CFD Modeling of Cold Trap Process in Drifts
Scientific Notebook No. 736E

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Prepared for: Southwest Research Institute, CNWRA

INITIAL ENTRIES

Scientific notebook: #736E
Issued to: Flavia Viana

By agreement with CNWRA QA, this notebook will be printed at approximate quarterly intervals. This computerized electronic notebook is intended to address the criteria of CNWRA QAP-001.

Account number: 20.06002.01.262

Description: Support Computational Fluid Dynamics (CFD) Modeling of Cold Trap Process in Drifts

Principal Investigator: C. Manepally

Collaborators: S. Green, C. Manepally, D. Bannon, and others.

Objective: CFD Modeling of Heat and Moisture Redistribution in Drifts

Personnel Qualification: All collaborators involved with the tasks detailed in this scientific notebook are familiar with the principles of unsaturated flow and heat transfer processes.

9/1/2005 – F.V.

TASK 2: 1/5 SCALE TEST AND CFD SIMULATIONS

Investigators:

~~Steve Green~~ F.V. 07/18/06 after QA surveillance.
Flavia Viana

Computers and Software:

CFD modeling and other miscellaneous computer tasks (data analysis, word processing, etc.) were performed with a Dell Precision PWS370 PC with Intel Pentium 4 processor and Windows XP Professional operating system version 2002.

The following software was used:

Software Name and Version	Description	Associated File Extension
Microsoft Word 2003	Word Processing	*.doc
Microsoft Excel 2003	Spreadsheet	*.xls
Flow-3D Version 9.0	Computational Fluid Dynamics	prepin.*; flsgrf.*; etc.

Objective: The objective of this task is to complete the 1/5 scale testing and FLOW-3D simulations for comparison, to validate the FLOW-3D model approach in preparation of full-scale repository simulations.

Subtask 1: Complete Testing

There have been several tests conducted to date in the 1/5 scale test facility. These tests will be reviewed to determine whether additional testing is warranted from the standpoint of providing adequate data for comparison to the FLOW-3D simulations of the test configurations. The planned activities are as follows:

1. Review test activities to date.
2. Plan more tests as needed.
3. Document test results.

Subtask 2: FLOW-3D Simulations – Dry Air, No radiation

The results obtained to date from previous simulations would be reviewed and documented. It is not possible to test without the effects of thermal radiation; however, these simulations will serve as a baseline for estimating the importance of heat radiation as well as moisture transport effects. The activities planned for this subtask are:

1. Review simulations to date.
2. Complete simulations as needed.
3. Process CFD data.
4. Compare test and CFD results.

Review of test activity to date

The Scientific Notebook # 616, prepared by Steven Svedeman was reviewed. It contains the documentation of the 1/5 scale tests completed to date. From the review four files containing the test data were identified. The data files for different heating and moisture conditions are summarized in the following table.

Fluid Condition	Heat distribution in waste packages (Watts)	Parameters Measured	File Name
Dry air	50 each and 75 each	Temperature	Fifth Scale Test Data 6-24-2004.xls
Dry air	50 each; 75 each; 75-25-25-75; 80-60-40-20	Temperature	Fifth Scale Test Data 9-3-2004.xls
With moisture	50 each	Temperature and Relative Humidity	Fifth Scale Test Data 12-14-2004.xls
With moisture	50 each	Temperature and Relative Humidity	Fifth Scale Test Data 2-6-2005.xls

For the dry test, only the data found in the file named **Fifth Scale Test Data 9-3-2004.xls** will be used since it contains the latest data for all four cases of heat distribution in waste packages. From the results of testing with moisture the data contained in the file **Fifth Scale Test Data 2-6-2005.xls** would be used since it contains the most recent data.

Plan more tests

There is only one set of test data with moisture. Additional tests should be conducted to include the effect of non-uniform heat distribution and to provide enough data to establish a comparison between experimental and CFD results obtained with the moisture module to be developed by Steve Green. The proposed tests cases with moisture are:

- Uniform heating: 75 watts each
- Non-uniform heating: 75-25-25-75 watts and 80-60-40-20 watts.

The 1/5 scale drift facility is not operative at this time. The testing would be completed as needed when the experimental set up is ready to be used. The Test vs. CFD comparison would be done with the data collected to date.

9/2/2005 – F.V.

Review of FLOW-3D Simulations to date

A list of the simulation results files was found in the scientific notebook # SN576 page 64, prepared by David Walter. The following table summarizes the name and status of those files and indicates the corresponding test data file available.

File Name	Case Name	Status of Simulation	Mesh Size	Associated Test Data File
prepinr.Dry50b flsgrf.Dry50b	Dry-50w	Completed	250x; 57y; 64z	Fifth Scale Test Data 9-3-2004.xls
prepinr.Dry75a flsgrf.Dry75a	Dry-75w	Completed	250x; 57y; 64z	Fifth Scale Test Data 9-3-2004.xls
prepinr.Dry75a-rmesh flsgrf.Dry75a-rmesh	Dry-75w-rmesh	Completed	275x; 66y; 76z	Fifth Scale Test Data 9-3-2004.xls
prepinr.Dry75a-rmesh2 flsgrf.Dry75a-rmesh2	Dry-75w-rmesh2	Incomplete	275x; 72y; 91z	Fifth Scale Test Data 9-3-2004.xls
prepinr.Dry80-60-40-20 flsgrf.Dry80-60-40-20	Dry-80-60-40-20w	Completed	250x; 57y; 64z	Fifth Scale Test Data 9-3-2004.xls

Each simulation has been assigned a case name for future referral. The input (prepin.*) file contains the settings of the simulation (i.e., physics, geometry, mesh, fluid properties, etc.); and the output (flsgrf.*) file contains the full results from the solution and can be reproduced using the input file.

9/6/05 – F.V.

Complete Simulations – Case: Dry-75-25-25-75w

Simulation of the cold trap process with a heat distribution on the waste packages of 75-25-25-75 watts would be done to compare with experimental values collected in the 20-percent drift scale experimental facility. The existing **prepinr.Dry50b** file was modified to incorporate the new values of heating and boundary conditions. Boundary conditions were taken from experimental data collected on 9/08/2004 in the Excel file **Fifth Scale Test Data 9-3-2004.xls.**

Simulation settings may be found in the input file **prepinr.Dry75-25-25-75.** The last output file for the 50w case **flsgrf.Dry50b** was used as an initial condition to accelerate de convergence of the solution.

9/15/05 – F.V.

Complete Simulations – Case: Dry-75w-rmesh2

The simulation with a heat distribution of 75 watts on each waste package has been run with three different mesh sizes. The coarse mesh (mesh: 250x; 57y; 64z) was refined to obtain a grid with about 51% more cells (rmesh: 275x; 66y; 76z). A further refined mesh with about 31% more cells than the previous one was also obtained (rmesh2: 275x; 72y; 91z). Simulation with the finer mesh (rmesh2) is not at steady state.

Restarted simulation with the finer mesh **prepinr.Dry75a-rmesh2** to obtain a converge solution and compare with results from the two other runs prepinr.Dry75a and prepinr.Dry75a-rmesh and with test data.

9/16/05 – F.V.

Data Processing

Test data for all heating conditions for dry air experiments may be found in the file **Fifth Scale Test Data 9-3-2004.xls**. Average and processing of test data is made directly in this Excel workbook.

CFD data at the same locations as of the thermocouples for in-drift air had been extracted from the result files: **flsgrf.Dry50b; flsgrf.Dry75a; flsgrf.Dry75a-rmesh; flsgrf.Dry80-60-40-20**. Average in time of the CFD data was made with the help of a VBA macro created by David Walter in the Excel file **A.xls**.

CFD average temperatures of the waste packages were also obtained from the CFD output files.

Average data (in time at steady state) for test and CFD simulations may be found in spread sheets of the Excel workbook called **Fifth Scale Test Data 9-3-2004.xls** for the following cases: Dry-50w ; Dry-75w-mesh; Dry-75w-rmesh; and Dry-80-60-40-20w.

9/26/05 – F.V.

Description of CFD Model

The solution domain of the CFD analysis performed with Flow-3D is defined by the rectangular mesh block which is 6.653 m long and has a square cross section with sides of 1.166 m. The geometry is defined by 8 components called obstacles; the first one is a fictitious obstacle in the form of a rectangular parallelepiped that fills up the entire space and is limited internally by a cylinder of 0.567 m radius that corresponds to the outer radius of the drift wall. This obstacle is used to prescribe a constant temperature to the outer wall of the drift (ambient temperature).

The second obstacle consists of a cylinder with and IR of 0.53m and OR of 0.567m and 6.51m of length and represents the drift wall (PVC pipe). The third and fourth obstacles correspond to the hot and cold end walls respectively and consist of cylinders with 0.567m of radius.

Finally, components 5 through 8 correspond to the four waste packages used in the 20-percent drift scale facility. These are cylinders of 0.152m radius and 1m long. A schematic of the geometry is shown in Figure 09/26/05-1.

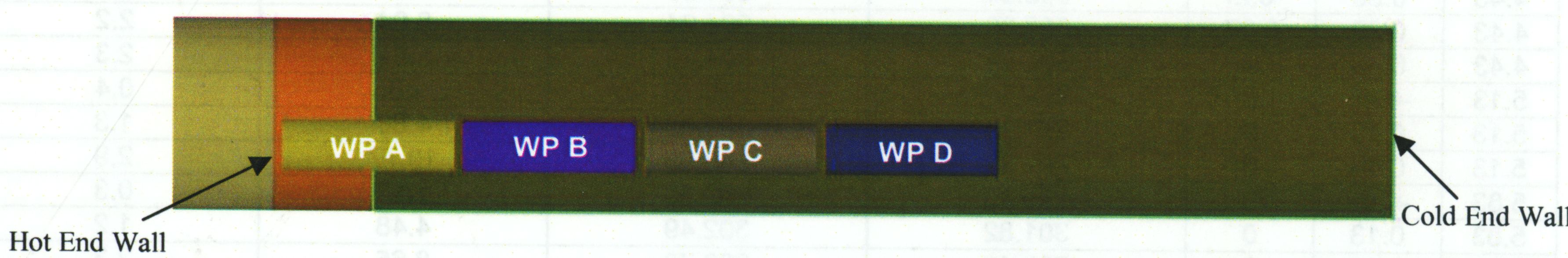

Figure 09/26/05-1. CFD Model of the 1/5 Scale Drift Facility [Source: prepinr.Dry50b]

9/29/05 – F.V.

CFD vs. Test Data Comparison - Case: Dry-50w

The results for the case with 50 watts on each waste package are shown in Table 09/29/05-1. The X, Y and Z values correspond to the Cartesian coordinates of the locations of thermocouples in the 1/5 scale drift facility. The measured and predicted values of temperature at each of those points are presented along with the absolute difference and the relative error.

The relative error is defined as the difference between the value predicted by the CFD simulation and the measured value, divided by the maximum temperature difference encountered in the system. The maximum temperature gradient is the difference between the highest average of temperatures measured on the waste packages and the ambient temperature.

Table 09/29/05-1. Comparison of Average Temperature Values from Test and CFD Simulation at Different Points along the 1/5 Scale Model – Case: Dry-50w [Source: Fifth Scale Test Data 9-3-2004.xls]

X	Z	Y	Avg. Test Temp. (K)	Avg. CFD Temp. (K)	Relative Error (%)	Abs. Diff. (°F)
0.55	0.13	0	304.20	305.95	11.56	3.1
0.55	0.46	0	303.01	305.19	14.49	3.9
1.6	-0.27	0.27	300.68	301.11	2.84	0.8
1.6	-0.27	-0.27	300.28	301.29	6.73	1.8
1.6	0.06	0.27	303.06	303.90	5.56	1.5
1.6	0.06	-0.27	302.68	303.67	6.57	1.8
1.6	0.13	0	304.80	305.75	6.37	1.7
1.6	0.38	0.27	303.65	304.89	8.20	2.2
1.6	0.38	-0.27	303.61	304.94	8.85	2.4
1.6	0.46	0	303.71	305.08	9.15	2.5
1.85	0.13	0	304.49	305.12	4.20	1.1
1.85	0.46	0	303.73	304.90	7.82	2.1
2.65	0.13	0	304.34	305.51	7.76	2.1
2.65	0.46	0	303.32	305.52	14.59	4.0
3.7	-0.27	0.27	300.40	301.10	4.64	1.3
3.7	-0.27	-0.27	300.27	301.27	6.64	1.8
3.7	0.13	0	303.46	304.74	8.52	2.3
3.7	0.06	0.27	301.26	302.76	9.99	2.7
3.7	0.06	-0.27	301.34	303.06	11.45	3.1
3.7	0.38	0.27	302.61	304.48	12.44	3.4
3.7	0.38	-0.27	302.61	304.51	12.64	3.4
3.7	0.46	0	302.13	304.52	15.89	4.3
3.95	0.46	0	303.11	304.22	7.42	2.0
3.95	0.13	0	303.56	304.77	8.04	2.2
4.43	-0.27	0.27	300.44	300.83	2.58	0.7
4.43	-0.27	-0.27	300.36	300.78	2.76	0.7
4.43	0.06	0.27	301.74	302.60	5.74	1.6
4.43	0.13	0	302.02	302.97	6.34	1.7
4.43	0.06	-0.27	301.69	302.77	7.18	1.9
4.43	0.38	-0.27	302.94	304.07	7.51	2.0
4.43	0.38	0.27	303.00	304.21	8.04	2.2
4.43	0.46	0	302.88	304.16	8.51	2.3
5.13	-0.46	0	299.40	299.15	-1.65	0.4
5.13	0.13	0	301.93	302.66	4.86	1.3
5.13	0.46	0	302.31	303.93	10.77	2.9
5.83	-0.46	0	299.43	299.60	1.12	0.3
5.83	0.13	0	301.82	302.49	4.48	1.2
5.83	0.46	0	302.40	303.70	8.65	2.3
2.125	0.13	0	303.25	304.81	10.36	2.8
2.125	0.46	0	303.41	304.40	6.58	1.8

The relative errors for this analysis go from -1.7% to about 16% while the absolute differences go from 0.3°F to 4.3°F.

Figure 09/29/05-1 shows the distribution of the relative errors along the 1/5 drift scale facility. This plot shows that most of the points fall within 4% and 12% of relative error. It is also observed that with exception of one point all predicted values are higher than the measured one.

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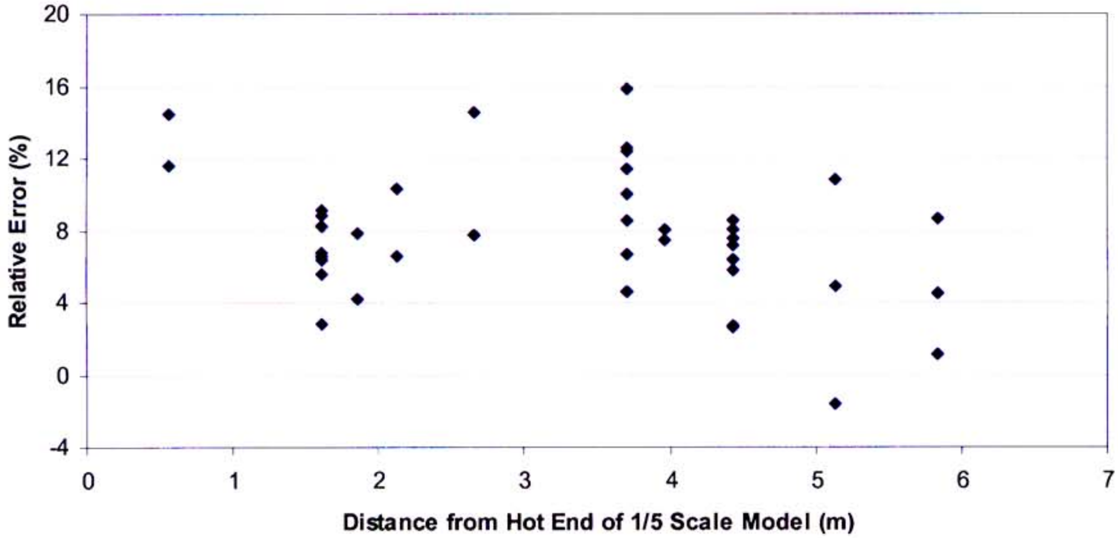

Figure 09/29/05-1. Relative Error Distribution along the 1/5 Scale Model – Case: Dry-50w [Source: Fifth Scale Test Data 9-3-2004.xls]

The average of measured temperatures at each of the ten cross sections along the 1/5 scale model are shown in Figure 09/29/05-2 together with the average of the predicted values at the same locations. The difference between predicted and measured values go from 1.3°F to 3.5°F and the CFD results closely follow the trend observed in experimental measurements.

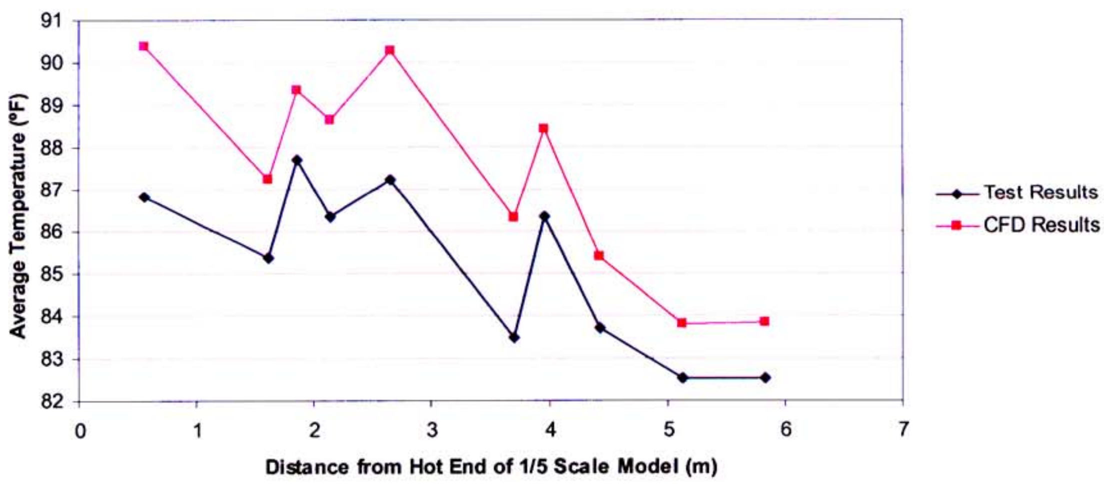

Figure 09/29/05-2. Average temperature at Different Cross Sections along the Pipe – Case: Dry-50w [Source: Fifth Scale Test Data 9-3-2004.xls]

Average temperatures for the waste packages obtained from experimental measurements and CFD simulations are shown in Table 09/29/05-2.

