Drift-Scale Thermohydrologic Process Modeling: In-Drift Heat Transfer and Drift Degradation

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Initial Entries

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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.

Purpose of Non-degradation Radiation Modeling:

- Set up a 2D unstructured METRA model to simulate the non-isothermal, multiphase flow for Yucca Mountain drift-scale model.
- Main approach and objectives:
    - Create an unstructured grid
    - Use existing thermal and hydrological parameters
    - Model radiation explicitly with the radiation module in METRA
    - Evaluate view factors from WP surfaces to drift/invert surfaces numerically.
    - Compare the results with previous results obtained via the effective thermal conductivity approach

Basic Concepts in Radiation Theory

Thermal radiation is electromagnetic radiation emitted by a material substance solely due to its temperature (Mahan, 2002, p.7). Radiation heat transfer concerns about the exchange of thermal radiation between two or more bodies. The Stefan-Boltzmann law of radiation heat transfer states that the heat flux (W) emitted from a blackbody at absolute temperature T_b is,

(1) $Q_{rad} = \sigma A T_b^4$

where σ is the Stefan-Boltzmann constant, and A is the total radiating area of the blackbody. For a real object, the radiation heat transfer is a function of several components. These include the object's surface reflectivity, emissivity, surface area, temperature, and geometric orientation with respect to other thermally participating objects. The Stefan-Boltzmann law for net radiation exchange between two non-black objects 1 and 2 is,

(2) $Q_{rad,1-2} = \varepsilon_1 \sigma A_1 F_{12}(T_1^4 - T_2^4)$

where ε_1 is the emissivity of object 1, F_{12} is called the view factor or the configuration factor. Emissivity, which has a value between 0 and 1, is introduced to account for the fact that the non-ideal surfaces/bodies emit and adsorb less heat than a blackbody at the same temperature. View factor is introduced to define the fraction of radiation that leaves object 1 and is intercepted by object 2. View factor is purely a function of the geometry of two-surfaces, their orientations and the spacing between them.

Note: Equation 2 is actually a simplified version of the following equation, which describes heat radiation between two surfaces 1 and 2, with surface 2 completely covering the surface 1 such that the view factor from 1 to 2 is 1, (Edwards et al., 1979),

(3) $$Q_{rad,1-2} = \frac{\sigma}{\dfrac{1-\varepsilon_1}{\varepsilon_1 A_1} + \dfrac{1}{A_1} + \dfrac{1-\varepsilon_2}{\varepsilon_2 A_2}}(T_1^4 - T_2^4)$$

Equation 3 reduces to 2 either when ε_2 is close to 1 or when the ratio of $\varepsilon_1 A_1$ and $\varepsilon_2 A_2$ is small. When these assumptions are not met, then Eq3 has to be used in lieu of 2.

Modeling the In-Drift Radiation in MULTIFLO

In this work, we use surface-to-surface approach (Edwards et al., 1979) to model radiation heat transfer between the waste package and the drift wall. The surfaces of waste package and drift wall are represented by a number of blocks. These surfaces are assumed to be non-diffusive. For any drift-wall block, the radiation power from the waste-package is assumed to be the dominant input. In other words, the radiation fluxes from other drift-wall blocks are assumed to be negligible. The latter assumption is deemed appropriate because the drift wall blocks tend to have similar temperatures and thus the radiation flux between drift wall blocks is small compared with the heat exchange between the waste package and the drift wall blocks. Under these assumptions, the net radiation flux between waste package and any drift wall node can be expressed by Eq(2).

Calculation of View Factor

View factor is defined as the fraction of radiation that leaves surface 1 and is intercepted by surface 2. Mathematically, this can be calculated as,

(4) $A_1F_{1-2} = \int_{A_1}\int_{A_2} \frac{\cos\theta_1 \cos\theta_2}{\pi r^2} dA_2 dA_1$

In a discrete form, for radiation between differential areas A_1 and A_2, the view factor is calculated as,

(5) $F_{1-2} = \frac{1}{A_1}\sum_{p=1}^{m}\sum_{q=1}^{n}\frac{A_{1p}A_{2q}}{\pi r_{pq}^2}\cos\theta_{1p}\cos\theta_{2q}$

where surface 1 is divided into m integration points and surface 2 is divided into n integration points. r_{pq} is the distance between A_{1p} and A_{2q}, θ_{1p} is the angle between A_{1p}'s normal vector and r_{pq}, and θ_{2q} is the angle between A_{2q}'s normal vector and r_{pq}. In this project, Eq.(5) was used to calculate view factors between the waste package and the drift-wall blocks. Note that the contribution of a segment on surface 1 to a segment on surface 2 is set to zero when the segment on surface 1 can not be seen by the segment on surface 2. A reciprocity relationship exists between view factors,

(7) $A_1F_{12} = A_2F_{21}$

Based on the reciprocity relationship, only the view factors from the waste package to the drift wall blocks need to be calculated.

