure inside the drift was treated as atmospheric, and in all the simulations, the drift was assumed to be initially filled with air.

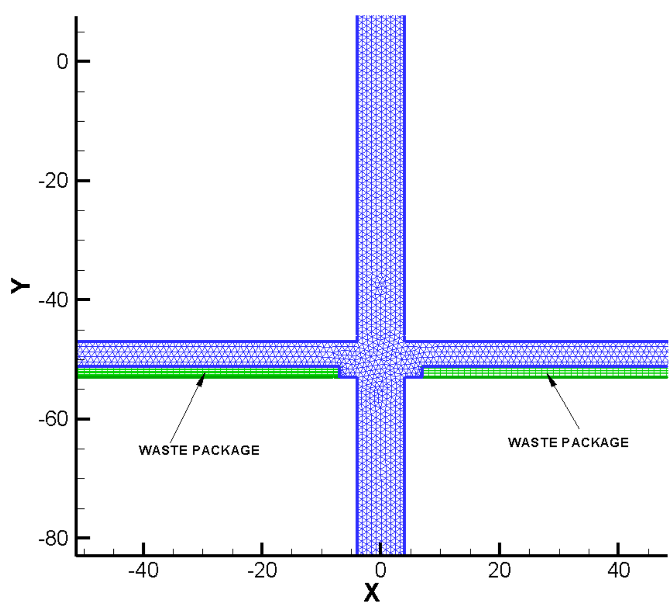


Figure 2-2. Schematic of the Computational Grid Used in the Simulations Overlain on the Dike-Drift Model. Waste Packages Are Shown in Green; Length Is in Meters.

Table 2-2. Details of the Computational Grid	
Construct	**Grid Dimension ($N_x \times N_y$)***
Drift	20×500
Dike	600×15
Waste Package (each)	290×8
*N_x = Number of cells in the x-direction and N_y = Number of cells in the y-direction	

2.3 Numerical Methods

The commercial software FLUENT® Version 6.3 [Fluent, Inc., 2006] was used for the simulations. FLUENT uses a control-volume-based technique to convert a general scalar transport equation to an algebraic equation that is solved numerically. It has a pressure-based solver and a density-based solver. While the pressure-based solver is normally used for incompressible flows, the density-based solver is recommended for compressible high Mach number flows. A variety of spatial and temporal discretization schemes as well as turbulence models are also available in FLUENT.

For these simulations, the solutions to the full two-dimensional Navier Stokes equations were obtained using an unsteady, implicit approach. The volume of flow (Hirt and Nichols, 1981) approach was used to properly simulate the two-phase magma-air interface. The Semi Implicit Pressure Linked Equations–Consistent (SIMPLEC) algorithm (Van Doormal and Raithby, 1984) was used to treat pressure-velocity coupling for stability. The third-order Monotone Upstream-Centered Schemes for Conservation Laws (MUSCL) (Van Leer, 1979) scheme was used to derive the face values of different variables for the spatial discretization, which were used to compute the convective fluxes. The upwind difference scheme was used for its enhanced numerical stability. The pressure based solver was used in conjunction with Green-Gauss cell based gradient option. An implicit time marching scheme was used for faster convergence. Temporal discretization was achieved through a second-order implicit method (second-order backward Euler scheme) (Gresho, et al., 1980). The flow Reynolds number (based on the magma viscosity and density) was 533, so the flow was considered laminar. The solutions were initiated in the unsteady mode. The timestep used for the unsteady simulations was varied between 0.01 to 0.05 seconds. The computations were conducted on a Sun Fire X4100 cluster configured with 10 dual-core AMD Opteron 200 series processors with 16 GB RAM per processor.

2.4 Material Properties

Properties of the interactive materials used in the simulations were obtained from Detournay, et al., (2003) and are listed in Table 2-3. The magma properties are for a magma with a temperature of 1,450 K [2,150 °F], the tuff properties for a tuff at 300 K [80.33 °F], and the Alloy-22 at 300 K [80.33 °F]. With one exception (Figure 3-4 depicts the temperature profile ~10 minutes after the drift is filled with magma), magma temperature and viscosity are held constant in these simulations, and latent heat is not considered.