Table 09/29/05-2. Waste Package Temperature – Case: Dry-50w [Source: Fifth Scale Test Data 9-3-2004.xls]

	Test Temperature (°F)	CFD Temperature (°F)	Difference (°F)
WP1	104.22	108.99	4.76
WP2	104.32	110.01	5.69
WP3	103.97	109.71	5.73
WP4	103.83	108.43	4.60

A graphical representation of the results in Table 09/29/05-2 may be observed in Figure 09/29/05-3. It can be concluded that the predicted temperature values for the waste packages are larger than the measured values; the differences go from 4.6°F to 5.73°F.

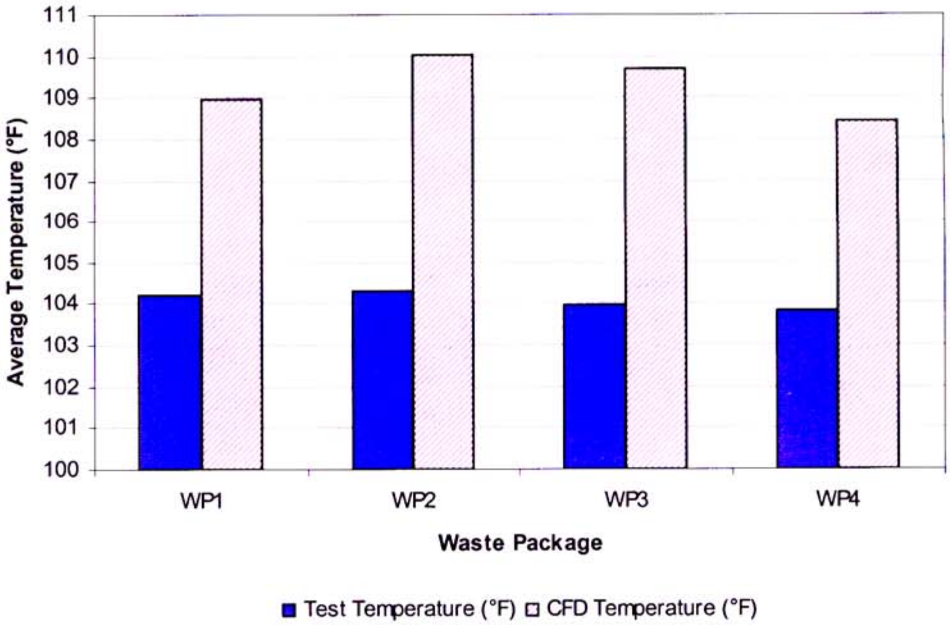

Figure 09/29/05-3. Bars Plot of the Predicted and Measured Temperature of Waste Packages – Case: Dry-50w [Source: Fifth Scale Test Data 9-3-2004.xls]

09/30/05 – F.V.

CFD vs. Test Data Comparison - Case: Dry-80-60-40-20w

In this case the total amount of energy supplied to the system is equal (200watts) to that used in the case where each waste package had 50 watts each. The difference is the non-uniform distribution of the heat. The heat is concentrated more to the left end of the pipe originating a higher temperature gradient in that region and a weak temperature gradient towards the end of the pipe. The temperatures at different locations along the pipe from tests and CFD simulations are presented in Table 09/30/05-1.

Table 09/30/05-1. Comparison of Average Temperatures from Test and CFD Simulation at Different Points along the 1/5 Scale Model – Case: Dry-80-60-40-20w [Source: Fifth Scale Test Data 9-3-2004.xls]

X	Z	Y	Avg. Test Temp. (K)	Avg. CFD Temp. (K)	Relative Error (%)	Abs. Diff. (°F)
0.55	0.13	0	305.25	307.57	11.61	4.18
0.55	0.46	0	304.41	306.90	12.45	4.48
1.6	0.13	0	304.80	307.43	13.16	4.73
1.6	0.46	0	303.82	306.33	12.56	4.52
1.6	-0.27	0.27	300.75	301.86	5.54	1.99
1.6	0.06	0.27	303.18	304.97	8.93	3.21
1.6	0.38	0.27	304.28	306.06	8.91	3.21
1.6	-0.27	-0.27	300.29	301.87	7.90	2.84
1.6	0.06	-0.27	302.84	304.78	9.73	3.50
1.6	0.38	-0.27	304.00	306.14	10.71	3.85
1.85	0.13	0	304.73	306.30	7.86	2.83
1.85	0.46	0	304.22	305.92	8.51	3.06
2.65	0.13	0	303.99	305.51	7.58	2.73
2.65	0.46	0	303.00	305.47	12.36	4.44
3.7	0.13	0	301.78	303.97	10.96	3.94
3.7	0.46	0	301.63	304.39	13.81	4.97
3.7	-0.27	0.27	300.45	301.49	5.22	1.88
3.7	0.06	0.27	301.33	303.70	11.84	4.26
3.7	0.38	0.27	302.26	304.57	11.58	4.17
3.7	-0.27	-0.27	300.33	301.51	5.94	2.14
3.7	0.06	-0.27	301.26	303.58	11.60	4.17
3.7	0.38	-0.27	302.31	304.77	12.29	4.42
3.95	0.13	0	302.36	303.48	5.59	2.01
3.95	0.46	0	302.59	304.29	8.51	3.06
4.43	0.13	0	301.94	303.56	8.10	2.92
4.43	0.46	0	302.66	304.23	7.86	2.83
4.43	-0.27	0.27	300.46	301.20	3.74	1.35
4.43	0.06	0.27	301.67	303.07	6.99	2.51
4.43	0.38	0.27	302.68	304.15	7.35	2.64
4.43	-0.27	-0.27	300.36	301.34	4.91	1.77
4.43	0.06	-0.27	301.63	303.14	7.58	2.73
4.43	0.38	-0.27	302.67	304.21	7.74	2.78
5.13	-0.46	0	299.51	299.72	1.06	0.38
5.13	0.13	0	301.84	303.20	6.84	2.46
5.13	0.46	0	302.20	304.05	9.22	3.32
5.83	-0.46	0	299.59	299.94	1.72	0.62
5.83	0.13	0	301.67	303.04	6.87	2.47
5.83	0.46	0	302.30	303.79	7.50	2.70
2.125	0.13	0	303.85	306.55	13.53	4.87
2.125	0.46	0	303.40	305.86	12.28	4.42

The relative error was calculated as explained on 09/29/05. The relative error distribution along the pipe for a non-uniform heating of 80-60-40-20 watts is shown in Figure 09/30/05-1. The relative error goes from 1% through 14%. All predicted temperatures are higher than the correspondent measured values.

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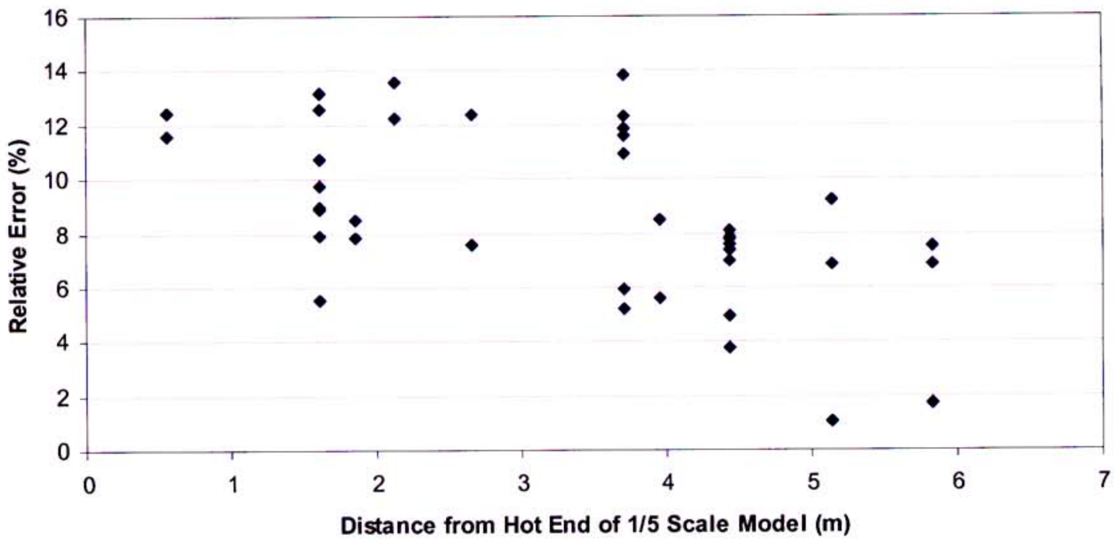

Figure 09/30/05-1. Relative Error Distribution along the 1/5 Scale Model – Case: Dry-80-60-40-20w[Source: Fifth Scale Test Data 9-3-2004.xls]

Figure 09/30/05-2 shows the plot lines of the average temperatures at ten cross sections along the pipe. The maximum difference between test and CFD average temperature is about 4.6 °F. The CFD line shows the same trend as that of the test line except at x = 2.125m where the test line shows a drop in temperature with respect to the previous value at x = 1.85m; while the CFD results indicate a slight increase in temperature at that point.

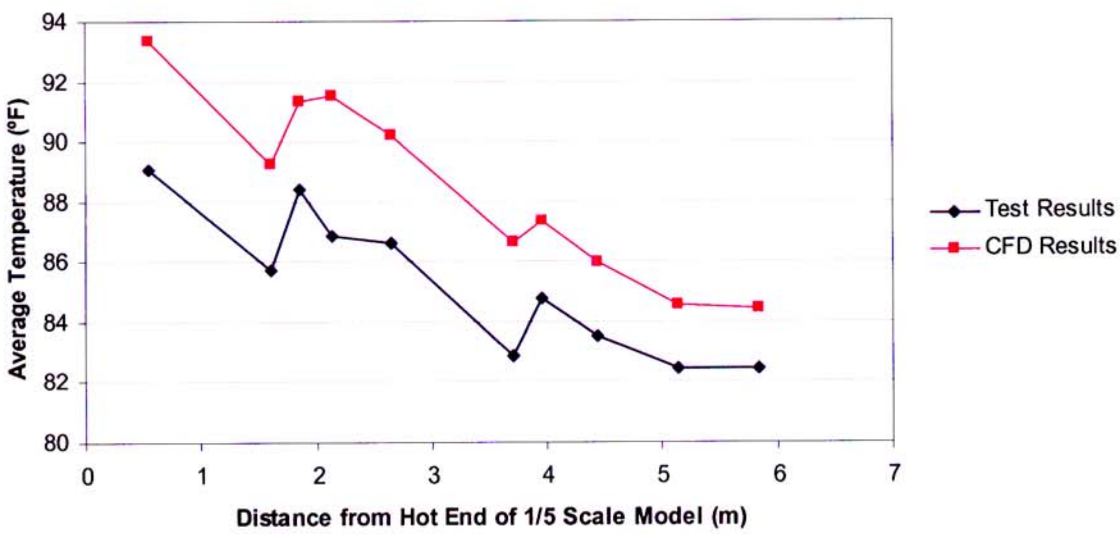

Figure 09/30/05-2. Average temperature at Different Cross Sections along the Pipe – Case: Dry-80-60-40-20w [Source: Fifth Scale Test Data 9-3-2004.xls]

A summary of the test and CFD temperatures for each of the four waste packages is shown in Table 09/30/05-2; and a bar plot with these results is presented in Figure

09/30/05-3. Again, the predicted temperatures are higher than the measured values the difference goes from about 3°F to 6°F.

Table 09/30/05-2. Waste Package Temperature – Case: Dry-80-60-40-20w [Source: Fifth Scale Test Data 9-3-2004.xls]

	Test Temperature (°F)	CFD Temperature (°F)	Difference (°F)
WP1	113.59	118.59	4.99
WP2	106.25	112.11	5.86
WP3	99.59	104.45	4.86
WP4	92.17	95.22	3.05

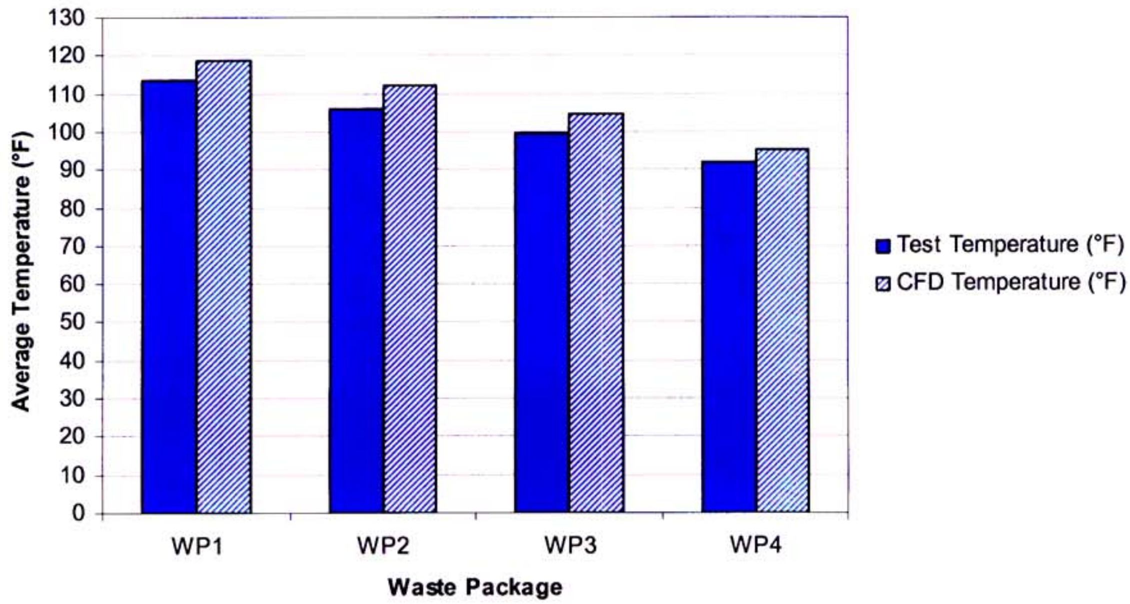

Figure 09/30/05-3. Bars Plot of the Predicted and Measured Temperature of Waste Packages – Case: Dry-80-60-40-20w [Source: Fifth Scale Test Data 9-3-2004.xls]

10/3/05 – F.V.

Symmetry about the z-axis

The test and CFD data is plotted about the symmetry plane to determine whether or not the temperature distribution across the drift would be symmetric about the axial plane. Two heating distribution cases are analyzed: uniform heating with 50 watts on each waste package and non-uniform heating with 80-60-40-20 watts applied on waste package.

Figure 10/03/05-1 shows the temperature profiles along the drift with a uniform heating of 50 watts per waste package. The lines represent the average temperature obtained from CFD simulation along the pipe (along x-axis) at specific locations (y and z coordinates are fixed for each line). There is three pair of points of measurement located symmetrically along the pipe; these are: T5 – T8; T7 – T10 and T6 – T9. The experimental values are represented by points in Figure 10/03/05-1.

As may by observed in Figure 10/03/05-1, the lines of temperature profile at two symmetric locations are very close to one another and follow about the same trend. Also the experimental data shows that symmetry would be a good approximation to reality. Temperature values at two symmetric points are either very close or almost identical in value.

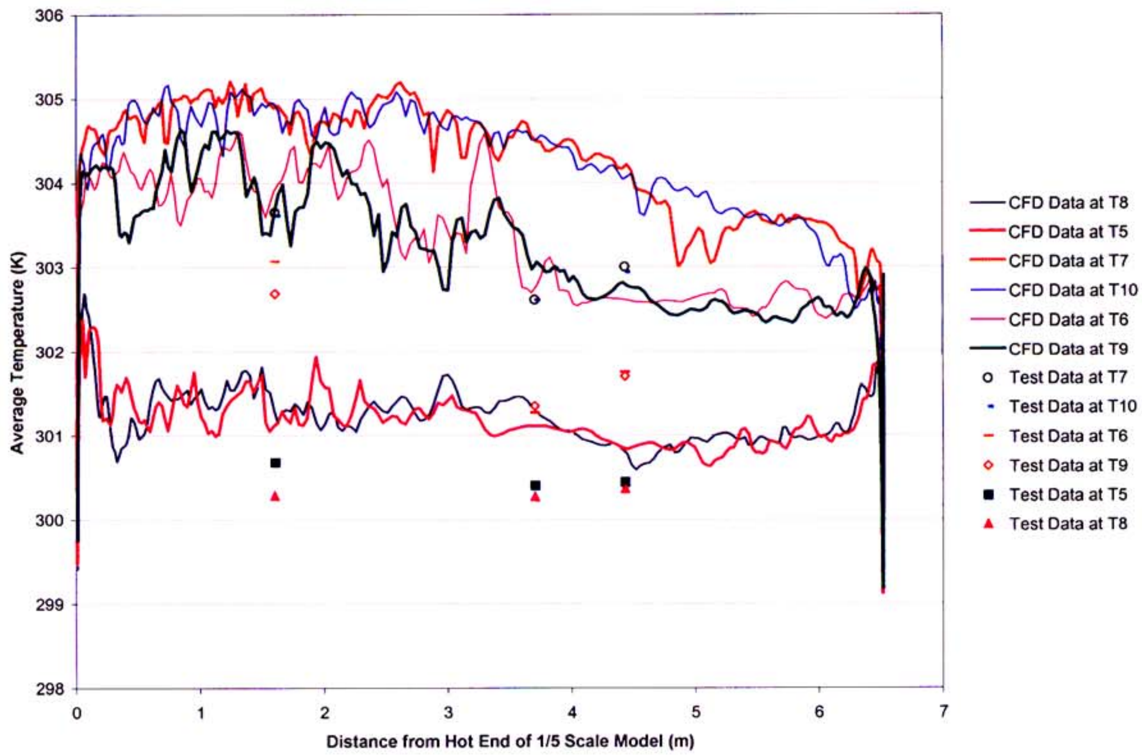

Figure 10/03/05-1. Temperature Profile along the 1/5 Drift Scale Model at Different Locations with a Uniform Heating of 50 watts per WP [Source: 50w_SYMM.xls]

For the case with non-uniform heat distribution (80-60-40-20 watts per WP) shown in figure 10/03/05-2. The symmetry is even more apparent since each symmetric pair of temperature profile line fall very close one to another as well as the experimental values.

These results could greatly simplify the computational time by running simulations with only one half of the geometry and assuming that the other half would have the same value at each position symmetric about the z-plane.