To check the result of simulation, the following relationship can be very useful:

(8) $\sum_{j=1}^{N} F_{ij} = 1$

The equation says for any area i that is within an enclosure (which is divided into N segments) the sum of view factors between i and j (j=1,N) is equal to 1.

Note:

A. In the current problem, surface *1* represents the whole WP surface. Surface 2 represents the combined areas of drift wall and the invert. Surface *2* is divided into N segments. A good check to the view factor calculation is fixing i and summing up all the ij's. The sum of these terms should be equal to 1 according to Equation (8).

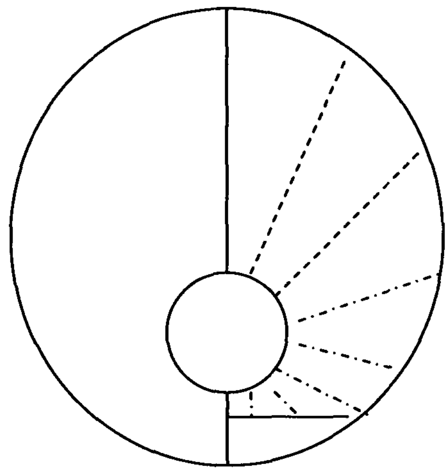
B. METRA computes the arithmetic average of the emissivities between two blocks, i.e., the formula used by METRA is,

(9) $Q_{rad,1-2} = 0.5(\varepsilon_1 + \varepsilon_2)\sigma A_1 F_{12}(T_1^4 - T_2^4)$

This averaging scheme may give erroneous results when $\varepsilon 1$ and $\varepsilon 2$ are very different.

<u>AS2004615 entry</u>

The following diagram illustrates the construction of view factors. The dashed lines (not to scale) represent the links to the pseudo nodes. The view factor from WP to each of the pseudo node is calculated.



For this project, the perimeter of WP is divided into 6 elements. The enclosure surface (i.e., drift wall and invert surface) is divided into 8 elements, the first 5 of which are on the drift wall and the last 3 are on the invert surface. This requires the calculation of 6x8=48 terms. To calculate the portion of WP power that is intercepted by a segment on the enclosure surface, the contributions of all WP segments to the specific segment needs to be summed up.

The detailed calculation has been documented in the spreadsheet, *.\Rubble\No_DD\viewfactor.xls*.

Reference

1. Mahan, J.R., Radiation heat transfer: a statistical approach. John Wiley & Sons, New York, 2002.
2. Edwards, D. K, V. E. Denny and A. F. Mills, Transfer Processes: An introduction to diffusion, Convection, and Radiation, 2nd Edition. Hemisphere Publishing Company, Washington, 1979.

Appendix

Detailed description for setting up radiation in MULTIFLO 2 for the no-drift degradation case

<u>Pre-processing</u>

Step 1. Generation of the grid. A two-D numerical grid is generated for the entire domain (from the ground surface to the water table) using the Mathematica notebook, *mtn_grid.nb*. The output from *mnt_grid.nb* serves as the input file to AMESH. The output from AMESH (consists of *eleme*, *conne* and *segmt*), together with *bcon_a* and *phik_a* serve as inputs to Amesh2Mflo. Amesh2Mflo generates *multi.phk* and *multi.bc* files. Input data are taken from DOE's MSTHM Table 4-1 (ANL-EBS-MD-000049 REV01).

Important: when preparing for the fracture permeability and fracture boundary flux data, must divide the reported data by the intrinsic fracture porosity.