Table 2-3. Materials and Properties Used in the Simulations

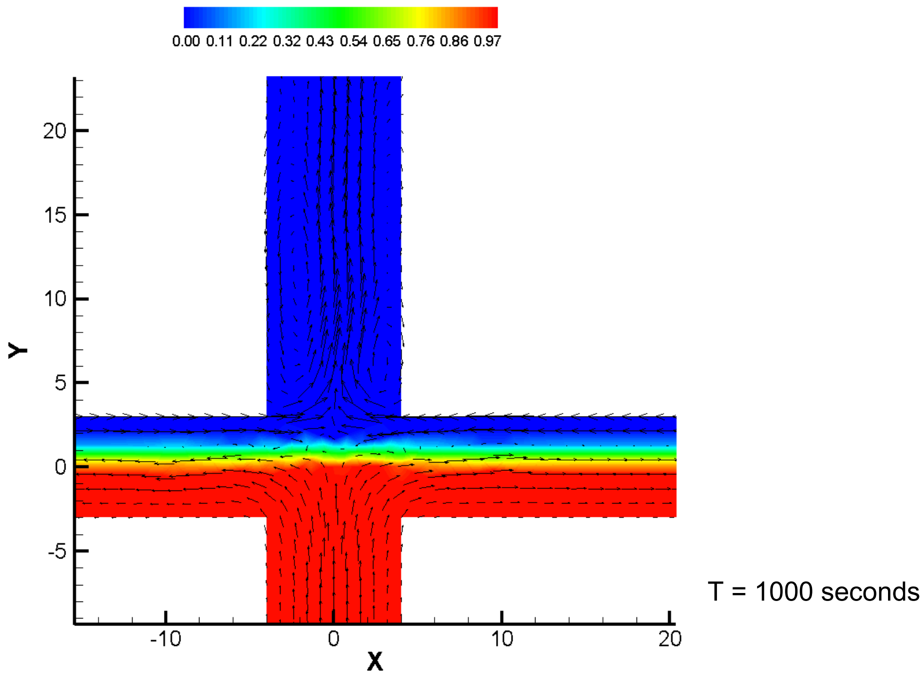
	Density		Specific Heat		Thermal Conductivity		Viscosity	
	Kg/m^3	lbm/ft^3	J/kg-K	BTU/lb-°F	W/m-K	Btu/(ft h °F)	Pa-s	lbf-s/ft^2
Magma	2,663	166.23	1,945	0.465	0.6	0.35	40	0.835
Air	1.225	0.0764	1,005	0.24	0.0242	0.014	1.78 e-05	3.72 e-07
Tuff	2,043	127.416	985	0.235	1.18	0.668	-----	-----
Alloy-22	3,495	218	378	0.09	1.5	0.8491	-----	------

3 RESULTS AND DISCUSSIONS

To gain insights about the flowfield(s) occupying the dike and drift after intersection, simulations focused primarily on two scenarios: (i) magma entering and eventually filling a drift both with and without the presence of waste packages and (ii) a magma filled drift including waste packages under conditions of constant magma supply and ascent (steady-state). Under these two scenarios, the velocity, vorticity, circulation patterns, and temperature profiles that develop and possibly dictate the conditions imposed on the waste packages were investigated.

