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September 16, 2011
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Attn: Document Control Desk
U.S. Nuclear Regulatory Commission
Dr. King Stablein
Office of Nuclear Material Safety and Safeguards
Division of High-Level Waste Repository Safety
Mail Stop EBB-2-BO2
Washington, DC 20555

Subject: In-Drift Heat Transfer—Final Report (IM 14002.01.441.136)

Dear Dr. Stablein:

This letter retransmits the subject report, incorporating the comments provided by the U.S. Nuclear Regulatory Commission (NRC) on the original report transmitted on July 25, 2011. Please note that the title of the report has been changed to “Numerical and Experimental Study of In-Drift Heat and Mass Transfer Processes.”

The Center for Nuclear Waste Regulatory Analyses (CNWRA®) received NRC comments on the original draft report as an attachment to an email. The NRC staff comments and CNWRA staff responses are in a document provided with this letter. The changes to the report can be seen in Version 6.0 (dated September 13, 2011) of the following SharePoint file:

YM Licensing Review > Knowledge Management > Knowledge Capture Reports >
Das_In-Drift Heat Transfer_136 > Das_In-Drift Heat and Mass Transfer_136

The NRC staff indicated in an email dated September 12, 2011, that the revised report was acceptable. The final formatted version of the report is preserved at the SharePoint location shown above.

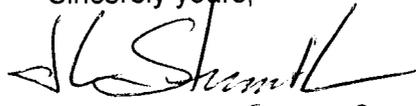


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Dr. King Stablein
September 16, 2011
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Please contact Jude McMurry at (210) 522-6935 or me at (210) 522-5582 if you have any questions regarding this report.

Sincerely yours,



For DP.

David Pickett
Senior Program Manager
Integrated Spent Fuel Regulatory
Program—Geologic Disposal

DP/ar

Enclosure

cc:

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COMMENTS ON THE REPORT TITLED “NUMERICAL AND EXPERIMENTAL STUDY OF IN-DRIFT HEAT AND MASS TRANSFER PROCESSES”

(8/30/2011)

This report discusses the heat and mass transfer process in a drift. Wall condensation and evaporation and volumetric condensation (equilibrium and nonequilibrium models) are numerically modeled using the software FLUENT for computational fluid dynamics (CFD). The boundary conditions are specified through customized functions, in which the condensation rate is assumed to be controlled primarily by the diffusion process in the vapor phase. Two different experimental studies were conducted for benchmarking the simulated data. The first experiment was carried out in a laboratory test chamber with closely controlled environment, where a single condensation-evaporation cycle was generated within a rectangular space. Computed results were compared with experimental data which established the validity of the adopted customized modules. The second experiment developed a 20-percent drift scale model of the repository using electrically heated cylinders to create the effect of heated waste packages and dripping water to replicate seepage. The calculated results were also compared with the measurements.

This report used the well tested software and boundary conditions. The numerical modeling results are supported by the experimental results. The experiment for the scaled-down drift is very pertinent to our program. The report is well organized and clearly written. So I conclude that this report is acceptable. The following are my comments, suggestions, questions, and typo corrections for the authors to consider in revision.

- (1) Although it is described in section 2.1 (page 2-1) that “The simulation boundary conditions could be defined using the options available with the solver, or users can define it through customized functions.” The relation between the baseline solver and customized functions in FLUENT may not be very clear for many readers. In your report for the wall condensation (section 2.2.2) and wall evaporation (section 2.2.3) modeling, the customized functions provided by equations 2-1 to 2-10 are simply the boundary conditions of the condensing wall and evaporating wall to the baseline solver. To indicate this will help the readers truly understand the relation between baseline solver and the customized functions.

Separate subsections have been added in section 2.2.2 and 2.2.3 to address the boundary condition issue more clearly. Actually equations 2-1 through 2-9 are used to calculate source terms in the governing equations that arise as a result of adding and removing mass from the system due to condensation and evaporation and also to estimate the condensed or evaporated water mass. Equations 2-10 and 2-12 have been added (numbers according to the modified document) to show how boundary conditions are specified. The added write up also says that this boundary condition was not available in the standard solver, hence the UDFs were developed.