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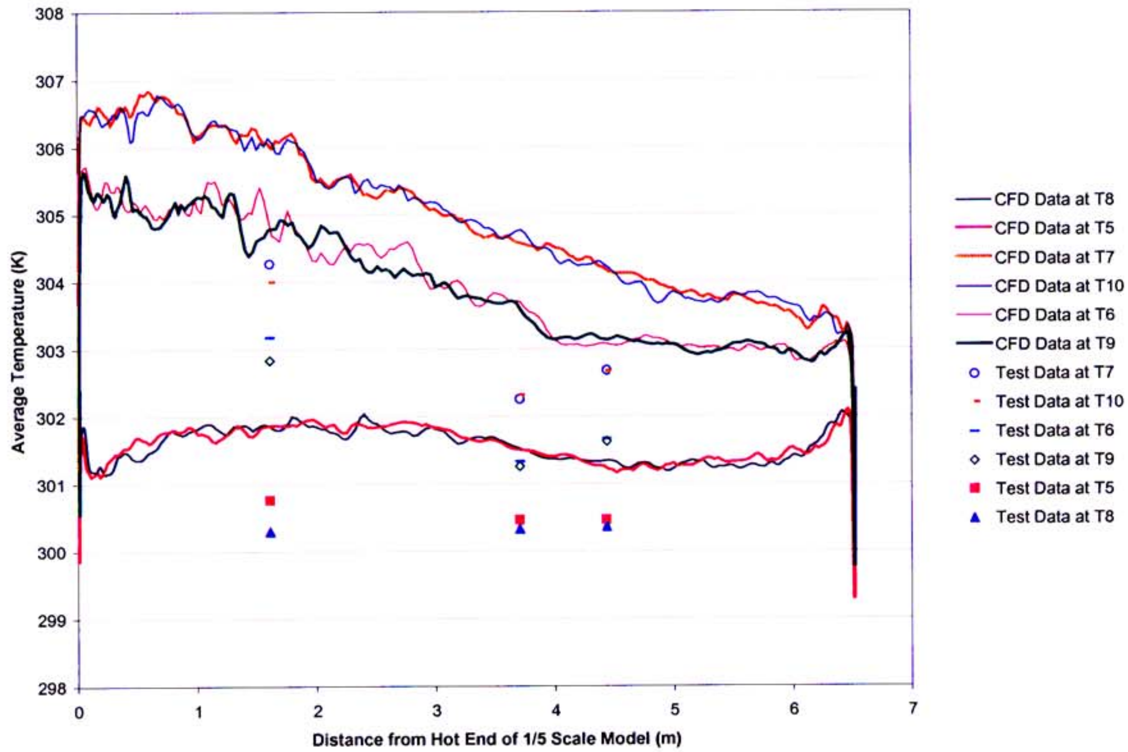

Figure 10/03/05-2. Velocity Profile along the 1/5 Drift Scale Model at Different Locations with a Non-Uniform Heating of 80-60-40-20 watts [Source: 80-60-40-20w_SYMM.xls]

10/6/05 – F.V.

Review of Test Activities with Moisture – Case: Wet-50w

One set of experimental data is available with a uniform heating of 50 watts per waste package (File: **Fifth Scale Test Data 2-6-2005.xls**). The data includes temperatures and relative humidity measurements at different locations within the drift. This case would be referred to as **Wet-50w**.

Figure 10/06/05-1 shows the measured values of relative humidity and temperature at different locations along the pipe. There is a significant difference in relative humidity between different points along the drift going from 78.4% to 91.8%.

The relative humidity is higher closer to the hot end wall and lowers towards the center of the pipe; and it is closer to saturation point at a level below the waste package and closer to the cold end wall.

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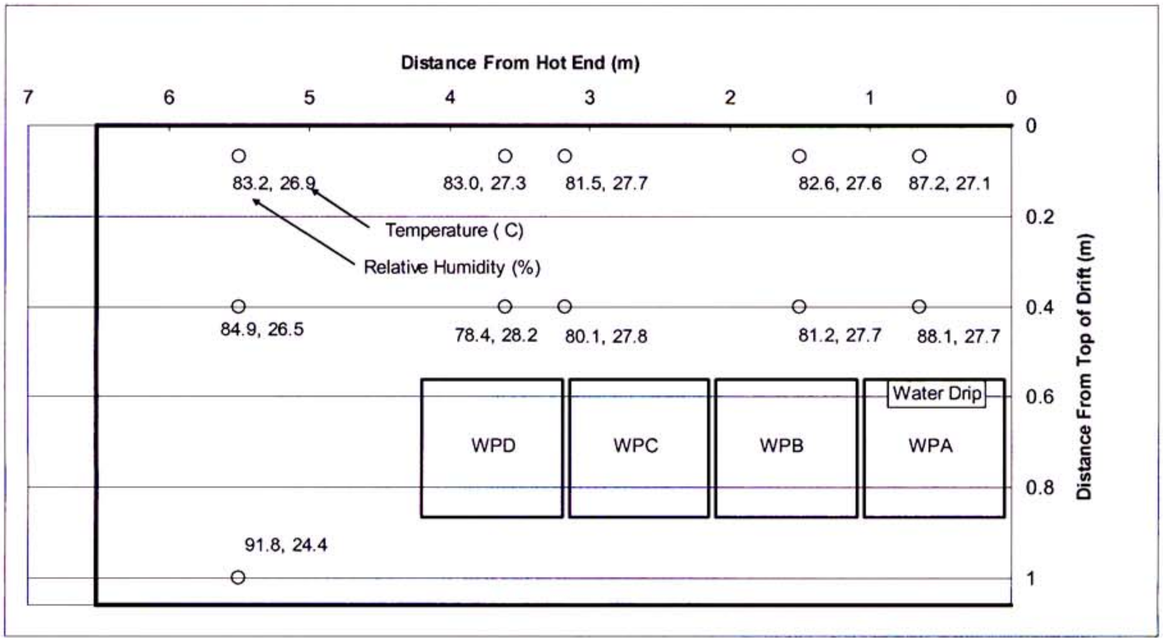

Figure 10/06/05-1. Relative Humidity and Temperature Measured along Drift Centerline- Case: Wet-50w [Source: Fifth Scale Test Data 2-6-2005.xls]

10/7/05 – F.V.

Review of Test Activities with Moisture – Case: Wet-75-25-25-75w

Another set of experimental data with temperature and relative humidity measurements has been reviewed and processed. The spread sheet with the data and average values was named **Fifth Scale Test Data 3-16-2005.xls**. The experiments were carried out on March 16, 2005 with a non-uniform heat distribution of 75-25-25-75 watts.

However, the relative humidity measurements for this test are limited to one unique location. Further measurements of relative humidity at different locations along the drift should be maid in order to obtain the moisture distribution along the pipe. The average value of the relative humidity measured at the center of the pipe (x=3.18; y=0.0; z=0.46) was 81.7%.

10/7/05 – F.V.

Completing Simulations – Case: Dry-75w-rmesh2

The simulation with a uniform heating of 75 watts using a refined mesh (rmesh2: 275x; 72y; 91z) has been restarted from the previous results using the files **prepinr.Dry75rmesh2** and **flsgrf.Dry75a-rmesh2**. For details on the simulation read annotations in **prepinr.Dry75rmesh2**.

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10/13/05 – F.V.

CFD vs. Test Data Comparison – Cases: Dry-75w and Dry-75w-rmesh

Tables 10/13/05-1 and 10/13/05-2 show the measured and predicted temperatures at 120 locations along the drift. The CFD results in Table 10/13/05-1 were obtained with a coarse mesh #1 (250x; 57y; 64z) and the CFD results in Table 10/13/05-2 were obtained with mesh #2 (275x; 66y; 76z) that contains 51% more cells than mesh#1.

Table 10/13/05-1. Comparison of Average Temperature Values from Test and CFD Simulation at Different Points along the 1/5 Scale Model – Case: Dry-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

X	Z	Y	Avg. Test Temp. (K)	Avg. CFD Temp. (K)	Relative Error (%)	Abs. Diff. (°F)
0.55	0.13	0	306.94	310.27	16.10	5.98
0.55	0.46	0	305.39	309.47	19.73	7.33
1.6	0.13	0	307.61	309.60	9.62	3.57
1.6	0.46	0	305.99	308.93	14.21	5.28
1.6	-0.27	0.27	302.10	303.64	7.45	2.77
1.6	0.06	0.27	305.35	307.73	11.51	4.28
1.6	0.38	0.27	306.16	308.88	13.15	4.89
1.6	-0.27	-0.27	301.51	303.84	11.30	4.20
1.6	0.06	-0.27	305.06	307.41	11.40	4.24
1.6	0.38	-0.27	306.04	308.87	13.70	5.09
1.85	0.13	0	307.27	310.24	14.40	5.35
1.85	0.46	0	306.25	309.00	13.33	4.95
2.65	0.13	0	307.02	310.70	17.83	6.63
2.65	0.46	0	305.77	309.26	16.91	6.28
3.7	0.13	0	305.97	310.06	19.82	7.37
3.7	0.46	0	304.26	308.91	22.52	8.37
3.7	-0.27	0.27	301.78	303.57	8.68	3.22
3.7	0.06	0.27	303.01	306.38	16.31	6.06
3.7	0.38	0.27	304.86	308.36	16.92	6.29
3.7	-0.27	-0.27	301.63	303.48	9.00	3.34
3.7	0.06	-0.27	303.13	306.09	14.35	5.33
3.7	0.38	-0.27	304.85	308.49	17.62	6.55
3.95	0.13	0	306.08	309.07	14.48	5.38
3.95	0.46	0	305.49	308.22	13.22	4.91
4.43	0.13	0	304.06	306.41	11.38	4.23
4.43	0.46	0	305.21	307.86	12.84	4.77
4.43	-0.27	0.27	301.88	303.27	6.72	2.50
4.43	0.06	0.27	303.66	305.91	10.86	4.04
4.43	0.38	0.27	305.35	307.87	12.22	4.54
4.43	-0.27	-0.27	301.74	303.12	6.70	2.49
4.43	0.06	-0.27	303.59	305.92	11.31	4.20
4.43	0.38	-0.27	305.29	307.60	11.17	4.15
5.13	-0.46	0	300.36	300.18	-0.89	0.33
5.13	0.13	0	303.92	306.21	11.10	4.12
5.13	0.46	0	304.45	307.65	15.50	5.76
5.83	-0.46	0	300.45	300.82	1.77	0.66
5.83	0.13	0	303.78	305.95	10.51	3.91
5.83	0.46	0	304.57	307.12	12.35	4.59
2.125	0.13	0	305.27	309.80	21.92	8.14
2.125	0.46	0	305.87	309.28	16.55	6.15

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Table 10/13/05-2. Comparison of Average Temperature Values from Test and CFD Simulation at Different Points along the 1/5 Scale Model – Case: Dry-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

X	Z	Y	Avg. Test Temp. (K)	Avg. CFD Temp. (K)	Relative Error (%)	Abs. Diff. (°F)
0.55	0.13	0	306.94	308.80	9.00	3.34
0.55	0.46	0	305.39	308.30	14.07	5.23
1.6	0.13	0	307.61	309.19	7.66	2.85
1.6	0.46	0	305.99	308.94	14.26	5.30
1.6	-0.27	0.27	302.10	303.71	7.79	2.90
1.6	0.06	0.27	305.35	306.84	7.21	2.68
1.6	0.38	0.27	306.16	308.42	10.93	4.06
1.6	-0.27	-0.27	301.51	303.82	11.22	4.17
1.6	0.06	-0.27	305.06	307.66	12.60	4.68
1.6	0.38	-0.27	306.04	308.61	12.41	4.61
1.85	0.13	0	307.27	309.24	9.57	3.56
1.85	0.46	0	306.25	308.69	11.79	4.38
2.65	0.13	0	307.02	309.31	11.10	4.13
2.65	0.46	0	305.77	308.92	15.25	5.67
3.7	0.13	0	305.97	308.72	13.33	4.95
3.7	0.46	0	304.26	307.72	16.75	6.22
3.7	-0.27	0.27	301.78	303.19	6.85	2.54
3.7	0.06	0.27	303.01	306.25	15.73	5.85
3.7	0.38	0.27	304.86	307.69	13.67	5.08
3.7	-0.27	-0.27	301.63	303.27	7.98	2.96
3.7	0.06	-0.27	303.13	306.20	14.87	5.53
3.7	0.38	-0.27	304.85	307.78	14.19	5.27
3.95	0.13	0	306.08	306.15	0.35	0.13
3.95	0.46	0	305.49	307.42	9.37	3.48
4.43	0.13	0	304.06	306.37	11.19	4.16
4.43	0.46	0	305.21	307.21	9.69	3.60
4.43	-0.27	0.27	301.88	303.10	5.92	2.20
4.43	0.06	0.27	303.66	305.70	9.85	3.66
4.43	0.38	0.27	305.35	307.05	8.23	3.06
4.43	-0.27	-0.27	301.74	303.02	6.23	2.32
4.43	0.06	-0.27	303.59	305.63	9.90	3.68
4.43	0.38	-0.27	305.29	307.06	8.56	3.18
5.13	-0.46	0	300.36	301.17	3.93	1.46
5.13	0.13	0	303.92	305.82	9.21	3.42
5.13	0.46	0	304.45	306.85	11.62	4.32
5.83	-0.46	0	300.45	301.45	4.84	1.80
5.83	0.13	0	303.78	305.52	8.43	3.13
5.83	0.46	0	304.57	306.50	9.36	3.48
2.125	0.13	0	305.27	308.80	17.08	6.35
2.125	0.46	0	305.87	308.64	13.44	5.00

Table 10/13/05-3. Waste Package Temperature [Source: Fifth Scale Test Data 9-3-2004.xls]

	Test Temperature (°F)	Dry-75w		Dry-75w-rmesh	
		CFD Temperature (°F)	Difference (°F)	CFD Temperature (°F)	Difference (°F)
WP1	115.43	123.96	8.53	120.32	4.89
WP2	115.23	124.70	9.47	122.22	7.00
WP3	114.94	124.90	9.96	121.87	6.92
WP4	115.28	123.99	8.72	120.73	5.46

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10/14/05 – F.V.

CFD vs. Test Data Comparison – Case: Dry-75w-rmesh2

The simulation case 75w-rmesh2 has been finalized.
With a heat distribution of 75 watts on each waste package the total energy (250 watts) in the system is higher than for the other cases (200 watts). This increase in energy demands a more refined mesh to capture the convection phenomena. Table 10/14/05-1 shows the test and CFD results of the 75w-rmesh2 simulation together with the relative error as defined on 9/29/05 in this Scientific Notebook.

Table 10/14/05-1. Comparison of Average Temperature Values from Test and CFD Simulation at Different Points along the 1/5 Scale Model – Case: Dry-75w-rmesh2 [Source: Fifth Scale Test Data 9-3-2004.xls]

X	Z	Y	Avg. Test Temp. (K)	Avg. CFD Temp. (K)	Relative Error (%)	Abs. Diff. (°F)
0.55	0.13	0	306.94	309.62	12.96	4.81
0.55	0.46	0	305.39	308.04	12.81	4.76
1.6	0.13	0	307.61	309.89	11.04	4.10
1.6	0.46	0	305.99	308.84	13.76	5.11
1.6	-0.27	0.27	302.10	303.51	6.83	2.54
1.6	0.06	0.27	305.35	306.53	5.72	2.13
1.6	0.38	0.27	306.16	308.25	10.11	3.76
1.6	-0.27	-0.27	301.51	303.15	7.96	2.96
1.6	0.06	-0.27	305.06	307.10	9.90	3.68
1.6	0.38	-0.27	306.04	308.58	12.30	4.57
1.85	0.13	0	307.27	309.11	8.95	3.32
1.85	0.46	0	306.25	308.45	10.67	3.96
2.65	0.13	0	307.02	309.44	11.74	4.36
2.65	0.46	0	305.77	308.49	13.17	4.89
3.7	0.13	0	305.97	307.60	7.89	2.93
3.7	0.46	0	304.26	307.85	17.37	6.46
3.7	-0.27	0.27	301.78	303.11	6.47	2.40
3.7	0.06	0.27	303.01	305.59	12.51	4.65
3.7	0.38	0.27	304.86	307.80	14.21	5.28
3.7	-0.27	-0.27	301.63	302.72	5.31	1.97
3.7	0.06	-0.27	303.13	306.17	14.73	5.47
3.7	0.38	-0.27	304.85	307.72	13.89	5.16
3.95	0.13	0	306.08	306.28	0.96	0.36
3.95	0.46	0	305.49	307.30	8.78	3.26
4.43	0.13	0	304.06	305.74	8.17	3.04
4.43	0.46	0	305.21	307.09	9.13	3.39
4.43	-0.27	0.27	301.88	303.00	5.42	2.01
4.43	0.06	0.27	303.66	305.38	8.31	3.09
4.43	0.38	0.27	305.35	307.13	8.60	3.20
4.43	-0.27	-0.27	301.74	302.87	5.48	2.04
4.43	0.06	-0.27	303.59	305.48	9.16	3.40
4.43	0.38	-0.27	305.29	306.80	7.31	2.72
5.13	-0.46	0	300.36	300.86	2.41	0.90
5.13	0.13	0	303.92	305.40	7.14	2.65
5.13	0.46	0	304.45	306.51	9.97	3.71
5.83	-0.46	0	300.45	301.12	3.23	1.20
5.83	0.13	0	303.78	305.32	7.46	2.77
5.83	0.46	0	304.57	306.19	7.87	2.93
2.125	0.13	0	305.27	308.18	14.10	5.24
2.125	0.46	0	305.87	308.55	12.99	4.83

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Table 10/14/05-2. Waste Package Temperature – Case: Dry-75w-rmesh2 [Source: Fifth Scale Test Data 9-3-2004.xls]

	Test Temperature (°F)	CFD Temperature (°F)	Difference (°F)
WP1	115.43	119.22	3.79
WP2	115.23	121.25	6.03
WP3	114.94	120.84	5.90
WP4	115.28	119.89	4.62

10/19/05 – F.V.

Comparison of Measured Temperatures and CFD Results for Cases: Dry-75w; Dry-75w-rmesh and Dry-75w-rmesh2

Figure 10/19/05-1 shows the relative error at the different points along the drift. The errors obtained with the coarse mesh (Dry-75w) go from -1% through 23% while the range of relative error for the cases with refined mesh (Dry-75w-rmesh and Dry-75w-rmesh2) is about the same, between 0% and 15%.