A scenario in which magma enters and fills the drift [scenario (i)] was investigated in configurations that included and excluded waste packages so that the effects of an obstacle on the floor of a drift could be ascertained. Under the presence of gravity, a single-phase magma ascends the dike at 1 m/s [3.28 ft/s], intersects and intrudes into a drift, and begins filling the drift from the bottom [Figure 3-1(a)(b)]. As the drift is filling with magma, air is displaced and escapes up the dike. Counter-rotating vortices of air develop in the dike due to the temperature difference between the hot air and the cold air. Notice, too, a small volume fraction of air remains inside the drift after magma has completely filled the drift. This remnant air is the result of assuming a closed-end drift with zero-permeability walls. Magma continues its ascent up the dike once the drift is completely filled, and counter-rotating vortices attributable to viscous coupling develop at the intersection of the dike and the drift in the magma. Beyond these small vortices in the magma adjacent to the dike, the larger circulation pattern established is characterized by magma flowing away from the dike along the lower portion of the drift and back towards the dike along the upper portion at very low velocities. In these simulations, magma ascending along the sides of the dike above the intersection has a much lower velocity than magma ascending along the dike center, but this profile reflects the no-slip boundary condition applied to the dike walls. Figures 3-1(a) and (b) demonstrate these flow patterns develop with and without waste packages in the drift.

Given the above-described circulation inside a magma filled drift, investigations performed under the auspices of scenario (ii) (with waste packages) included variations in the distance between the dike and the waste packages and in the ascent rate of the magma. Figures 3-2(a) and (b) illustrate changes in flow resulting from a distance of ~4 m [~13 ft] and ~7 m [~22.56 ft] between the dike and the end of the waste packages. At 4 m [13 ft] circulation in the drift and the velocity profile in the dike look much the same as Figure 3-1(b). Counter-rotating vortices develop in the space between the dike and the obstacle (waste package), and a long, low-velocity cell develops in the drift beyond these vortices. However, if the space is increased from ~4 m [~13 ft] to ~7 m [~22.56 ft] [Figure 3-2(b)], a second, more distinct clockwise vortex develops above the waste package adjacent to the counter-clockwise vortex that largely occupies the gap between the obstacle and the dike. As in the ~4 m [~13 ft] case [Figure 3-2(a)], these smaller vortices decrease away from the dike and are replaced by a larger low velocity cell. In Figure 3-3, magma velocity at the inlet was varied between 1–3 m/s [3.3–9.8 ft/s] to examine its affect on the vorticity field. At 1 m/s [3.3 ft/s], the results are equivalent to those previously discussed [Figures 3-1(b) and 3-2(a)]. With increasing magma ascent velocity, the strength and size of the primary, counter-rotating vortices that occupy the space between the dike and the obstacle increases, and at 3 m/s [9.8 ft/s], two counter-rotating vortices develop, one on top of the other, in the gap between waste package and dike.