- (2) It is very easy to derive equation (2-6) from equations (2-2) and (2-4) assuming that mass flow rate of air is zero or the left side of equation (2-2) is zero. But I got equation (2-6) with an extra "-" (minus sign), please check. This also affects equation (2-10).

Thanks for the review. The equations have been corrected. Actually the area vector within the solver takes care of the sign convention and adds or subtracts mass accordingly. The convention is to use negative sign for condensation and positive for evaporation. The area vector and the gradient calculation within the solver take care of the direction of the flow. Equations (2-1) and the following equations are changed. The evaporation equation (2-11) was correct. Also some other corrections were made, such that equations 2-1 and 2-2 used volumetric source terms instead of fluxes.

- (3) In the beginning of section 2.2.2 Wall Condensation you describe the general physics process of condensation which includes "contact with the cold surface". The reader will expect this will be modeled or clearly indicated in the assumptions for why not included in the model. On pages 2-4 and 2-6 you provided many assumptions for the wall condensation and wall evaporation modeling respectively. But I think you missed the most important one, which is that although condensation is a multiphase process involving flow and coupled heat and mass transfer in both the liquid film and vapor, under certain conditions the condensation rate may be controlled primarily by the diffusion process in the vapor phase. This is exactly shown in the equations (2-1) to (2-10), where there are only two terms controlling the process (for example the two terms on right side of equation 2-1), one is for the diffusion process and the other for the convection process. Without indicating this assumption, it is very surprising why the described temperature dependence for condensation and evaporation as we usually expect is completely missing in equations (2-1) to (2-10). In the general discussion for the physical process, such as on page 1-1, you emphasized for the cold trap process that "condensation at cooler locations". Including this assumption will avoid confusions. The validity of this assumption or this simplified modeling approach is, as indicated in the report and in Bell (2003), demonstrated by comparing the results with theoretical and experimental results.

The assumptions are rewritten. The very first assumption for both condensation and evaporation now states that these processes have been assumed to be diffusion controlled and the diffusion rate depends on the difference in concentration across the boundary layer. The diffusion process, however, depends on the wall temperature and has included the thermal effect albeit indirectly. The rewrite of this section attempts to clear that understanding. As mentioned, equation (2-1) and (2-11) has two terms. The first term is the diffusive process and the second term the convective process. The thermal effects are hidden in the species concentration term ω_{H_2O} . The species concentration at the wall depends on the wall temperature (which is equal to the liquid film temperature adjacent to the wall) as a saturation concentration is assumed. Similarly the concentration at the bulk flow is dependent on all the flow parameters including temperature. Hence the diffusive process that is responsible for condensation and evaporation is getting influenced by the wall temperature.

The previous write up was probably not explicit in indicating the wall thermal effect on the evaporation/condensation process. The separate boundary condition section attempts to clearly demonstrate the dependence on wall temperature.

- (4) Equation (2-7) is simply given without reference. The definitions of $A_{\text{cell wall}}$ and V_{cell} were not given. I guess the former is the area of the cell cross section and latter the cell volume. The ratio of the latter vs. the former is the cell dimension d in the normal direction to the wall and v/d is the velocity gradient. So equation (2-7) is the mass continuity equation from mass conservation. I suggest some explanations to be added here to help the reader to understand what it is.

Yes it is indeed the continuity equation. Explanation has been added for $A_{\text{cell wall}}$ and V_{cell} in the nomenclature section. Some text has also been added to describe equation (2-7) more clearly and spell out some of the assumptions that went into specifically formulating equation 2-7)

- (5) In the text on top of page 2-11, you say Figs 2-4 to 2-7 are for equilibrium model and Figs 2-8 to 2-11 for nonequilibrium model. But the figure captions show otherwise. Your section 2.4.2 (nonequilibrium) and section 2.4.3 (equilibrium) are consistent with the figures and captions. You also have typos in section 2.4.3, such as Figures 9-9 and 9-10. Please check.

Agree with the suggestion and changed the document to specify nonequilibrium model for Figs 2-4 through 2-7. I could not find any mention about Fig 9-9 and 9-10, you may have already corrected it

- (6) For the nonequilibrium model, the reference to equations (2-13) to (2-16) should be provided. I tried to skim the ANSYS FLUENT Theory Guide 12.0 (816 pages) and did not find similar formulas. It must be from Fox, et al. (1997a, b). The definition of parameter K_B in equation (2-15) is never provided.