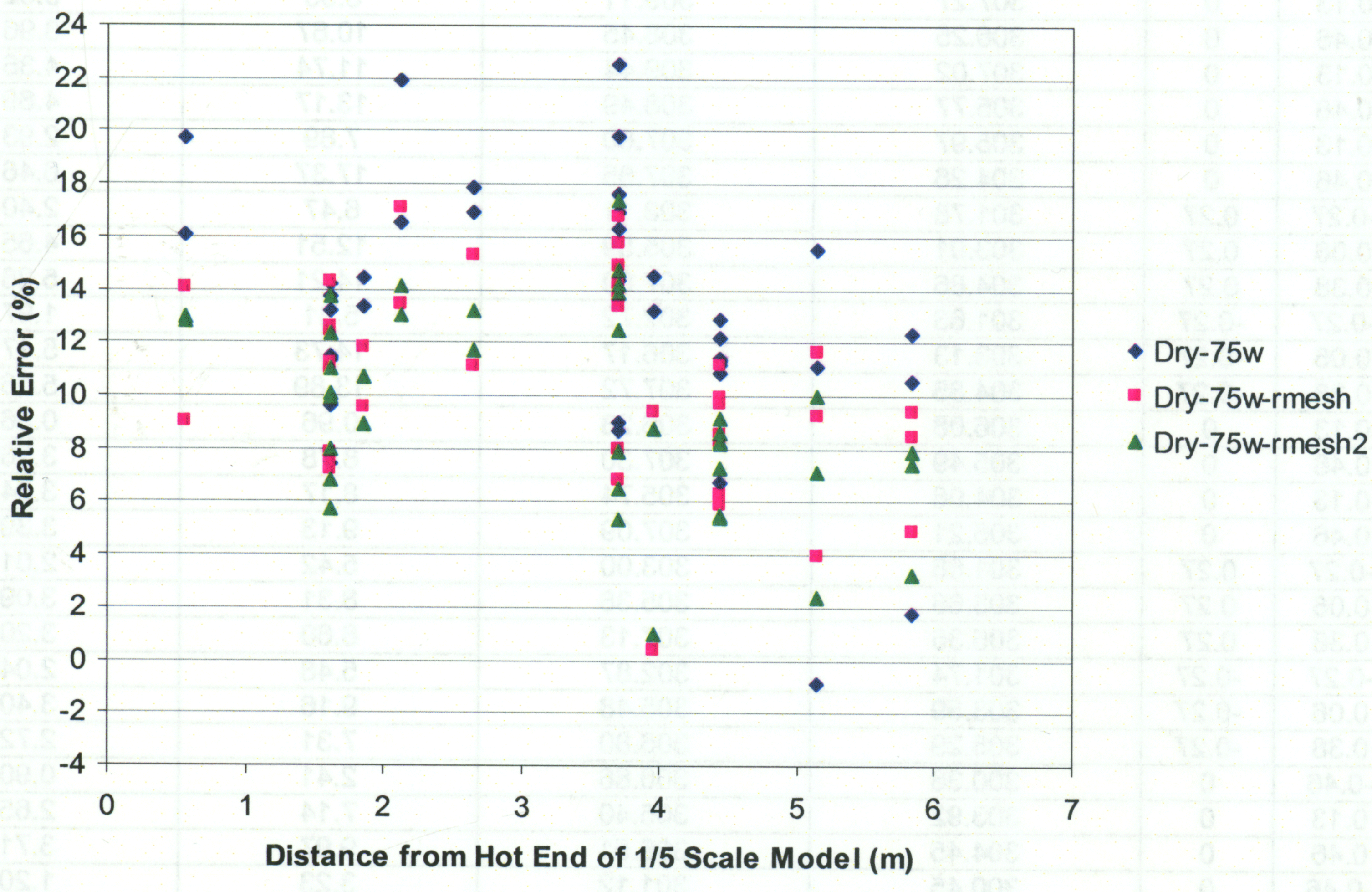

Figure 10/19/05-1. Relative Error Distribution along the 1/5 Scale Model – Cases: Dry-75w; Dry-75w-rmesh; Dry-75w-rmesh2 [Source: Fifth Scale Test Data 9-3-2004.xls]

Since the numerical results with both refined meshes give about the same error; the mesh with less cells from these two should be used in order to reduce computational time.

Figure 10/19/05-2 shows the temperature profile along the drift. The average temperatures at ten cross sections along the pipe are plotted as a function of the distance. The numerical results with the three different meshes are plotted together with the average of the measured values. All three lines of the CFD results follow the trend of the experimental line.

As can be noticed from Figure 10/19/05-2, the numerical results with the two refined meshes (Dry-75w-rmesh and Dry-75w-rmesh2) are very close to one another. The maximum temperature difference between these two lines is about 0.65°F. It shows again that the mesh used in the case Dry-75w-rmesh is as accurate as the one use in case Dry-75w-rmesh2, with the advantage of running faster.

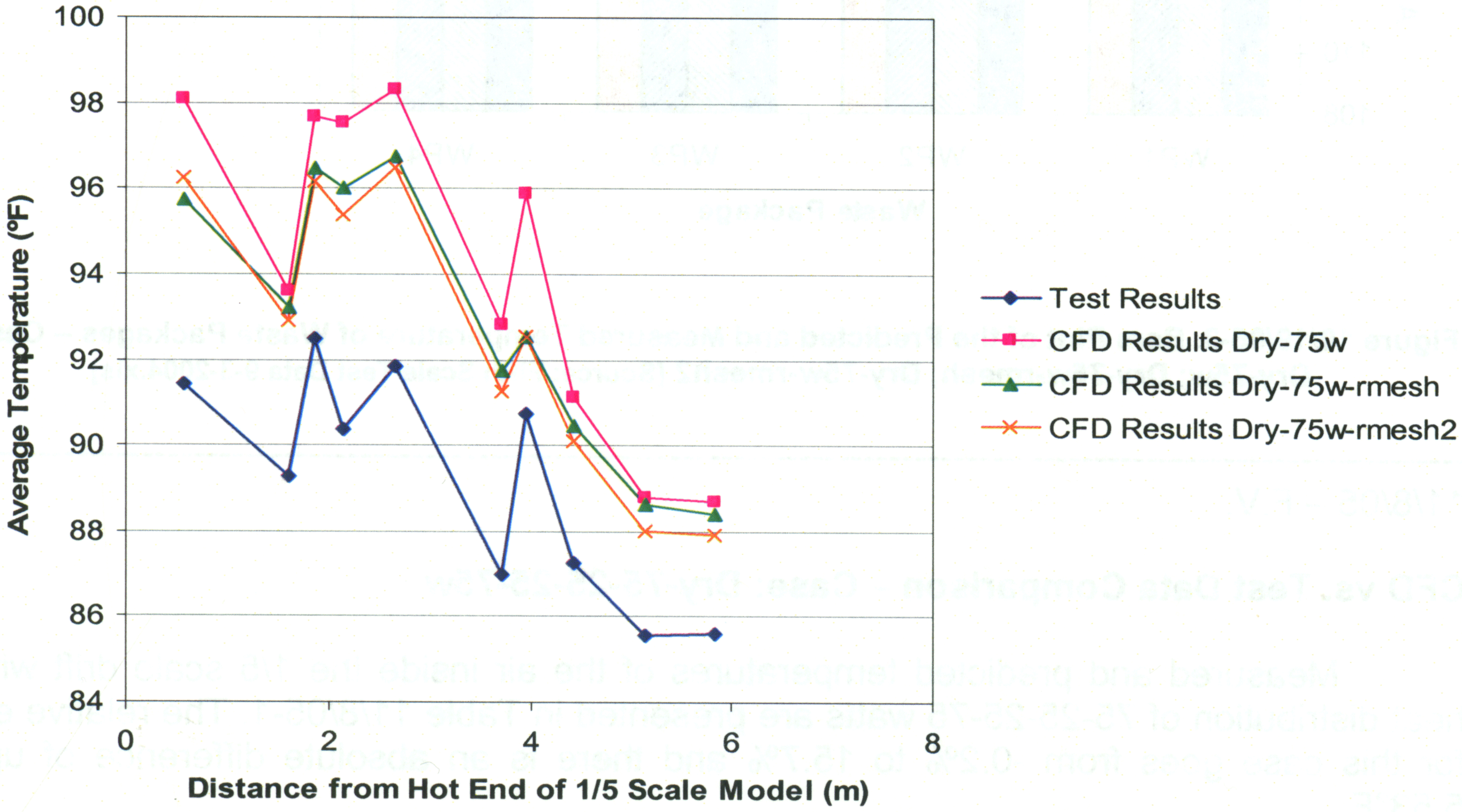

Figure 10/19/05-2. Average temperature at Different Cross Sections along the Pipe – Cases: Dry-75w; Dry-75w-rmesh; Dry-75w-rmesh2 [Source: Fifth Scale Test Data 9-3-2004.xls]

Figure 10/19/05-3 shows the average temperature of the waste packages from measurements, and from the three numerical results with different mesh sizes. In any case the predicted values are higher than the measured ones. There is a significant difference (up to 10°F) between the results from the case Dry-75w and measured values.

The maximum difference between the numerical results Dry-75w-rmesh and Dry-75w/rmesh2 is about 1°F; between Dry-75w-rmesh and test results is 7°F; and between Dry-75w-rmesh2 and test results is about 6°F.

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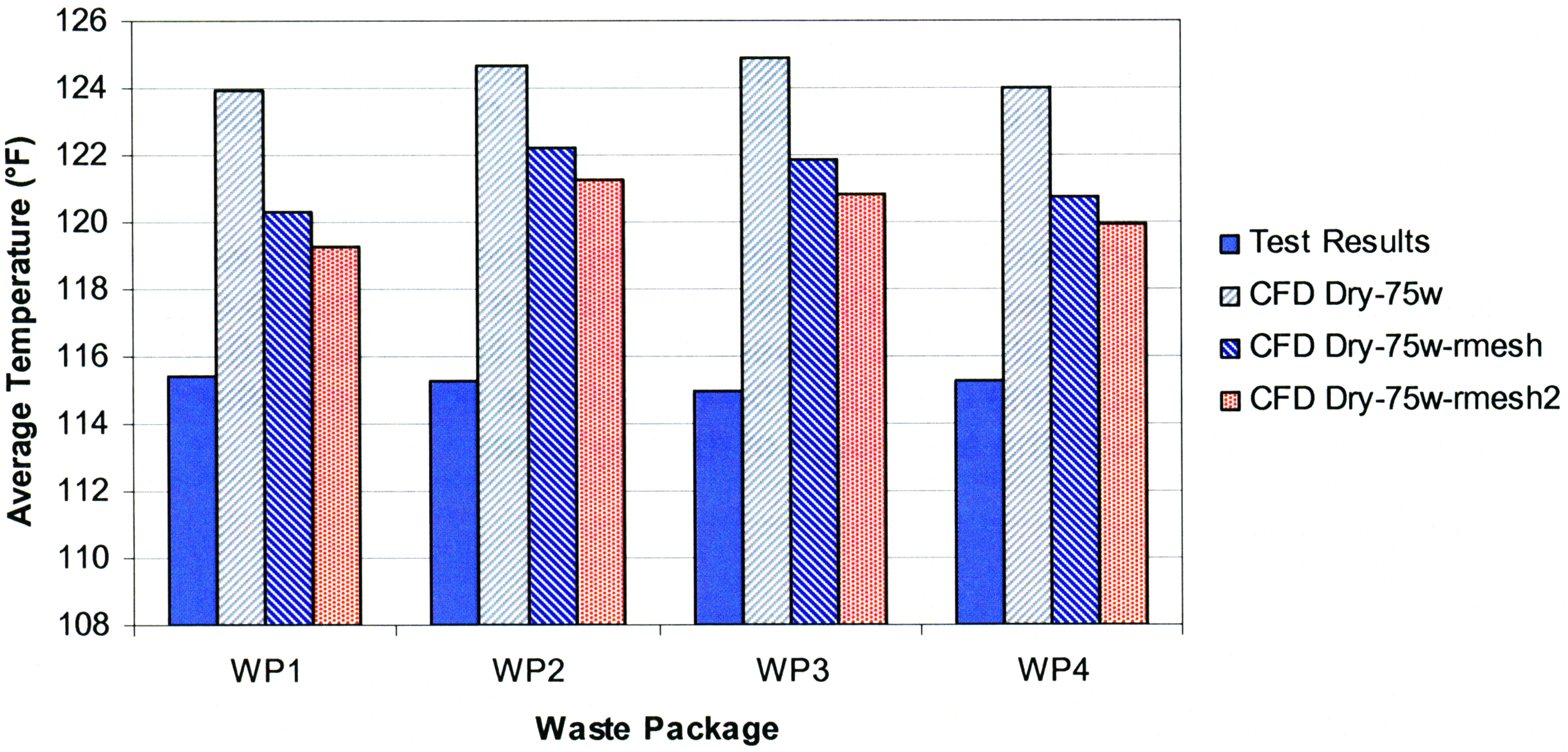

Figure 10/19/05-3. Bars Plot of the Predicted and Measured Temperature of Waste Packages – Cases: Dry-75w; Dry-75w-rmesh; Dry-75w-rmesh2 [Source: Fifth Scale Test Data 9-3-2004.xls]

11/8/05 – F.V.

CFD vs. Test Data Comparison – Case: Dry-75-25-25-75w

Measured and predicted temperatures of the air inside the 1/5 scale drift with a heat distribution of 75-25-25-75 watts are presented in Table 11/8/05-1. The relative error for this case goes from -0.2% to 15.7% and there is an absolute difference of up to 5.53°F.

Table 11/8/05-1. Comparison of Average Temperature Values from Test and CFD Simulation at Different Points along the 1/5 Scale Model – Case: Dry-75-25-25-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

X	Z	Y	Avg. Test Temp. (K)	Avg. CFD Temp. (K)	Relative Error (%)	Abs. Diff. (°F)
0.55	0.13	0	305.85	307.6	8.73	3.1
0.55	0.46	0	304.14	306.6	12.39	4.4
1.6	0.13	0	303.15	304.7	8.03	2.8
1.6	0.46	0	302.54	304.7	11.02	3.9
1.6	-0.27	0.27	300.56	301.4	4.24	1.5
1.6	0.06	0.27	302.67	304.2	7.95	2.8
1.6	0.38	0.27	303.32	304.8	7.43	2.6
1.6	-0.27	-0.27	299.99	301.4	7.10	2.5
1.6	0.06	-0.27	302.52	304.1	7.96	2.8
1.6	0.38	-0.27	303.21	304.6	7.04	2.5
1.85	0.13	0	303.02	304.1	5.41	1.9
1.85	0.46	0	302.60	304.3	8.68	3.1
2.125	0.13	0	302.30	304.3	10.00	3.5
2.125	0.46	0	301.98	304.2	11.22	4.0
2.65	0.13	0	302.90	304.3	7.27	2.6
2.65	0.46	0	302.09	304.0	9.82	3.5
3.7	0.13	0	304.63	307.2	12.98	4.6
3.7	0.46	0	302.73	305.8	15.65	5.5
3.7	-0.27	0.27	300.35	301.1	3.86	1.4
3.7	0.06	0.27	301.18	303.2	10.22	3.6
3.7	0.38	0.27	302.70	305.3	13.33	4.7

3.7	-0.27	-0.27	300.22	301.2	5.06	1.8
Continuation of Table 11/8/05-1						
X	**Z**	**Y**	**Avg. Test Temp. (K)**	**Avg. CFD Temp. (K)**	**Relative Error (%)**	**Abs. Diff. (°F)**
3.7	0.06	-0.27	301.20	303.1	9.83	3.5
3.7	0.38	-0.27	302.73	305.4	13.44	4.8
3.95	0.13	0	304.00	305.8	8.93	3.2
3.95	0.46	0	303.57	305.3	8.64	3.1
4.43	0.13	0	301.87	303.4	7.87	2.8
4.43	0.46	0	303.06	304.6	7.89	2.8
4.43	-0.27	0.27	300.30	300.9	2.98	1.1
4.43	0.06	0.27	301.63	303.1	7.63	2.7
4.43	0.38	0.27	303.10	304.7	8.16	2.9
4.43	-0.27	-0.27	300.19	301.0	4.09	1.4
4.43	0.06	-0.27	301.57	303.0	7.46	2.6
4.43	0.38	-0.27	303.02	304.5	7.51	2.7
5.13	-0.46	0	299.15	299.1	-0.19	0.1
5.13	0.13	0	301.86	303.3	7.46	2.6
5.13	0.46	0	302.36	304.2	9.42	3.3
5.83	-0.46	0	299.21	299.2	0.11	0.0
5.83	0.13	0	301.73	303.0	6.61	2.3
5.83	0.46	0	302.42	304.0	7.95	2.8

Average values of the measured and predicted temperatures of the waste packages are shown in Table 11/8/05-2. The difference between predicted and measured varies between 4.3°F and 6.9°F.

Table 11/8/05-2. Waste Package Temperature – Case: Dry-75-25-25-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

	Test Temperature (°F)	CFD Temperature (°F)	Difference (°F)
WP1	112.15	119.07	6.92
WP2	93.71	98.30	4.58
WP3	94.12	98.44	4.31
WP4	112.61	118.98	6.38

11/16/05 – F.V.

Running Simulations with Moisture Model

To start the CFD analysis with the new moisture model the simulation file **prepin.Dry50b** would be modified. Some of the changes include:

- Modify the geometry of the waste package "A" that is located closer to the hot end. The modification consists of creating separate obstacles for about ¼ of the upper part of the horizontal cylinder and another obstacle for the rest of the waste package. This is necessary to specify the region where water is injected.
- Fluid Properties
- Boundary conditions obtained from experimental data contained in file **Fifth Scale Test Data 2-6-2005.xls.**

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11/17/05 – F.V.

CFD vs. Test Data Comparison – Case: Dry-75-25-25-75w

Figure 11/17/05-1 shows the relative error distribution along the 1/5 scale drift, that varies between about 0% and 16%.