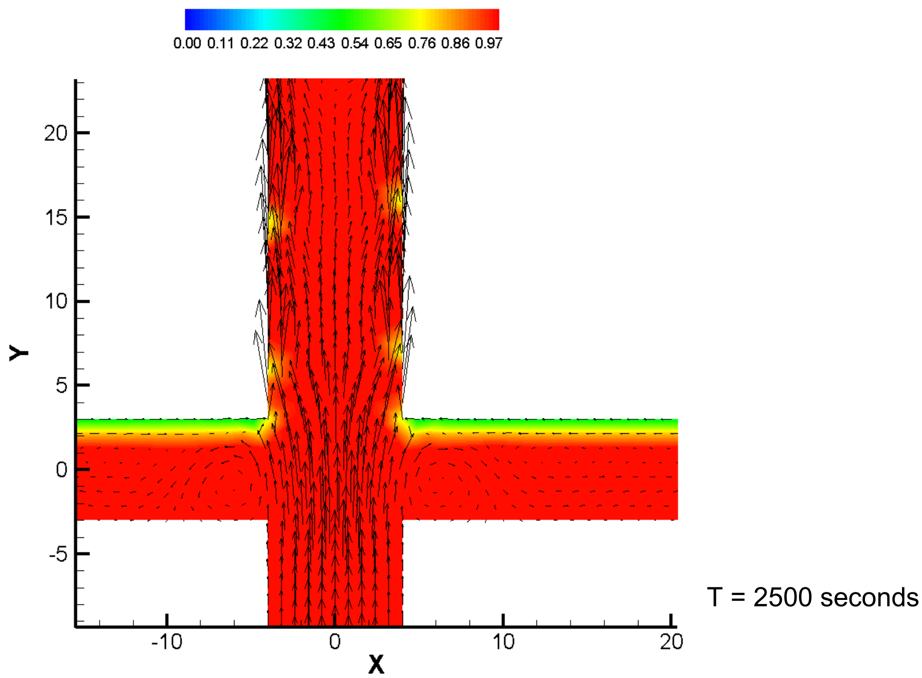


Figure 3-1(a). Time Sequence of Magma Filling Drift Without Waste Packages. Color Contours Show Magma Volume Fraction Superimposed With Velocity Vectors; Magma Inlet Velocity = 1 m/sec [3.28 ft/sec]; Length Is in Meters.