Step 2. Adding pseudo nodes. pseudo nodes are added to the *multi.phk* and *multi.con* files. The connectivity and element property data related to the pseudo nodes are generated by the script, *pseudolink.cxx*. Radiation is implemented through pseudo nodes. Basically these nodes enable us to add additional logics in an ad-hoc fashion. In the current context, WP is represented by a single pseudo node. Several pseudo nodes are added to the surface of drift wall and invert to form a pseudo layer. The pseudo layer is attached to the real nodes by adding necessary connection information to the *multi.con* file. WP node is connected to each of the node in the pseudo layer. The connections between WP node and pseudo layer, however, are not geometric connections. They are the products of element surface areas and view factors. Inside MULTIFLO, they are used to calculate the radiation flux given in Eq 1. The outputs from *pseudolink.cxx* is *multiextra.con* and *viewfactor.phk*. The contents of these two files are pasted to the end of *multi.con* and *multi.phk*, respectively.

Step 3. Assembling MULTIFLO input files. The DCMParam parameters are calculated in the spreadsheet, *\rubble\dd\airdensity.xls*. The initial condition file, *multi.int.* is generated by a steady-state run. See *\thc\mtn\initrun*. The steady-state run simulates the ambient condition for the given boundary and hydraulic property data.

<u>Post-processing</u>
Post-processing is done using a modified version of Mathematica package, *mfloPlot.m*, which was created by Scott Painter for MULTIFLO 2. The modified version is in *H:\asun\mathbook\mfloPlotRad.m*. The plotting package can plot any variable listed in the METRA field file. The modified version prints out the max value and year information. Also one can use the modified package to track the change of a node over all time steps. The Mathematica notebook, *initrun0415.nb*, shows examples of *mfloPlotRad.m* in action.

<u>AS20040604Entry Summary of Results</u>
The results of the ambient run that established the initial conditions for the site-scale model are contained in the folder,
`\thc\mtn\initrun`

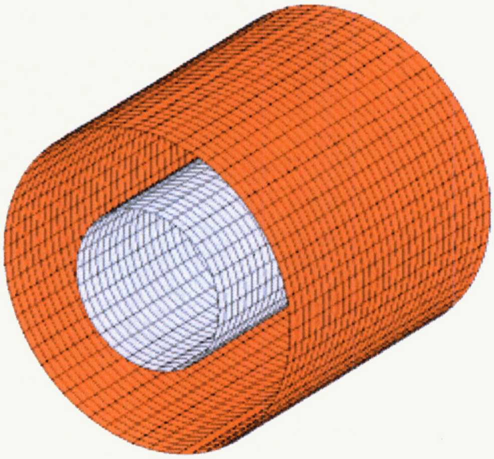
The final results of the radiation run are stored in the folder `\thc\mtn\run0415`. Inside the folder, the Mathematica notebook, `radrun0415.nb`, plots temperature and saturation distributions at various time periods.

<u>AS20040701 entry</u>

Revisit the radiation problem. This thinking is inspired by one of the validation problems reported by ThermoAnalytics, Inc.
(http://www.thermoanalytics.com/support/validation/example004.html)
Part I:

Consider the problem of two finite-length concentric cylinders. To calculate view factors, one needs to consider all four surfaces involved, i.e.,

- A1: outer surface of the inner cylinder
- A2: inner surface of the outer cylinder
- A3: outer surface of the outer cylinder
- A4: environment surrounding the cylinders



Some terms can be eliminated based on visual examination.
Since A2 cannot see A3 at all,
(1) F23 = 0, F32=0,
Since room surrounding the geometry is very large,
(2) F41=0, F42=0, F43=0, F34=1

The following equations exist for the remaining terms

(3)F14+F12=1, F13 = 0, F11= 0, F31=0, F33=0

(4)F21+F22+F23+F24=1

The view factors between surfaces 1 and 2 can be computed using the following equations,

$$(5)\ F_{21} = \frac{1}{R} - \frac{1}{\pi R}\left\{\cos^{-1}\left(\frac{B}{A}\right) - \frac{1}{2L}\left[\cos^{-1}\left(\frac{B}{RA}\right)\right]\sqrt{(A+2)^2-(2R)^2} + B\sin^{-1}\left(\frac{1}{R}\right) - \frac{\pi A}{2}\right\}$$

(6)

$$F_{22} = 1 - \frac{1}{R} + \frac{2}{\pi R}\tan^{-1}\left(\frac{2\sqrt{R^2-1}}{L}\right)$$

$$-\frac{L}{2\pi R}\left[\frac{\sqrt{4R^2+L^2}}{L}\sin^{-1}\left(\frac{4(R^2-1)+(L^2/R^2)(R^2-2)}{L^2+4(R^2-1)}\right) - \sin^{-1}\left(\frac{R^2-2}{R^2}\right) + \frac{\pi}{2}\left(\frac{\sqrt{4R^2+L^2}}{L}-1\right)\right]$$

where

$$R = \frac{r_2}{r_1},\ L = \frac{l}{r_1}$$

$A = L^2 + R^2 - 1$, $B = L^2 - R^2 + 1$

r_1 is the radius of the inner cylinder, r_2 is the radius of the outer cylinder and l is the length of the cylinders.