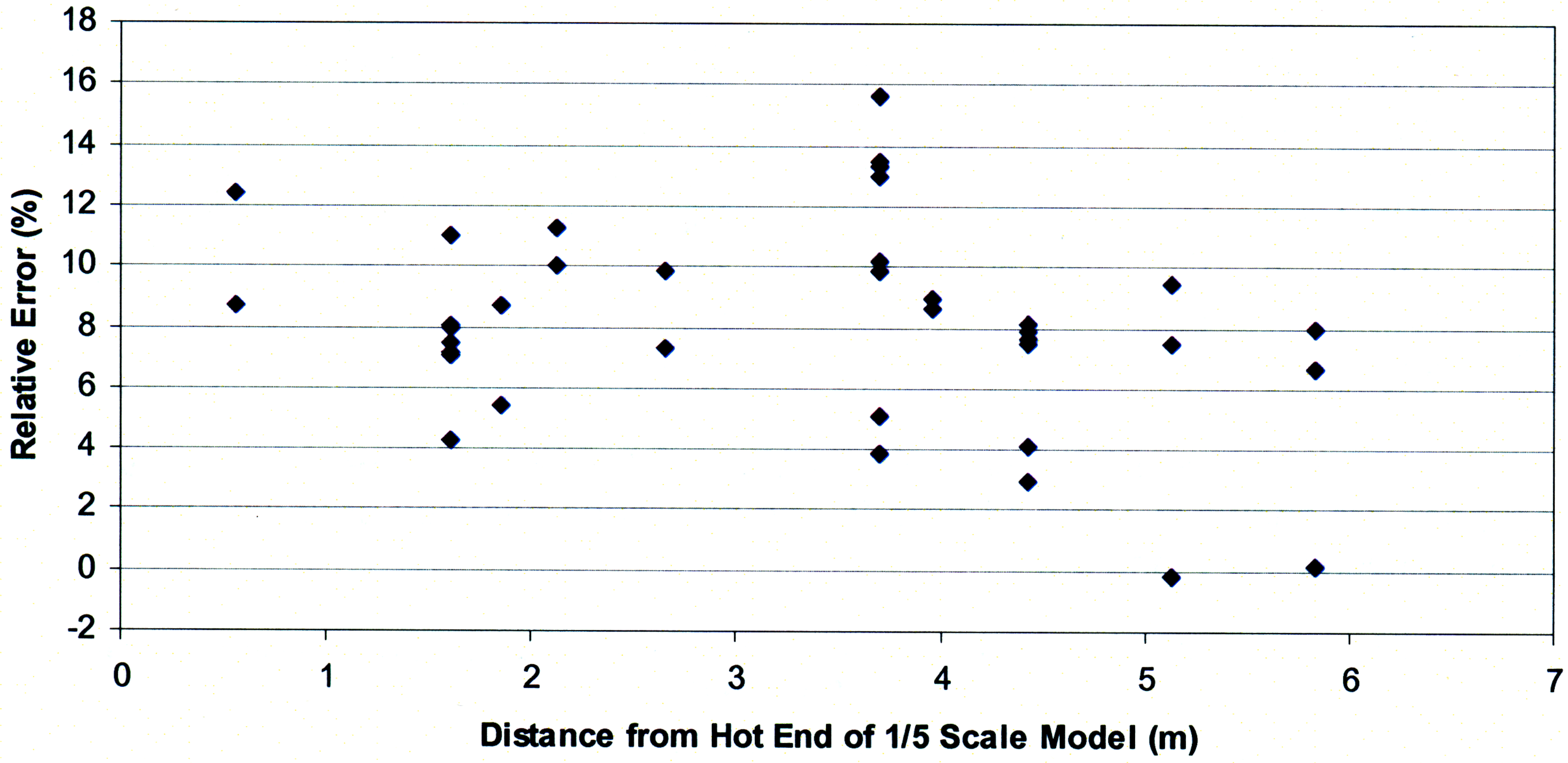

Figure 11/17/05-1. Relative Error Distribution along the 1/5 Scale Model – Case: Dry-75-25-25-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

Figure 11/17/05-2 shows the average temperature at ten cross sections along the pipe. The CFD results follow the same trend as that of the test results, except at x=2.125m.

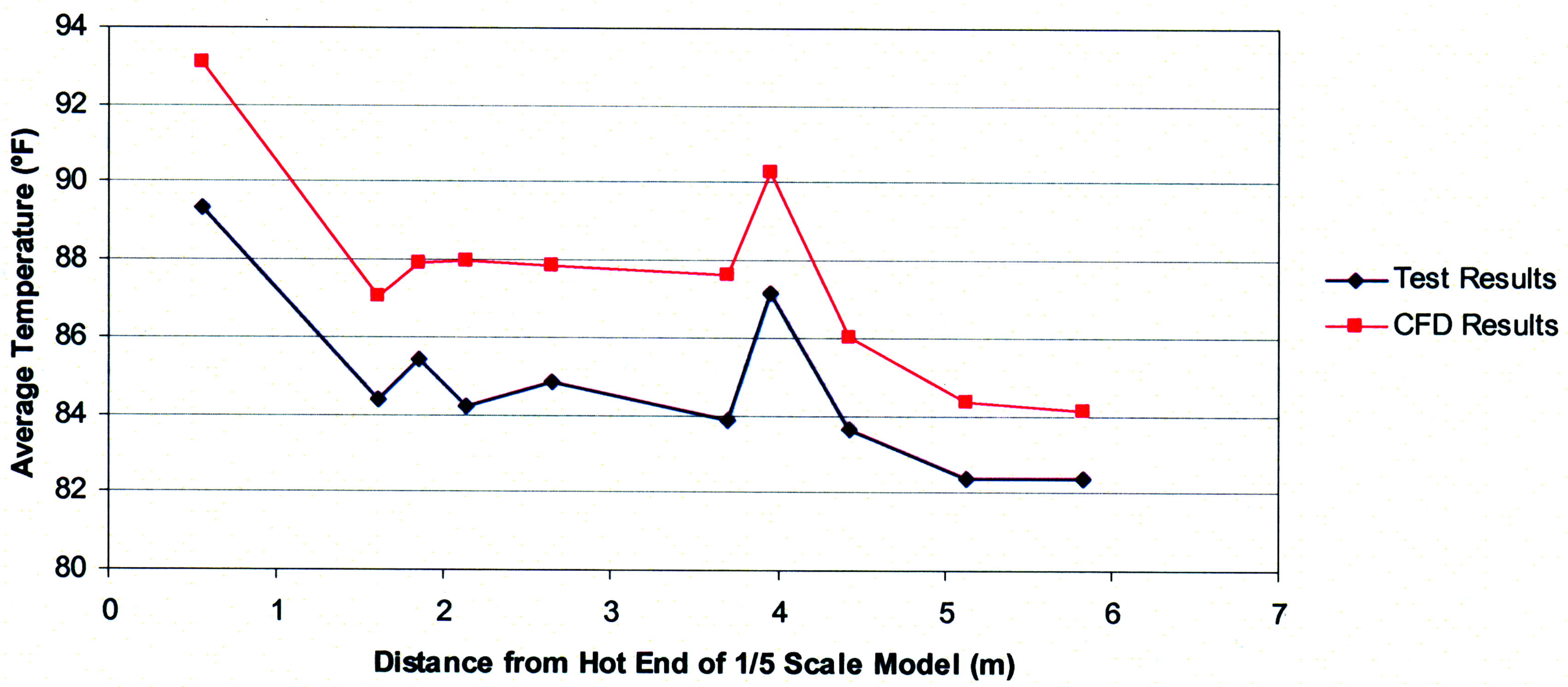

Figure 11/17/05-2. Average temperature at Different Cross Sections along the Pipe – Case: Dry-75-25-25-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

Figure 11/17/05-3 is the graphical representation of the difference between the predicted and measured waste package temperature. The predicted temperature is up to 6.9°F higher than the measured value.

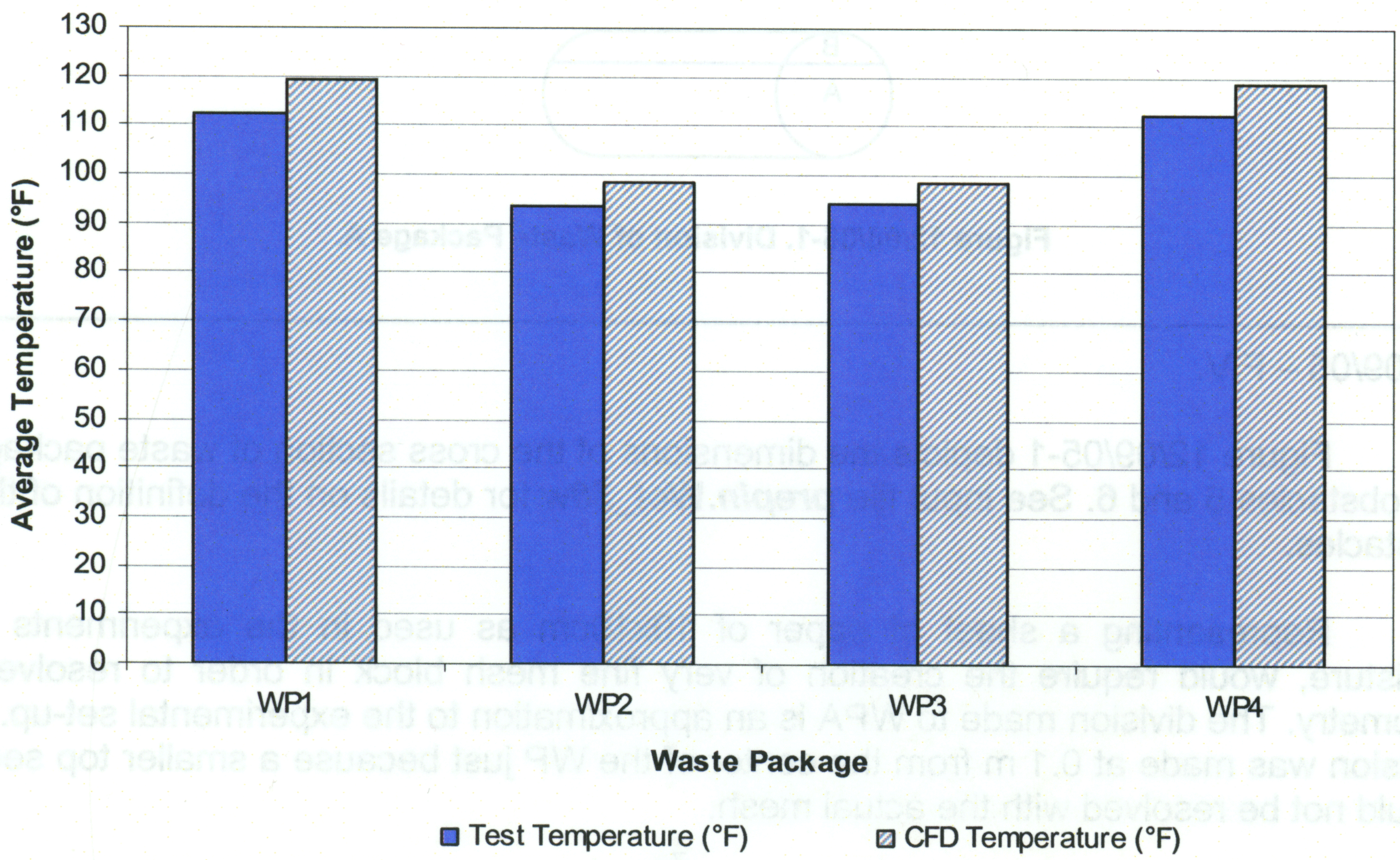

Figure 11/17/05-3. Bars Plot of the Predicted and Measured Temperature of Waste Packages – Case: Dry-75-25-25-75w [Source: Fifth Scale Test Data 9-3-2004.xls]

12/08/05 – F.V.

1/5-scale Drift CFD Simulations with Moisture Transport Model

The following entries correspond to the set-up of the input file to be used in the runs with the new version of FLOW-3D that includes moisture transport calculations. The results from this simulations would be compared with the results obtained in the 1/5 scale drift for the cases where water was added.

As explained on SN616 page 58, the water is added to the system from the drift wall over the waste package A (WPA; the one closest to the hot end wall); by dripping water directly over a 10x10 cm sheet of paper located on top and at the center of the WPA.

The moisture transport model requires the number(s) of the obstacle(s) that contains and gives water. In order to better represent the experimental conditions, the obstacle that defines the WPA in the input file must be changed. Instead of one, two obstacles should be defined. One would represent the top of WPA where water is being added and the other one would represent the bottom part.

--END OF PAGE--

Figure 12/08/06-1 depicts the division of the original obstacle No. 5 in sections A (bottom of waste package) and B (top of waste package). In the new input file (***prepin.Wet_50w***) these two sections correspond to obstacles 5 and 6 respectively.

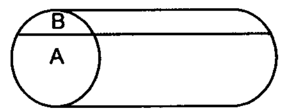

Figure 12/08/06-1. Division of Waste Package A.

12/09/05 – F.V.

Figure 12/09/05-1 depicts the dimensions of the cross section of waste package A or, obstacles 5 and 6. See input file ***prepin.Wet_50w*** for details on the definition of these obstacles.

Representing a sheet of paper of 10x10cm as used in the experiments with moisture, would require the creation of very fine mesh block in order to resolve the geometry. The division made to WPA is an approximation to the experimental set-up. The division was made at 0.1 m from the center of the WP just because a smaller top section would not be resolved with the actual mesh.

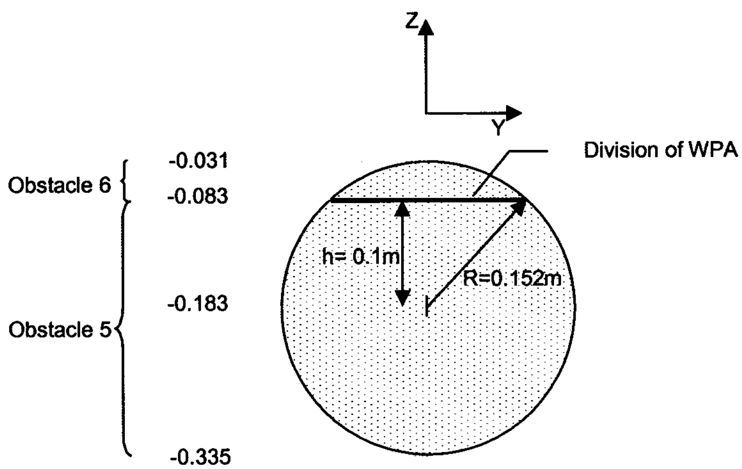

Figure 12/09/05-1. Cross Section of Obstacles 5 and 6 Representing WPA.

01/05/06 – F.V.

Calculation of Heat Rate on Obstacles 5 and 6

The 50 watts originally assigned to waste package A must be multiplied by the volume fraction of obstacles 5 and 6. The total volume of WPA represented by a cylinder of 0.152m radius and 1 m long is:

$V_T = \pi r^2 l = 0.0726 m^3$

The volume obstacle 6 is calculated as follows:

$$V_6 = \frac{1}{2} r^2 (\theta - \sin\theta) l \,,$$

where: $\theta = 2\arccos\left(\frac{h}{r}\right) = 2\arccos\left(\frac{0.1}{0.152}\right) = 1.706$.

Substituting θ into V_6 yields:

$$V_6 = \frac{1}{2}\left(0.152^2\right)\left(1.706 - \sin 1.706\right)(1) = 0.008255 m^3$$

The fraction of the volume of the waste package A represented by obstacles 6 (X_6) and 5 (X_5) are computed as follows:

$$X_6 = \frac{V_6}{V_T} = \frac{0.008255}{0.0726} = 0.113735$$

$$X_5 = 1 - X_6 = 0.886265$$

In turn, the amount of energy assigned to obstacles 5 and 6 is calculated.

$$\boxed{Q_5 = 0.886265(50 watts) = 44.31 watts}$$

$$\boxed{Q_6 = 0.113735(50 watts) = 5.69 watts}$$

01/10/06 - F.V.

See new input file ***prepinr.Wet_50w*** for a list of scalar functions and user defined parameters that must be entered in order to predict the moisture redistribution using FLOW-3D with the added moisture transport model.

02/03/06 – F.V.

The second case to be simulated is the one with a heat rate distribution of 75-25-25-75 watts on WPA-WPD respectively.

The geometry definition would be the same one used on ***prepinr.Wet_50w***. The heat rate for obstacles 5 and 6 in this case are calculated as follows:

$$\boxed{Q_5 = 0.886265(75 watts) = 66.47 watts}$$

$$\boxed{Q_6 = 0.113735(75 watts) = 8.53 watts}$$

03/27/06 – F.V.

The input file for a heating rate of 75-25-25-75 watts with moisture is ***prepinr.Wet_75-25-25-75***. See this file for a complete list of entries.

03/29/06 – F.V.

CFD Simulations with Moisture and Radiation Models

The input file ***prepinr.Wet_50w*** was used as a starting point since it contains all the parameters required to run the moisture transport model. The new input file is named ***prepin.Wet+Rad_50w.***

The first step to incorporate radiation heat transfer into the calculations is to define the radiation surfaces. FLOW-3D does not allow for the selection of surfaces, only obstacles can be assigned properties and boundary conditions. The radiation subroutine recently added to FLOW-3D accounts for the definition of the surfaces that would participate in the radiation process.

The number of radiation surfaces for each obstacle was assigned as follows:

Table 03/29/06. Radiation Surfaces per Obstacle

Obstacle Number and Description	Number of Radiation Surfaces
Obstacle 2 – Drift Wall	52
Obstacle 3 – Hot End Wall	4
Obstacle 4 – Cold End Wall	2
Obstacle 5 – Bottom Part of WPA	12
Obstacle 6 – Top Part of WPA	12
Obstacle 7 – WPB	24
Obstacle 8 – WPC	24
Obstacle 9 – WPD	24
Total Radiation Surfaces	**154**

--END OF PAGE--

03/30/06 – F.V.

Limits of Radiation Surfaces

Low and high values of the radiation surface limits in the x, y and z directions should be determined. This operation would be done by obstacle, by assigning limits to the each of the radiation surfaces indicated on the right column of Table 03/29/06.

The surface of the hot end wall would be divided in 4 equal-size surfaces and the cold end wall is divided horizontally in two pieces. The inner surface of the drift wall would be cut in 13 cross sections and each cross section is divided in four. These 13 cross sections would be limited by the following x-locations:

Surface	xl	xh
1	0	0.441
2	0.441	0.882
3	0.882	1.323
4	1.323	1.764
5	1.764	2.205
6	2.205	2.646
7	2.646	3.087
8	3.087	3.528
9	3.528	3.969
10	3.969	4.41
11	4.41	5.11
12	5.11	5.81
13	5.81	6.51

The surface of the four waste packages would be divided in six cross sections. The first and last divisions are located very close to the edges in an attempt to capture the area of the circles at both ends of the cylindrical object. The rest of the body is divided in another four equally spaced slices.

For a complete list of the radiation surface limits, see the input file ***prepin.Wet+Rad_50w***.

03/31/06 – F.V.

The run of the input file ***prepin.Wet+Rad_50w*** failed due to pockets or abnormal fluid trapped into two solid obstacles. To avoid this from happening touching obstacles have been overlapped. The length of the drift wall (obstacles 2) was slightly increased (zl(2)=-0.01, zh(2)=6.520) to overlap the hot and cold end wall (obstacles 3 and 4 respectively)

After a close look at the contact between the bottom and top parts of waste package A, no fluid pockets were observed indicating that overlapping of obstacles 5 and 6 is not necessary.

04/13/06 – F.V.

The latest version of the combined moisture-radiation model is been used. The executable files are hydr3d_rad_pcg_4-13-06.exe and prep3d_rad_pcg_4-13-06.exe. This new version contains a check-terminate sentence that allows to detect possible problems on the radiation surfaces by writing out the number of surface where and error is encountered and closing the check file.