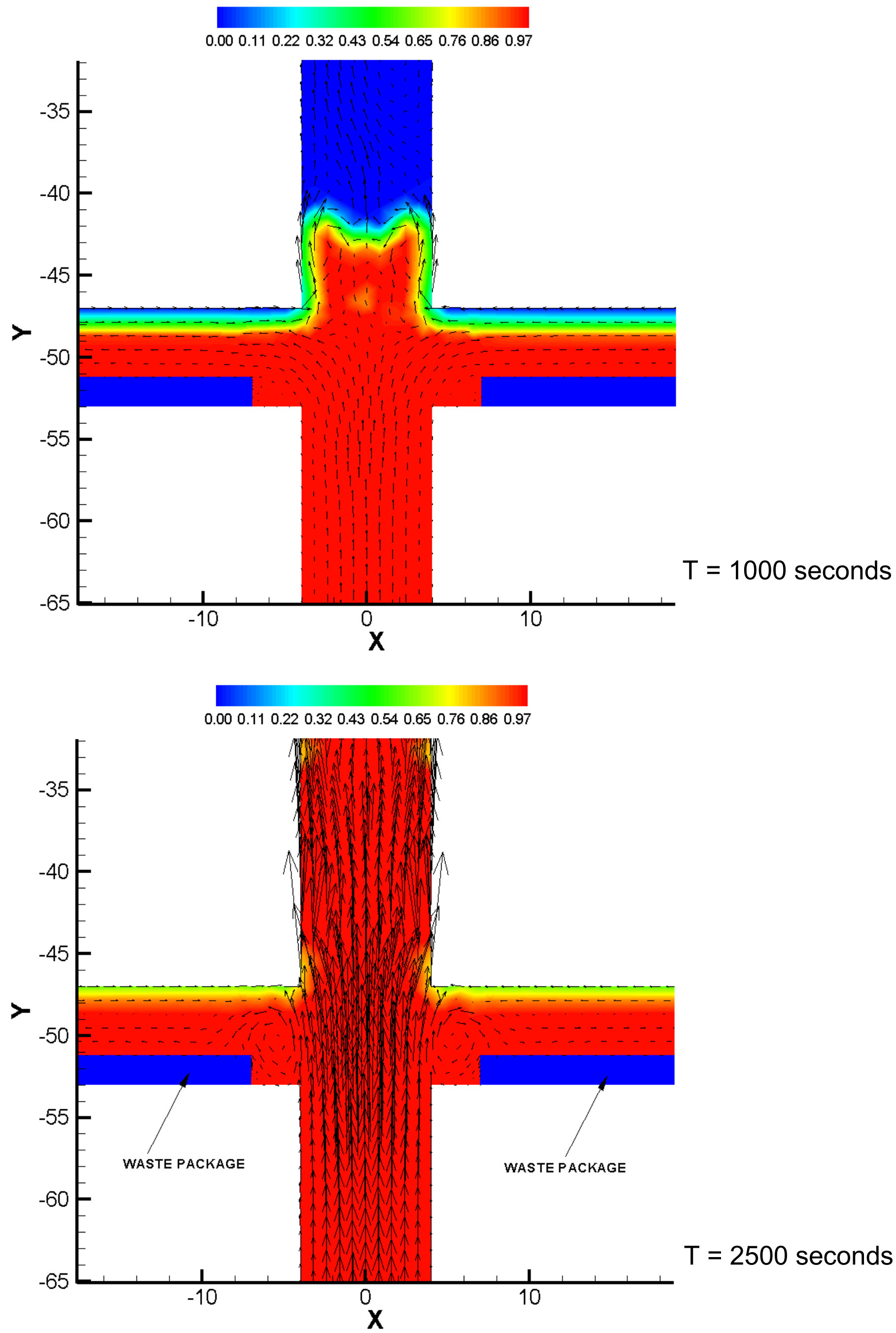


Figure 3-1(b). Time Sequence of Magma Filling Drift With Waste Packages. Color Contours Show Magma Volume Fraction Superimposed With Velocity Vectors; Magma Inlet Velocity = 1 m/sec [3.28 ft/sec]; Distance Between Dike and Obstacle = 4 m [13.12 ft]; Length Is in Meters.

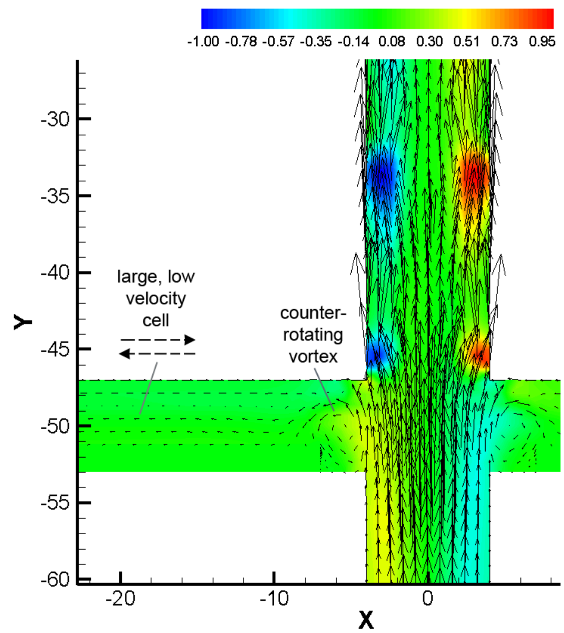


Figure 3-2(a). Color Contours Show Vorticity Superimposed With Velocity Vectors. Magma Inlet Velocity = 1 m/sec [3.28 ft/sec]; Distance Between Dike and Obstacle = 4 m [13.12 ft]; Length Is in Meters.