Based on the current YM repository in-drift geometry, r_1 is 0.835m and r_2 is 2.75m. The average length of a drift is ~1000m, which means the cylinders can be considered as of infinite length. This conjecture will be proven below. Also ε1=0.8, ε2=0.92, ε3=1.0, ε4=1.0

If we assume the WP and the drift are concentric cylinders, we can apply the above equations (5) and (6) and find the values for F21 and F22,

(7) F21= 0.3032 and F22 = 0.6947.

Substituting these values into (4) and noting F23=0, we get
(8) F24 = 0.0021

The reciprocity rule indicates A1 F12 = A2 F21. In this case, A1=$2\pi r_1 l$=5246 m^2 and A2=$2\pi r_2 l$=17279 m^2, so
(9) F12=0.9987
and from equation (3),
(10) F14 = 0.0013
The closeness of F12 to 1.0 confirms the "infinite length" conjecture.

Now all the view factors have been found, we can proceed to calculate the temperatures. (Seigel and Howell, equation 7-31)

$$(11)\ \sum_{j=1}^{N}\left(\frac{\delta_{kj}}{\varepsilon_j} - F_{kj}\frac{1-\varepsilon_j}{\varepsilon_j}\right)\frac{Q_j}{A_j} = \sum_{j=1}^{N}\left(\delta_{kj} - F_{kj}\right)\sigma T_j^4 = \sum_{j=1}^{N} F_{kj}\sigma\left(T_k^4 - T_j^4\right)$$

This yields the following system of equations,

$$\frac{1}{\varepsilon_1 A_1}Q_1 - \frac{F_{12}(1-\varepsilon_2)}{\varepsilon_2 A_2}Q_2 + F_{12}\sigma T_2^4 = \sigma T_1^4$$

$$-F_{21}\frac{(1-\varepsilon_1)}{\varepsilon_1 A_1}Q_1 + \frac{1-F_{22}(1-\varepsilon_2)}{\varepsilon_2 A_2}Q_2 - (1-F_{22})\sigma T_2^4 = -F_{21}\sigma T_1^4 - F_{24}\sigma T_4^4$$

$$\frac{1}{\varepsilon_3 A_3}Q_3 - \sigma T_3^4 = -F_{34}\sigma T_4^4$$

Part II

Before proceeding further, we have to revise the above conceptual model a bit to reflect the YM drift model. Since A3 is really the whole repository surface and A4 the space surrounding the repository, we shall choose to remove A3 and A4 completely from the model. The smallness of F24 and F14 supports the decision we make here. Q1 is the total flux emanates from all WPs in a drift. This renders the above system of equations into,

$$\frac{F_{12}(1-\varepsilon_2)}{\varepsilon_2 A_2}Q_2 + \sigma T_1^4 = F_{12}\sigma T_2^4 + \frac{1}{\varepsilon_1 A_1}Q_1$$

$$\frac{1-F_{22}(1-\varepsilon_2)}{\varepsilon_2 A_2}Q_2 + F_{21}\sigma T_1^4 = F_{21}\frac{(1-\varepsilon_1)}{\varepsilon_1 A_1}Q_1 + (1-F_{22})\sigma T_2^4$$

Assuming the length of the drift is 1000m, and the peak heat load per WP is 300 W/m, then Q1 is 3.0e5 W.

Using some representative T2 from the numerical simulation, here is the prediction about T1,

- If the peak T2 is 150C or 423 K, T1 is 154C.
- If the peak T2 is 130C or 403 K, T1 is 134C.

Entries into Scientific Notebook # 649E for this period have been made by

Name: Alexander Sun

Signature [signature] Date 5/16/06

I have reviewed this scientific notebook and find it in agreement with QAP–001.

EM: Dr. Gordon Wittmeyer

Signature [signature] Date 5/18/2006