A run was started at 3:16pm and terminated with an error on surface 58 at 8:06pm. This indicates that it took 4 hours 50 minutes for the program to compute the surface area of at least 57 surfaces.

04/14/06 – F.V.
Start running simulation with input file ***prepin.Wet+Rad_50w*** at 8:19am.

04/18/06 – F.V.
The current run started on 04/14/06 has been running for about 4 days and 7 hours and has not finished yet. It indicates that is still in progress.

04/24/06 – F.V.

The run started on 04/14/06 with input file ***prepin.Wet+Rad_50w*** has terminated due to the large amount of time that was taking just to compute the configuration factors for the radiation surfaces. Steve Green made some changes to the radiation module that resulted in a significant reduction of computational time. He was able to obtain the configuration factor for the input file ***prepin.Wet+Rad_50w*** in 5.5 hours.

The file ***Check_rad.Wet+Rad_50w_stg*** contains the surface area and configuration factor of each one of the 154 radiation surfaces. These values will be verified by opening the result file in MS Excel and performing simple arithmetic calculations to compare with.

05/02/06 – F.V.

Simulations with Moisture Model

The cases with uniform (50w) and non-uniform heating (75-25-25-75w), running with the FLOW-3D version that includes the moisture transport model have been taking very long time and have not yet reached steady state at least in moisture redistribution. In order to speed up the solution, a coarser mesh will be used. The actual mesh for both cases has 912,000 cells (250x; 57y; 64z) and the new coarse mesh has 172,140 cell (151x; 30y ;38;). For more details, see entries made in input files ***prepinr.Wet_50w_B*** and ***prepinr.Wet_75-25-25-75_B.***

--END OF PAGE--

05/03/06 – F.V.

In order to verify that the data from a coarse mesh can be overlayed on the fine mesh, the input file ***prepinr.Wet_50w_B1*** has been created. In this input file the mesh use has 250x; 57y; 64z elements and was restarted using the results file ***flsgrf.Wet_50w_B*** (696-813 sec) obtained with the coarse mesh (155x; 30y; 38z). The file restarted successfully.

05/04/06 – F.V.

Another coarse mesh would be used that is scalable with the fine mesh, it has 30% less cells in each Cartesian direction (175x; 40y; 45z), which represents a reduction of 67% in the total number of cells (172,140 cells in total). For more details, see entries made in input files ***prepinr.Wet_75-25-25-75_C*** and ***prepin.Wet+Rad_50w_B***.

The fluid properties used for the 1/5 scale simulations that have been entered in the past were verified and the following table shows a summary of all fluid properties been used, their current value and the valued I have found and its corresponding source.

Table 05/04/06. Properties of Air, Moist Air and Liquid Water Used in CFD Simulations

Description	FLOW-3D Parameter & Assigned Value	Parameter Value / Source
Dry Air Specific Heat (const. vol.) at 300 K and atmospheric pressure	cv1=717.7	717.7 J/kg K / Handbook of tables for Applied Engineering Science, 2nd edition 1973, Table 1-2
Dry Air Density at 300 K and atmospheric pressure	rhof=1.177	1.177 kg/m^3
Dry Air Conductivity at 300 K and atmospheric pressure	thc1=0.02624	0.02624 W/m K
Dry Air Thermal Expansion Coefficient (1/T) with T= 300 K	thexf1=3.33e-03	
Dry Air Viscosity	mu1=1.846e-05	18.46e-05 N.s/m^2
Heat of Vaporization or Latent Heat of Evaporation of Water	hvvap_stg = 2300000.	2,260,000 J/kg at 300 K and 101,325 N/m^2 Handbook of tables for Applied Engineering Science, 2nd edition 1973, Table 1-46
Water vapor specific heat (const. vol.)	cvvap_stg = 1411.	1,402.34 J/kg.K at 300K Handbook of tables for Applied Engineering Science, 2nd edition 1973, Table 1-5
Water liquid specific heat (const. vol.)	cvliq_stg = 4186.	4180 J/kg.K at 300 K and 101,325 N/m^2 Handbook of tables for Applied Engineering Science, 2nd edition 1973, Table 1-46
Gas constant for water vapor	rvap_stg = 416.	461.51 J/kg.K Handbook of tables for Applied Engineering Science, 2nd edition 1973, Table 1-5
Gas constant for air	rgas_stg = 289.	286.8 J/kg.K Handbook of tables for Applied Engineering Science, 2nd edition 1973, Table 1-14

05/08/06 – F.V.

Summary of Input and Results Files to Date

Table 05/08/06_1. Summary of Files for CFD Simulations with Vapor Calculations

FLOW-3D Executable File	Input File	Results Files	Mesh
hydr3d_vapor_11-4-05.exe prep3d_vapor_11-4-05.exe	prepin.Wet_50w	flsgrf.Wet_50w_t0-10	(250x; 57y; 64z)
"	prepinr.Wet_50w	flsgrf.Wet_50w_t10-93 flsgrf.Wet_50w_t93-119 flsgrf.Wet_50w_t119-150 flsgrf.Wet_50w_t150-172 flsgrf.Wet_50w_t172-300 flsgrf.Wet_50w_t300-398 flsgrfr.Wet_50w (398-666 sec)	"
"	prepinr.Wet_50w_B	flsgrf.Wet_50w_R_t398-666 flsgrf.Wet_50w_B_t666-696 flsgrfr.Wet_50w_B (696-813 sec)	(155x; 30y; 38z)
"	prepinr.Wet_50w_B1	flsgrf.Wet_50w_R50wB_t696-813 flsgrfr.Wet_50w_B1	(250x; 57y; 64z)
"	prepinr.Wet_50w_C	flsgrf.Wet_50w_RB1_t813-1004 flsgrf.Wet_50w_C_T1004-1015 flsgrfr.Wet_50w_C	(175x;40y;45z)
	prepin.Wet_50w_D		(175x;40y;45z) RHi=80% Frozen flow field
	prepinr.Wet_50w_D	NONE	(175x;40y;45z)
	prepinr.Wet_50w_E	NONE	(250x; 57y; 64z)
ydr3d_vapor_3-21-06.exe prep3d_vapor_3-21-06.exe	prepinr.Wet_75-25-25-75	flsgrf.Wet_75-25-25-75_R50w_t150 flsgrf.Wet_75-25-25-75_t150-160 flsgrf.Wet_75-25-25-75_t160-165 flsgrf.Wet_75-25-25-75_t165-200 flsgrf.Wet_75-25-25-75_t200-216 flsgrf.Wet_75-25-25-75_t216-248 flsgrf.Wet_75-25-25-75_t248-352 flsgrf.Wet_75-25-25-75_t352-372 flsgrf.Wet_75-25-25-75_t372-382 flsgrf.Wet_75-25-25-75 (382-397 sec)	(250x; 57y; 64z)
hydr3d_vapor_3-21-06.exe prep3d_vapor_3-21-06.exe	prepinr.Wet_75-25-25-75_B		(154x; 30y; 38z)
	prepinr.Wet_75-25-25-75_C		
	prepin.Wet_75-25-25-75_C		

None of the results files listed in Table 05/08/06_1 corresponds to steady state condition and are considered preliminary.

05/10/06 – F.V.

Table 05/10/06_1. Summary of Files for CFD Simulations with Vapor and Radiation Calculations

FLOW-3D Executable File	Input File	Results Files	Mesh
hydr3d_rad_pcg_4-13-06.exe prep3d_rad_pcg_4-13-06.exe	prepin.Wet+Rad_50w	Check_rad.Wet+Rad_50w_stg	(250x; 57y; 64z)
hydr3d_rad_pcg_5-10-06.exe prep3d_rad_pcg_5-10-06	prepinr.Wet+Rad_50 w_B	flsgrf.Wet+Rad_50w_R50wVa pOnly_t1004-1015 flsgrfr.Wet+Rad_50w_B (1015-running)	(175x;40y;45z)

See prepin.* files for additional inputs.

06/01/06 – F.V.

Simulations with Moisture Model

New executables with moisture and radiation modules are available:

hydr3d_pcg_rad_6-7-06.exe
prep3d_pcg_rad_6-7-06.exe

All previous simulations with moisture are preliminary.

06/07/06 – F.V.

Simulations with Moisture Model

In order to restart the simulation with moisture, using the results obtained for dry air a small subroutine was written by Steve Green to initialize the pressure and bring all conditions to a stage where the moisture calculations can be performed without conflicts. This subroutine is only available in a version of the executables named: hydr3d_5-12-06_pshift.exe.

Using the new results file with the initialized pressure, the run for the case with uniform heating (50w each WP) is restarted using the latest version of the flow-3d executable files also the case with non uniform heating was restarted in the same way.

See the files: prepinr.Moist+Rad_50w and prepinr.Moist+Rad_75-25-25-75w, for details on the simulation.

Note: ALL other prepin files for the simulation with moisture should be disregarded since they were used to debug the new version of the flow-3d executable files with the added moisture and radiation models and to refine the final input files.

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06/08/06 – F.V.

Location of Temperature Sensors for the Dry Tests

Ten cross sections along the 20-percent drift test model were selected for the positioning of thermocouples. The distance from the hot end wall to each one of these cross sections are shown in Figure 06/08/06-1. Table 06/08/06-1 summarizes the nomenclature used to identify each cross section and the distance in the x-direction given in meters.

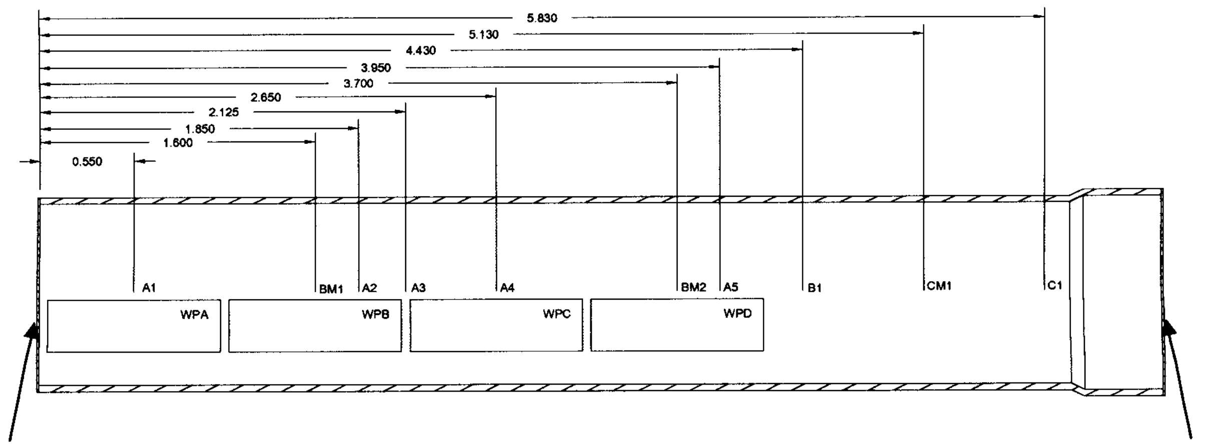

Figure 06/08/06-1. Schematic of the longitudinal cross section of the 20-percent scale experimental drift model.

The location of each thermocouple at each one of the ten cross sections is shown in the schematics presented in Figures 06/08/06-2 and 06/08/06-3. The location of the thermocouples on the surface of the waste package and on the hot and cold end walls is also shown on figure 06/08/06-3.

Table 06/08/06-1. Nomenclature and location ten cross sections of the 20-percent scale drift test model.

Cross Section	Distance from Hot End Wall (m)
A1	0.550
BM1	1.600
A2	1.850
A3	2.125
A4	2.650
BM2	3.700
A5	3.950
B1	4.430
CM1	5.130
C1	5.830

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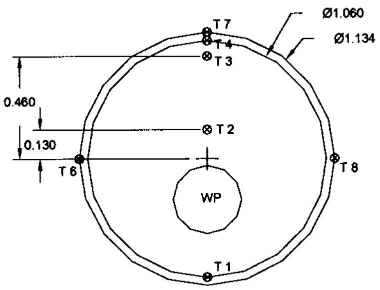
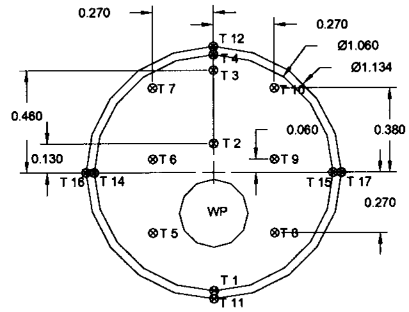
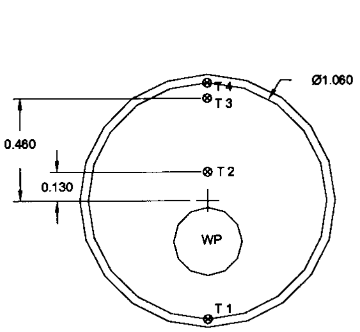


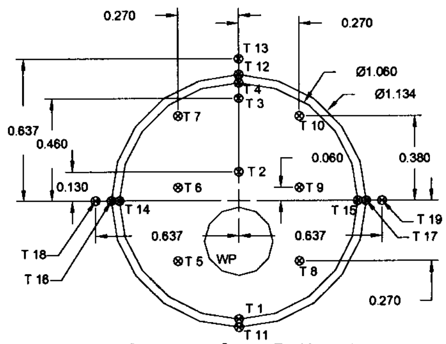
Temperature Sensor Positions at
Location A1



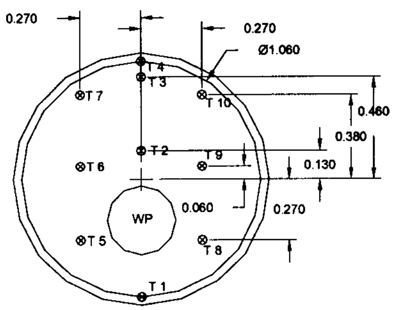
Temperature Sensor Positions at
Location BM1



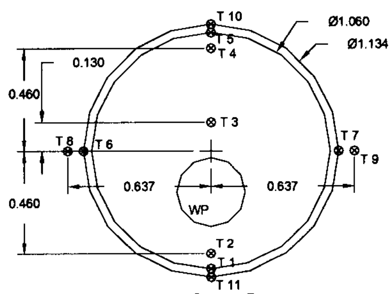
Temperature Sensor Positions at
Locations A2, A3, A4, and A5



Temperature Sensor Positions at
Location BM2



Temperature Sensor Positions at
Location B1



Temperature Sensor Positions at
Location CM1

Figure 16/18/06-2. Location of thermocouples at different cross sections of the 20-perfent scale drift test model.

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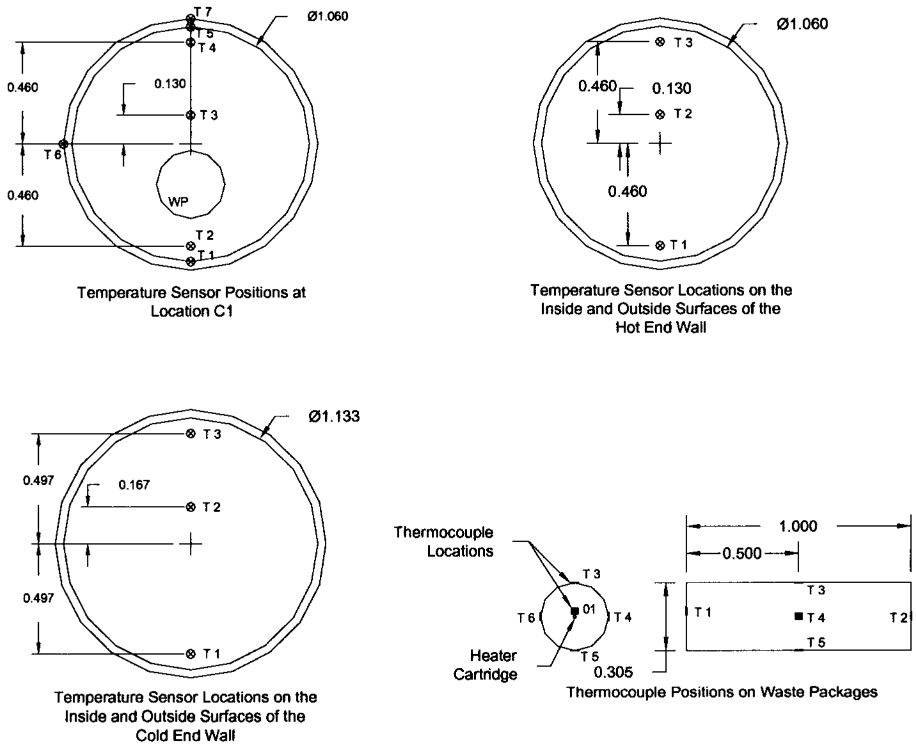

Figure 16/18/06-3. Location of thermocouples at cross section C1, hot end wall, cold end wall and on the waste package.

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4/11/2008

Location of Temperature Sensors for the Moist Tests

Eight of the ten cross sections selected for the location of temperature sensors during the dry tests were maintained during the moist tests. Changes made to the number and location of temperature sensors for the moist tests are indicated in Figures 06/08/06-4 and 06/08/06-5. The set of sensors located at cross sections A2 and A5 were all eliminated (Fig. 06/08/06-4). Some thermocouples were replaced by thermistors and some additional thermistors were added about ½" apart from thermocouples.

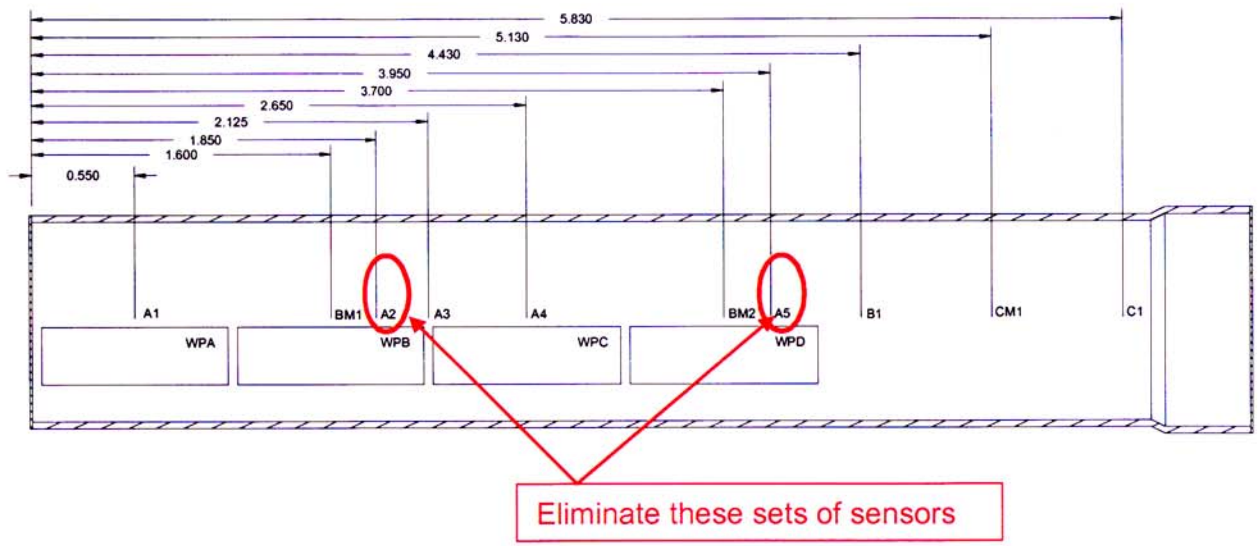


Figure 06/08/06-4. No temperature sensors were located at cross sections A2 and A5 during the moist test.