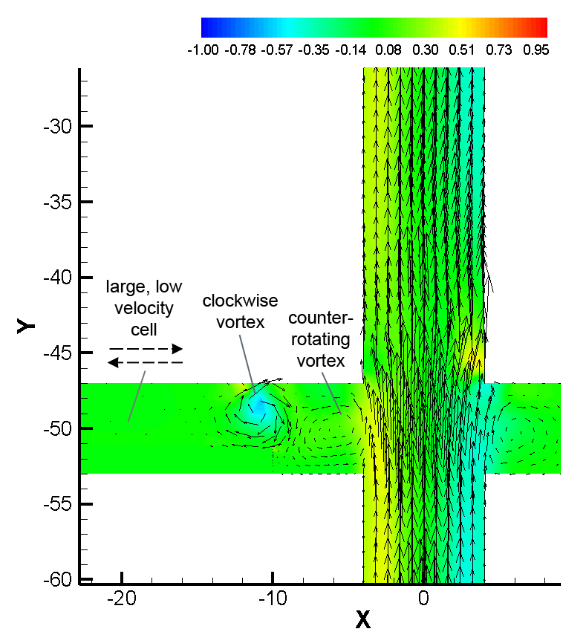
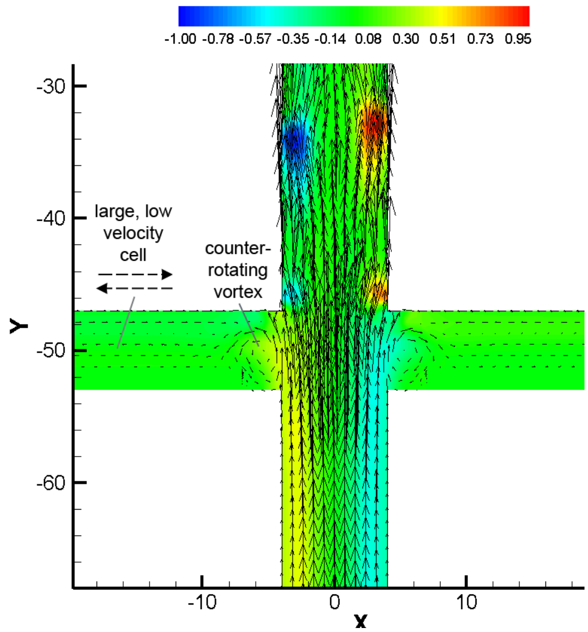
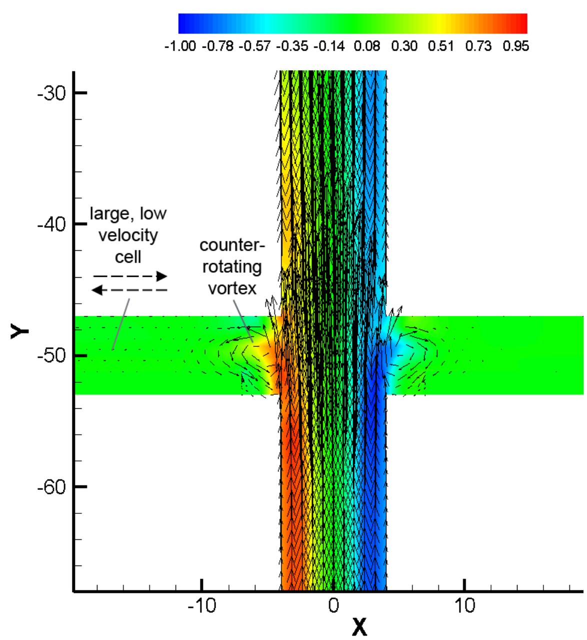


Figure 3-2(b). Color Contours Show Vorticity Superimposed With Velocity Vectors. Magma Inlet Velocity = 1 m/sec [3.28 ft/sec]; Distance Between Dike and Obstacle = 7 m [22.56 ft]; Length Is in Meters.

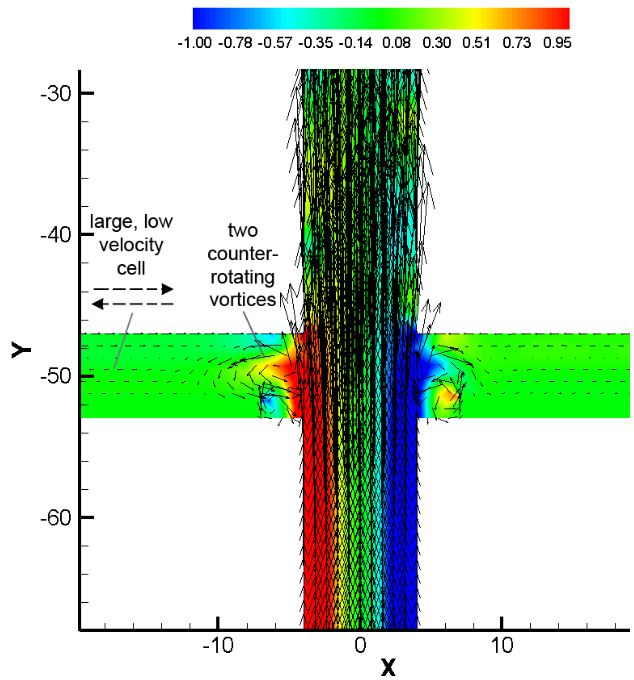


Magma Inlet Velocity = 1m/sec [3.28 ft/sec]