References for equations 2-13 through 2-16 (Carey and Fox) have been added. Also the parameter k_B has been defined in the nomenclature section (previously it was mistakenly specified as k_A)

- (7) I understand that data from Tests 4-15 (not tests 16 to 18) in Table 1 are summarized in Figure 3-4. How do you explain tests 16 and 17, which have the same T_6 and T_7 as test 11, and the range of T_1 and T_2 for tests 16 and 17 covers T_6 and T_7 for test 11, but test 11 has pretty high condensation rate and tests 16 and 17 have zero condensation rate.

Tests 16 through 18 were dry test, where there was no water in the evaporating water pan. Hence no condensation was observed, even though the test conditions were similar to some other tests. Rows for experiment 16 through 18 are deleted in order to avoid any confusion.

- (8) In Figs 3-6, 3-7, 3-8, 3-9, and 3-10, 3-11, you compared the velocity, temperature, and relative humidity distributions between equilibrium and nonequilibrium models respectively. In Figs 3-13 and 3-14 you compared the condensation rate as a function of temperature difference. But why the condensation rate should be a function of temperature difference is not revealed through the comparisons of velocity, temperature, and relative humidity distributions between different temperature differences. The

formulas provided in chapter 2, in which the condensation rate is assumed to be controlled primarily by the diffusion process in the vapor phase, the relation to the temperature difference is never provided or discussed. Although we all expect from fundamental physics that condensation rate should be a function of temperature difference, your formulation and comparison of experimental results did not establish such physical connection for the reader to understand how the temperature difference manifests its influence on condensation rate. I believe if you compare the velocity, temperature, and relative humidity distributions between different temperature differences the physical processes will be revealed. This is my main comment to this report.

The main issue is the inclusion of wall thermal effect into the evaporation/condensation process. As mentioned in bullet number 3, the assumption and formulation section has been rewritten to explicitly show how the wall temperature influences water vapor diffusion through boundary layer and how in turn the evaporation/condensation process is affected. The rewrite also shows how the thermal effects are considered into the model (through boundary conditions).

Figures 3-13 and 3-14 show the variation in rates of condensation with difference in temperature between the cold and hot walls. The conclusion is that the temperature difference between the cold and hot plate drives the quantity of water that moves from the hot to cold plates. How much water evaporates at the hot surface depends on the temperature difference between hot water pan and the bulk temperature. On the other hand, the condensation rate depends on the temperature difference between cold plate and the bulk. Under steady state conditions (this is the scenario we simulate and expect to take place in the repository), the rate of condensation will be equal to the rate of evaporation. So, in essence the bulk temperature will adjust so that the condensation and evaporation rates are the same. At this condition, the whole condensation evaporation cycle will just depend on the temperature difference between the hot and cold plates with the bulk temperature adjusting itself to a value that enables attaining a steady system. This is reflected in Figures 3-13 and 3-14.

The wall temperature is actually the primary driving force for the diffusion process and controls how much water gets transported. The velocity, temperature and relative humidity profiles for different temperature range showed different absolute values, but exhibited an analogous pattern. Hence only a representative set of contours are provided for a general understanding of the flow and thermal field within the domain. As mentioned, the developed methodology takes into account the thermal effects and that is what was primarily responsible for the variation in condensation rate with temperature difference.

- (9) On top of page 4-23, "Figure 3-18" must be a typo because there is no Figure 3-18. From the context it is like to be Figure 4-24. In the same paragraph, "A qualitative comparison of Figure 4-21(a) and 4-21(d) shows..." must be typos too because there are no Figure 4-21(a) and 4-21(d). There are likely to be Figure 4-25 (a) and 4-25 (d).

I tried to find out these typos but could not. You may have taken care of it already, thank you

- (10) In the last paragraph of page 4-23, there is no Table 4-2 (a, b). You only have Table 4-1. There is a typo in the title of Table 4-1 about 20%. You have a 2 there.

Again I tried to find it out the typos and could not find it. You may have taken care of it already, thank you