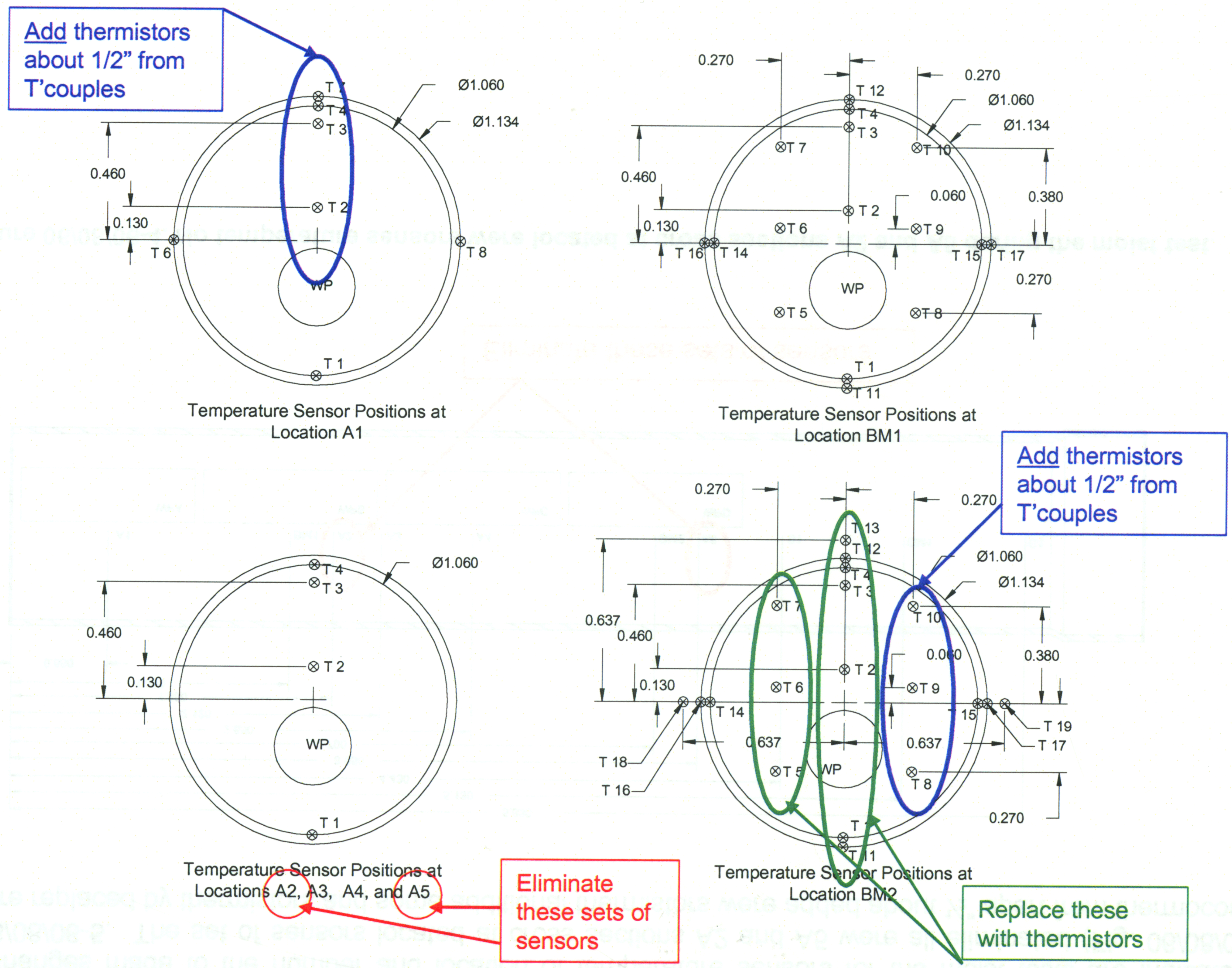
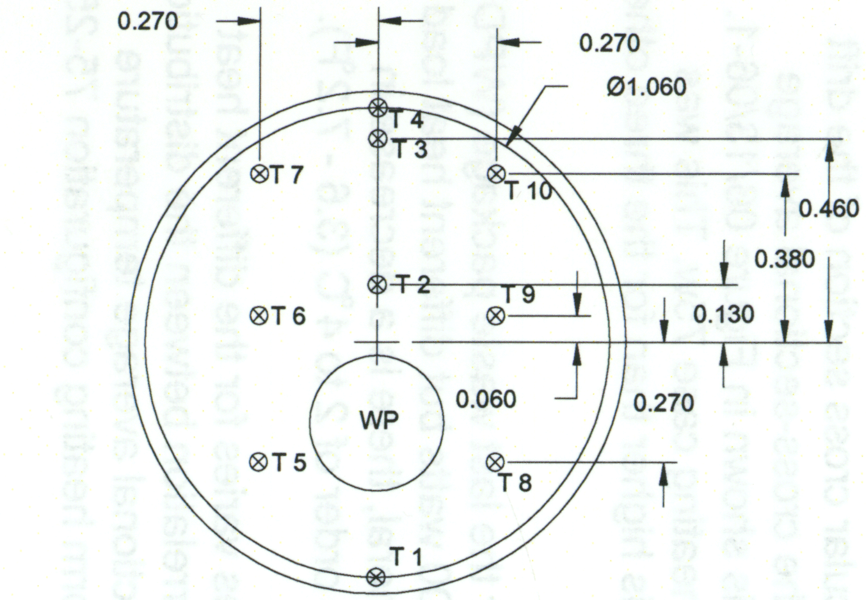
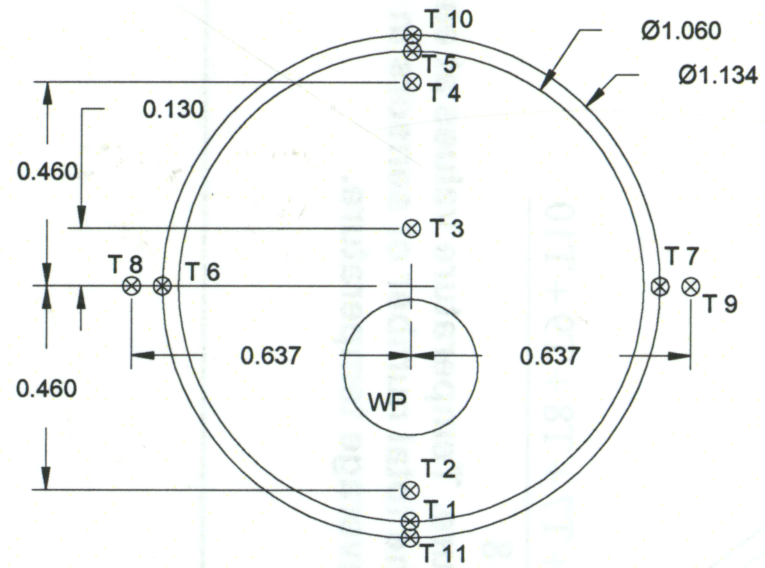


Figure 06/08/06-5. Some thermocouples were replaced by thermistors and some thermistors were added at about ½" from thermocouples.



Temperature Sensor Positions at Location B1

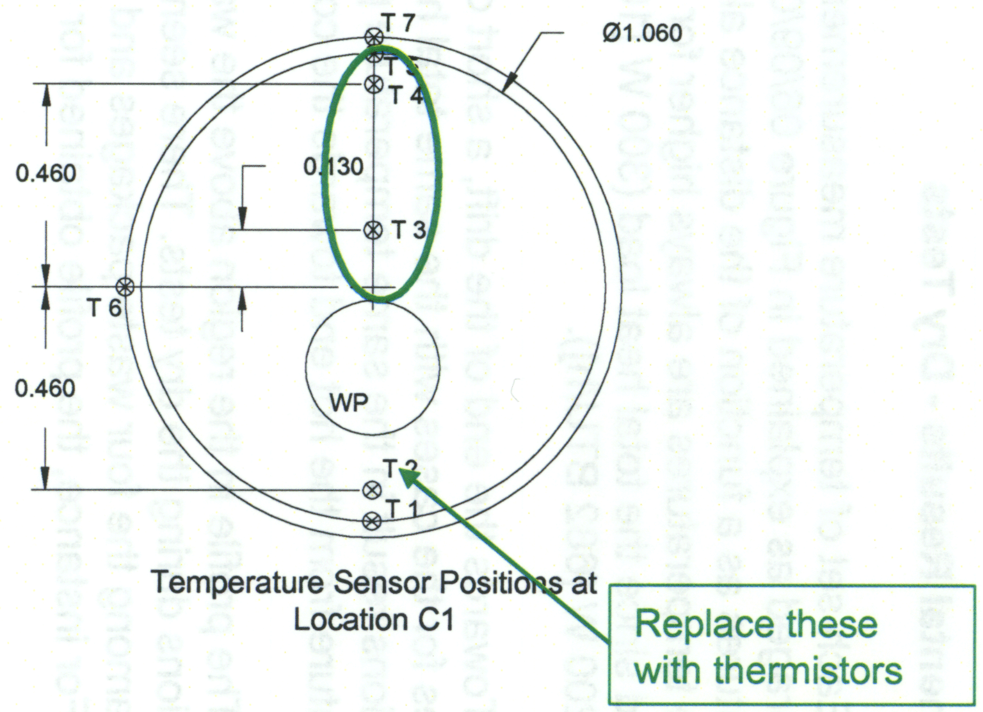


Temperature Sensor Positions at Location CM1

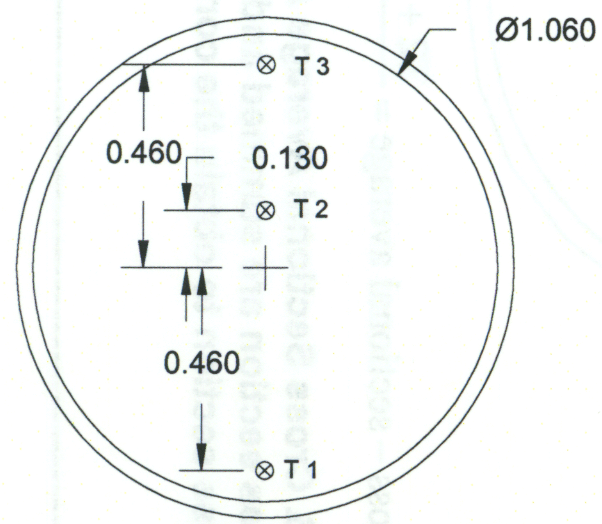
- Eliminate Thermocouples:
  - Location A2
    - T1,T2, T3, T4
  - Location A5
    - T1,T2, T3, T4

- Replace Thermocouples with Thermistors:
  - Location BM2
    - T1,T2, T3, T4, T5, T6, T7, T11, T12, T13
  - Location C1
    - T3, T4, T5

- Add Thermistors about ½" from Thermocouples:
  - Location BM2
    - T8,T9, T10
  - Location A1
    - T2, T3, T4, T7



Temperature Sensor Positions at Location C1



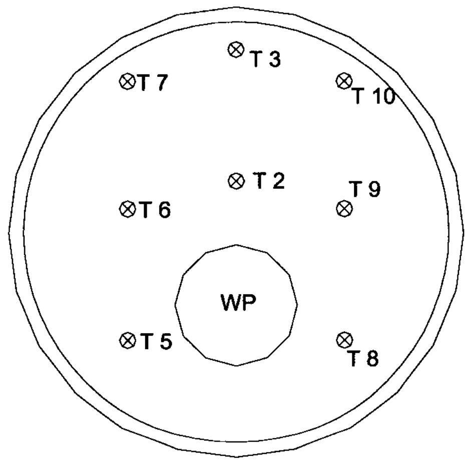
Temperature Sensor Locations on the Inside and Outside Surfaces of the Hot End Wall

Continuation of Figure 06/08/06-5. Some thermocouples were replaced by thermistors and some thermistors were added at about ½" from thermocouples.

06/09/06 – F.V.

Cross Sectional Average Temperature

The cross-sectional average temperature is the average of the individual measured or predicted temperature values at the different locations in a cross section as shown in Figure 06/09/06.



$$\text{Cross - sectional average} = \frac{T2 + T3 + T5 + T6 + T7 + T8 + T9 + T10}{8}$$

Figure 06/09/06. Cross Sectional Average Air Temperature. Temperature values at each location in a cross section are summed and divided by the total number of sensors in that cross section to obtain the corresponding average temperature.

06/13/06 – F.V.

Experimental Results - Dry Tests

Each set of temperature measurements in a particular cross section of the drift was averaged as explained in Figure 06/09/06. A plot of the cross-sectional average temperatures as a function of the distance along the drift is shown in Figure 06/13/06-1. Average temperatures are always higher for the uniform heating case 75w. This was expected since the total heat load (300 W [1024 BTU/h]) is higher than for the three other cases (200 W [682 BTU/h]).

Towards the end of the drift, a short distance after the last waste package (WPD), all curves for the cases with the same total heat rate of 200 watts but different heat load distributions result in the same temperature profile. In general, there is a decrease in temperature from the hot end towards the cold end in the order of 2 to 4℃ (3.6 - 7.2℉).

The profile in the region above the waste packages varies for the different heat distributions during the dry tests. There seems to be a correlation between the distribution of heat among the four waste packages and the cross-sectional average temperature profile. For instance, the profile obtained for the non-uniform heating configuration 75-25-

25-75w exhibits two maximums located above the waste packages with higher heat loads (WPA and WPD) and an approximately flat profile at a lower temperature above the two central waste packages (WPB and WPC) that have a heat load three times lower (25 W [85 BTU/h]) each) than the other two (75 W [256 BTU/h] each).

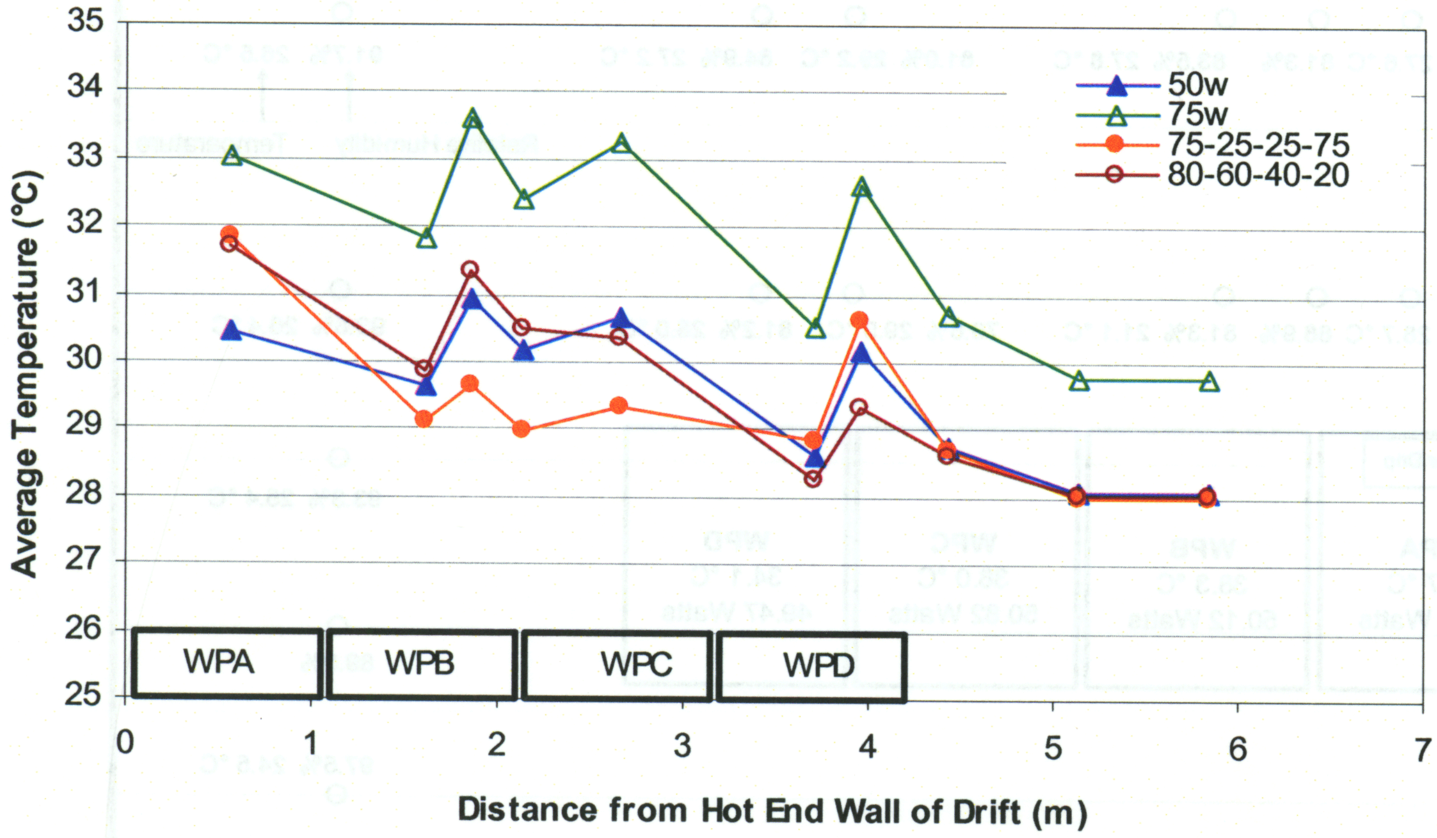


Figure 06/13/06-1. Cross-sectional average air-temperature profile for all dry tests with different heat load distribution between individual waste packages.
From Excel File "*Fifth Scale Test Data 9-3-2004 (version 4).xls*"

Relative Humidity and Temperature – Moist Test; Uniform 50W

The temperature and relative humidity were measured at 15 different locations in a plane along the centerline of the drift. The highest relative humidity values were measured towards the end of the drift in the region past the waste packages. Figure 06/13/06-2 shows the temperature and relative humidity measured during the moist test with a uniform heat distribution 50W and Figure 06/13/06-3 shows the temperature and relative humidity measured during the moist test with non-uniform heat distribution 75-25-25-75W.