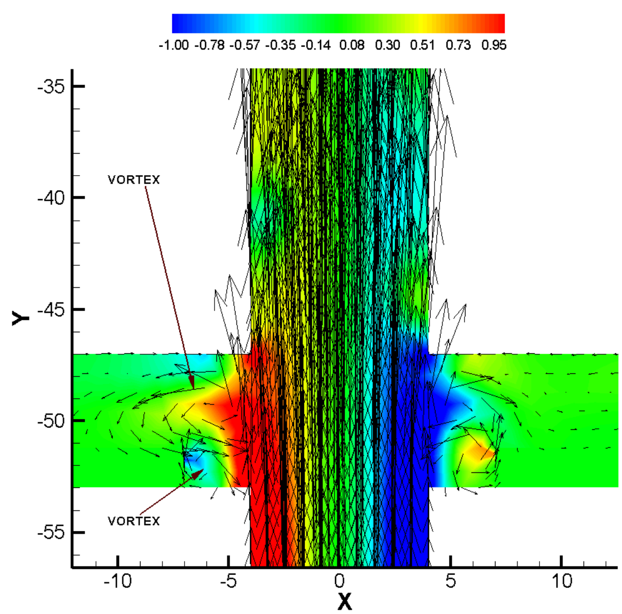


Magma Inlet Velocity = 2 m/sec [6.56 ft/sec]

Figure 3-3. Color Contours Show Vorticity Superimposed With Velocity Vectors. Distance Between Dike and Obstacle = 4 m [13.12 ft]; Length Is in Meters.



Magma Inlet Velocity = 3 m/sec [9.84 ft/sec]



Magma Inlet Velocity = 3 m/sec [9.84 ft/sec] (Enlarged)

Figure 3-3. Color Contours Show Vorticity Superimposed With Velocity Vectors (Continued). Distance Between Dike and Obstacle = 4 m [13.12 ft]; Length Is in Meters.

Also within the configuration of scenario (ii), the temperature profile of a magma-filled drift with waste packages was determined (Figure 3-4). The simulation had a magma ascent velocity of 1 m/s [3.28 ft/sec] and the distance between the dike and the obstacle was 4 m [13.12 ft]. In this simulation, heat transfer between magma and waste packages was purely conductive, and the effect of wall thermal boundary conditions on the predicted temperature field was not considered. Hence, the results provide only a qualitative assessment of the temperature field. Approximately 700 seconds after intersection and filling, the temperature at the boundary between the waste packages and the magma is ~700 K [800 °F]. Given an initial waste package temperature of 350 K [170.33 °F], the temperature has approximately doubled.

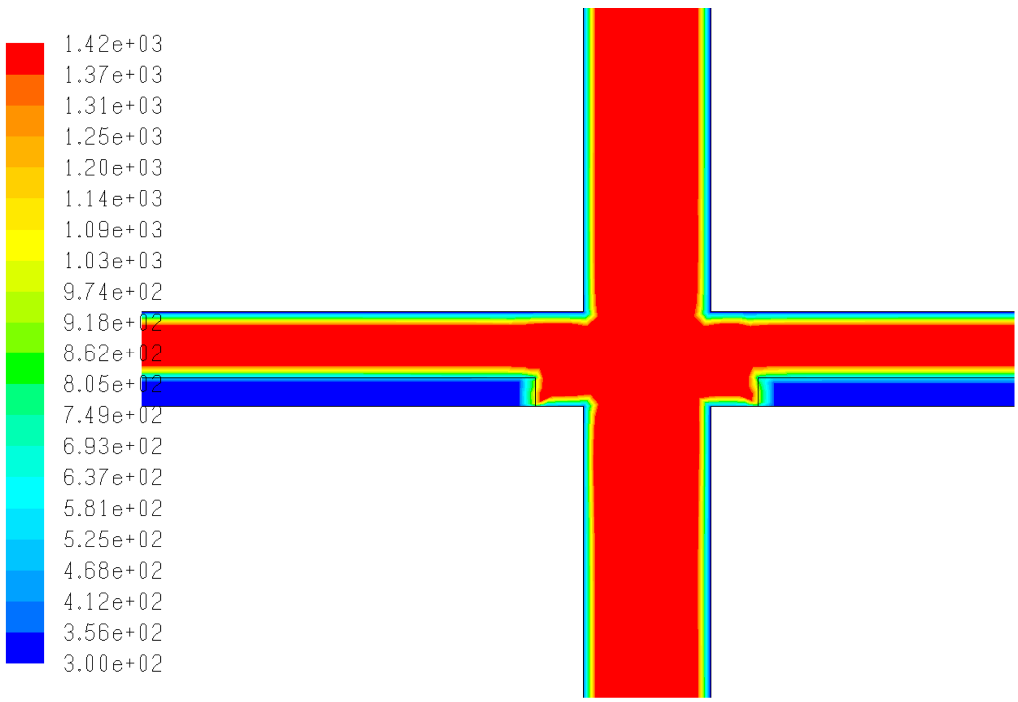


Figure 3-4. Temperature Distributions (K) for the Drift, Magma, and Waste Packages. Magma Inlet Velocity = 1 m/sec [3.28 ft/sec]; Distance Between Dike and Obstacle = 4 m [13.12 ft].

4 CONCLUSIONS

In Phillips, et al. (2008) the theoretical flow of a single-phase, viscous liquid in a configuration analogous to a drift without waste packages intersected by a dike was described. They surmised a series of counter-rotating vortices would develop in the drift, with the primary vortex closest to the entrance of the cavity being the strongest, and the strength of the successive vortices decreasing down the drift. Center for Nuclear Waste Regulatory Analyses (CNWRA) staff conducted computational modeling that added realism to the scenario and produced quantified results. Salient points of these analyses are:

- Magma ascending along a dike that intersects a drift will fill the drift under the influence of gravity from the base to the top and then continue upwards along the drift. Counter-rotating vortices adjacent to the dike that extend into the drift are driven by viscous coupling between the magma rising in the connected dike and the magma in the drift. In the drift beyond these primary vortices, a larger, low velocity circulation cell is established with magma flowing away from the dike along the base of the drift and toward the dike along the drift ceiling. This same pattern develops in the presence of an obstacle in the drift (i.e., waste packages).

- Flow patterns that develop in a magma-filled drift can be affected by the location of dike intersection, specifically relative to obstacles in the drift. Slight changes in the modeled distance between the dike and the waste package produced additional vortices adjacent to the primary vortices (i.e., those located directly next to dike) that extended higher-velocity circulating magma further down the drift.

- In addition to the strength and size of the primary vortices, the shape and distribution of the vortices that develop are affected by the ascent rate of the magma in the dike. At higher ascent rates, vertically coupled counter-rotating vortices develop in the space between the dike and the waste packages.

- The temperature of the waste packages rises in the presence of magma in a static environment. Depending on the time-span of the eruption, circulation of hot magma in a magma filled drift could represent a significant heat source that might affect the integrity of the waste package.

Performance assessment models often calculate the number of failed waste packages and the amount of waste released as a result of separate intrusive and extrusive igneous events. In nature, however, intrusive dikes and conduits that extend to the surface in a volcanic region are often connected. The complexity of volcanic plumbing can be obscured during model abstractions, thus alternative eruption scenarios that include a steady supply of magma (over a finite timeframe) filling a drift and continuing its ascent have been proposed (NRC, 2005). CNWRA staff constructed flow models to examine dike-drift interactions under such conditions in preparation of evaluating the assumptions and uncertainties inherent in model development and their consequences. In all cases, some pattern of circulation developed in the drift, and the pattern was largely influenced by the interplay between the ascending magma and location of the waste packages. These flow patterns provide a method to transport waste release from waste packages other than those directly intersected, which may affect the mass of spent fuel and high-level waste transported to the surface. The waste packages away from the dike intersection zone may also release radionuclides into the magma ascending the dike.

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