Comparison of Figures 06/13/06-2 and -3 indicate that there is not a significant difference in the humidity level between a uniform and non-uniform distribution of heat, except at those locations close to the waste packages were higher temperature gradients are expected.

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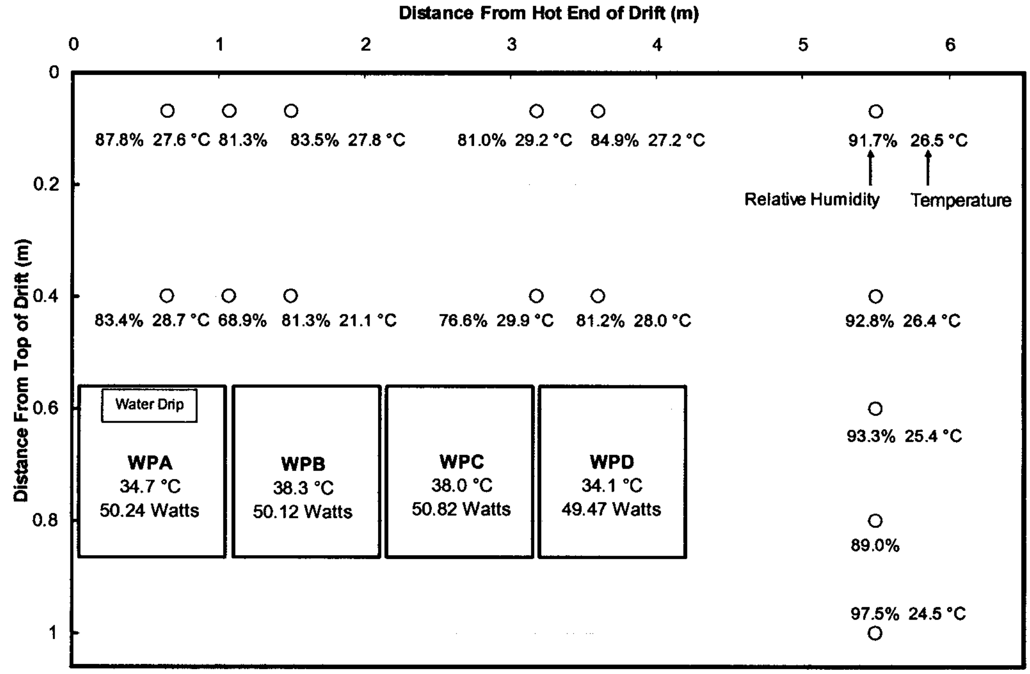

Figure 06/13/06-2. Measure Temperature and RH - Moist Test – Uniform Heating 50w.
From Excel File "*Fifth-scale Moist_50w.xls*"

Relative Humidity and Temperature – Moist Test; Non-uniform 75-25-25-75W

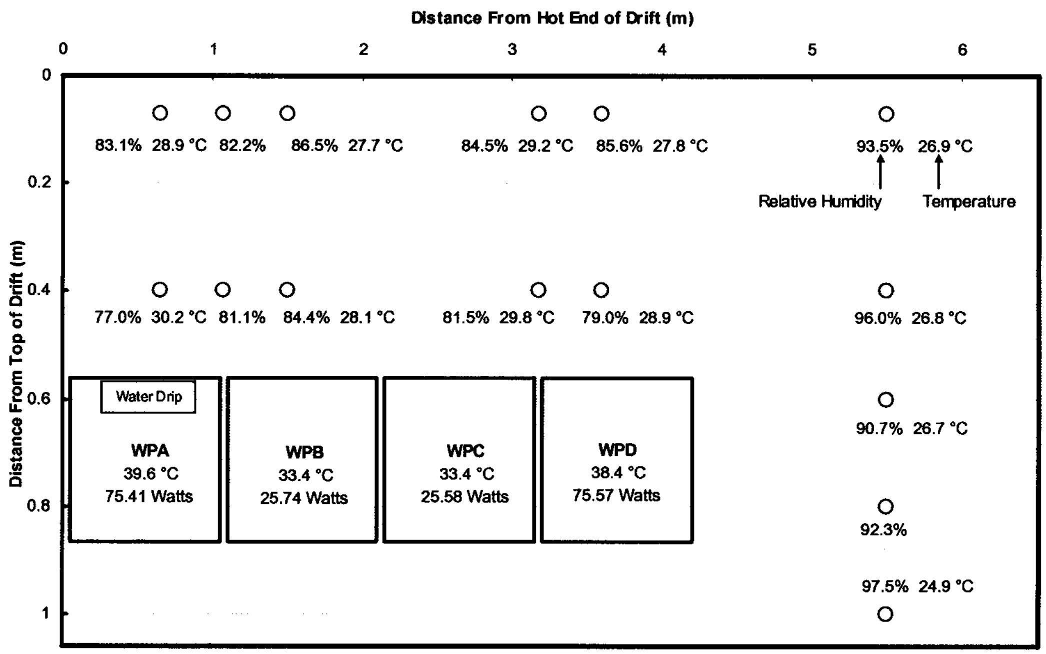

Figure 06/13/06-3. Measure Temperature and RH - Moist Test – Non-Uniform Heating 75-25-25-75w.
From Excel File "*Fifth-scale Moist_75-25-25-75w.xls*"

06/16/06 – F.V.

CFD Results – Dry Case 50w

The FLOW-3D input and result files are respectively: prepinr.Dry50b and flsgrf.Dry_50w. The CFD results for this case obtained from the results file, at a time of 850 seconds.

The contour plot of the air temperature inside the 20-percent scale drift model is shown in Figure 06/16/06-1, where temperatures are given in degree Kelvin. The highest temperatures are observed right on top of the waste packages and the lowest temperatures are observed below the waste packages. In the region past the waste packages temperature gradients are slightly higher in the z-direction than in the x-direction on a XZ plane along the centerline.

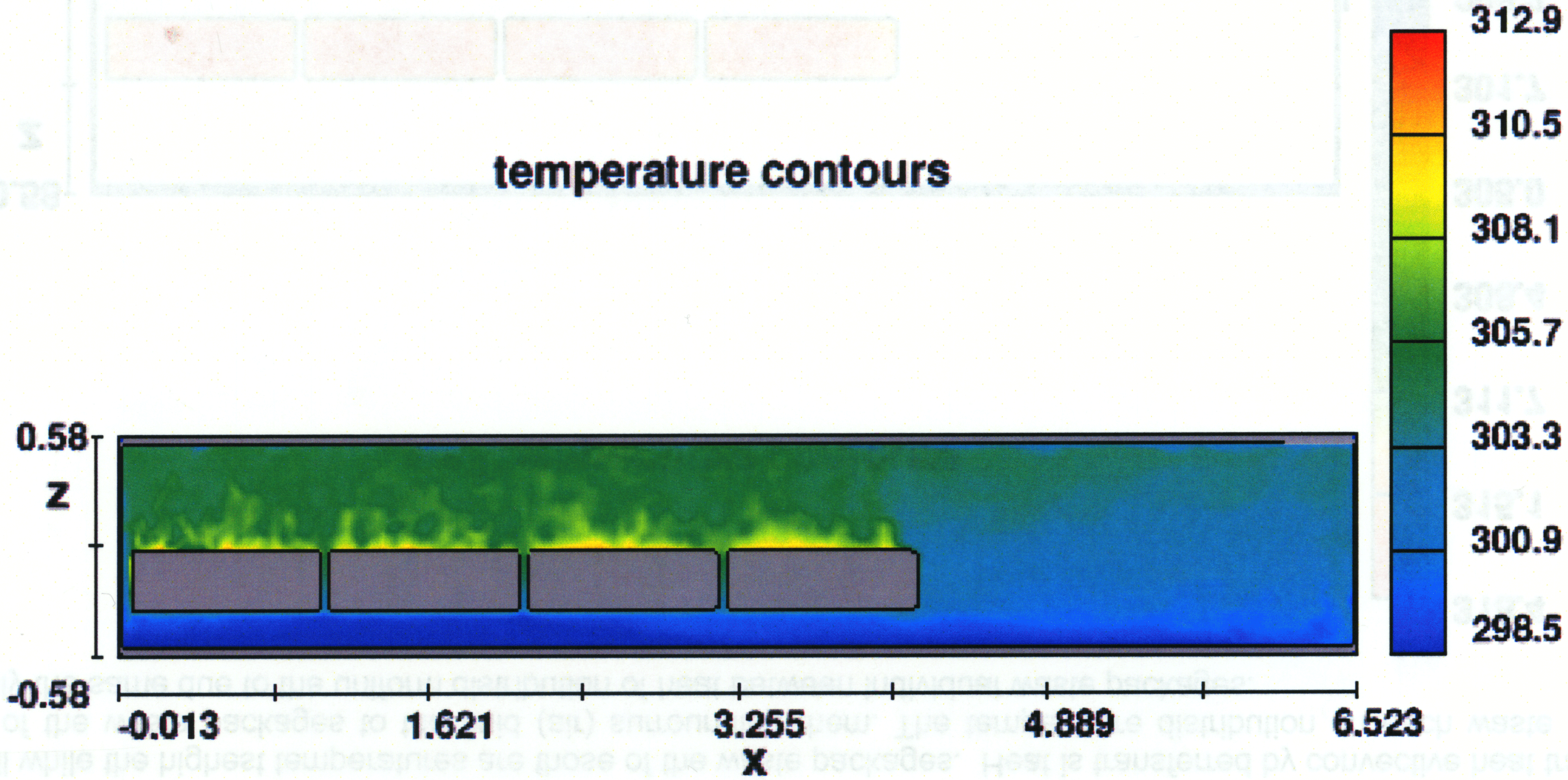

Figure 06/16/06-1. Contour Plot of the Air Temperature (K) – Dry Test – Uniform Heating 50W.

The contour plot of the wall temperature is shown in Figure 06/16/06-2. The lowest wall temperature is encounter on the cold end wall while the highest temperatures are those of the waste packages. Heat is transferred by convective heat transfer from the surface of the waste packages to the fluid (air) surrounding them. The temperature distribution on each waste package is approximately the same due to the uniform distribution of heat between individual waste packages.

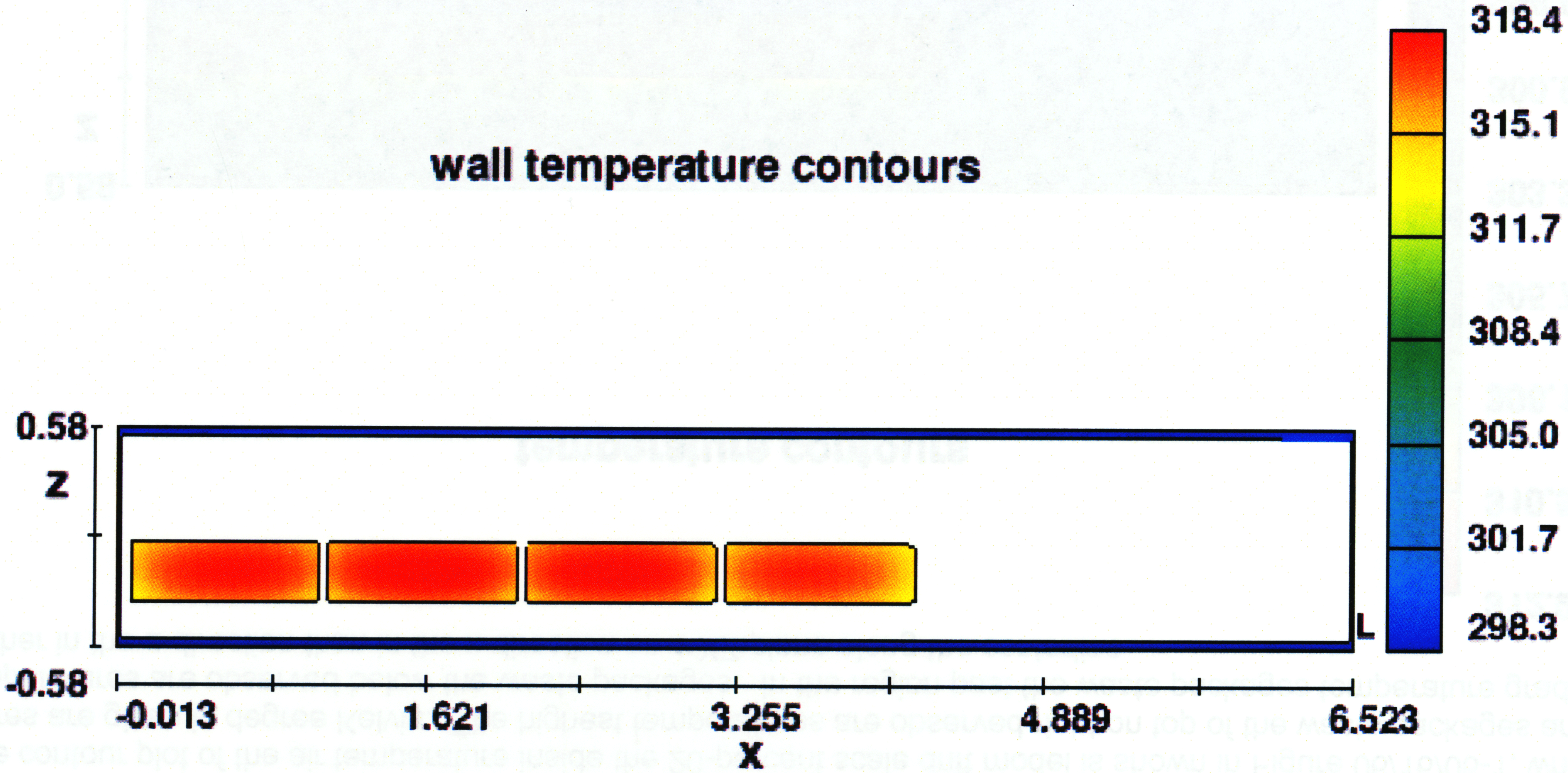

Figure 06/16/06-2. Contour Plot of the Wall Temperature (K) – Dry Test – Uniform Heating 50W.

The velocity field on the XZ plane along the centerline of the 20-percent scale drift model is shown in Figure 06/16/06-3 together with the contour plot of the y-velocity component. The fluid on top of the waste packages moves away from the waste packages and towards the top of the drift. There is a recirculation zone on top of WPA due to the presence of the cold end wall. In the region past the waste packages the flow moves in the cold to hot end wall direction at the top of the drift, and in the opposite direction, from cold to hot end wall, at the center and bottom of the drift. Velocity magnitudes are given in meters per second and distances are given in meters.

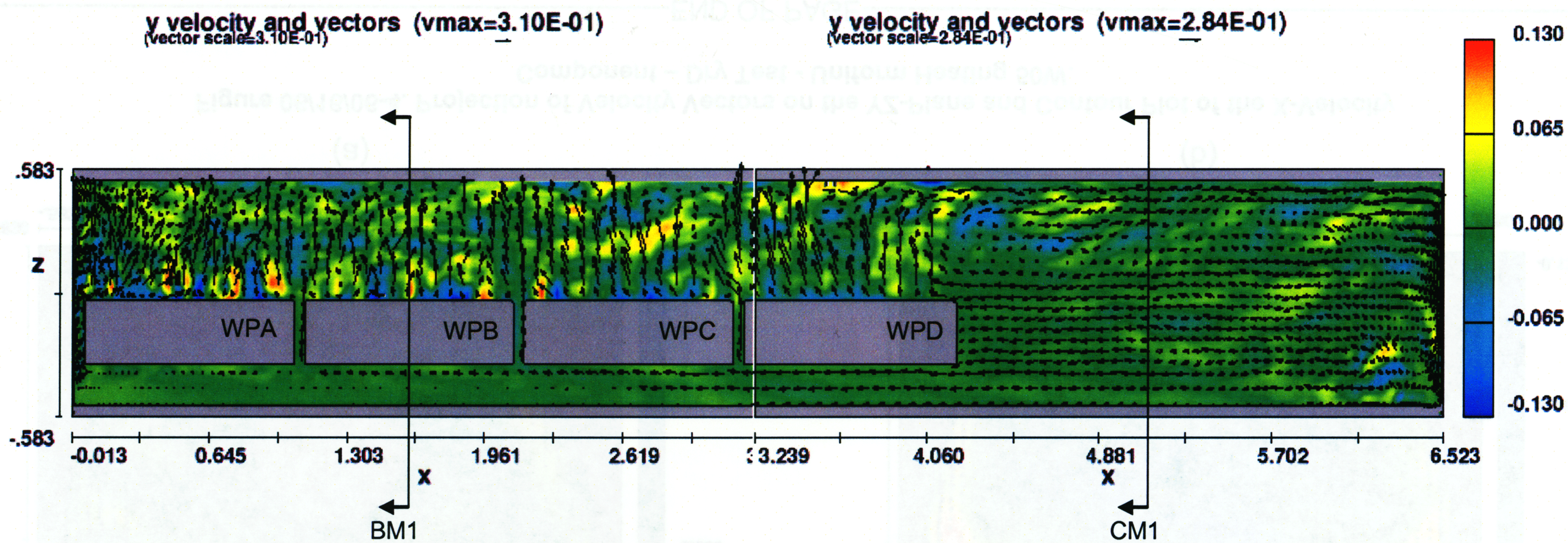

Figure 06/16/06-3. Projection of Velocity Vectors on the XZ-Plane and Contour Plot of the Y-Velocity Component – Dry Test - Uniform Heating 50W.

Figure 06/16/06-4 shows the projection of the velocity vectors on the YZ plane and the contour plots of the x-velocity component in two cross sections (BM1 and CM1) of the 20-percent drift model. Figure 06/16/06-4a shows that the fluid (air) inside the drift model moves in the cross sectional direction with a maximum velocity magnitude of 0.25 m/s. The air around the waste package moves upwards at the center and downwards along the walls, forming a circular pattern on each side of the plumb. Below the waste package the velocity vectors are very small, indicating a reduction on the movement of air in the cross-sectional direction. The contour plot of the x-velocity component in the region below the waste package indicates that the fluid in contact with the waste package is moving from cold to hot with very slow motion (maximum x-velocity magnitude is around -0.13m/s), while the fluid velocity at the bottom of the drift tends to zero.

The vector field on Figure 06/16/06-4b shows that the fluid moves from the center to the top of the drift and then downwards along the walls of the drift where the maximum velocity magnitude is around 0.143m/s. The contour plot also shows