

**DEVELOPMENT AND TESTING OF A METHOD FOR
EFFICIENT SIMULATION OF EVAPORATION
FROM A SEEPAGE FACE**

C. Fredrik Ahlers, Teamrat Ghezzehei, Stefan Finsterle

Earth Sciences Division
Lawrence Berkeley National Laboratory
1 Cyclotron Road
Berkeley, California 94720, United States

Paper presented at:

TOUGH Symposium 2003
Lawrence Berkeley National Laboratory
May 12–14, 2003

This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor The Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or The Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof, or The Regents of the University of California.

DEVELOPMENT AND TESTING OF A METHOD FOR EFFICIENT SIMULATION OF EVAPORATION FROM A SEEPAGE FACE

C. Fredrik Ahlers¹, Teamrat Ghezzehei, Stefan Finsterle

Earth Sciences Division
Lawrence Berkeley National Laboratory
1 Cyclotron Road
Berkeley, California 94720, United States
e-mail: Rick.Ahlers@lfr.com

ABSTRACT

Evaporation from the surface of a porous medium is a complex process, governed by interplay between (1) coupled liquid and vapor flow in the porous medium, and (2) relative humidity, temperature, and aerodynamic conditions in the surrounding air. In order to avoid the computational expense of explicitly simulating liquid, gas, and heat flow in the porous medium (and the possible further expense of simulating the flow of water vapor in the atmosphere), evaporative potentials can be treated in a simplified manner within a model where liquid is the only active phase. In the case of limited air mixing, evaporation can be approximated as a diffusion process with a linear vapor-concentration gradient.

We have incorporated a simplified scheme into the EOS9 module of iTOUGH2 to represent evaporation as isothermal Fickian diffusion. This is notable because the EOS9 module solves a single equation describing saturated and unsaturated flow, i.e., phase transitions and vapor flow are not explicitly simulated. The new approach was applied to three simple problems and the results were compared to those obtained with analytical solutions or the EOS4 module, which explicitly considers advective and diffusive vapor flow. Where vapor flow within the porous medium can be neglected, this new scheme represents significant improvement over the computational expense of explicitly simulating liquid, gas, and heat flow, while providing an adequate reproduction of the overall hydrologic system. The scheme is set up to allow parallel flow of liquid and vapor, so that evaporation from an actively seeping face can be simulated. In addition, dynamic relative humidity boundary conditions can be simulated using standard iTOUGH2 features.

INTRODUCTION

Seepage into underground openings, such as tunnels, is an issue that concerns several industries, including mining, transportation, and nuclear waste disposal. Methods for estimating seepage can be as simple as gauging the flow seeping into the tunnel, if condi-

tions for which the estimation is to be used are not expected to change. However, more complex methods of characterizing seepage are needed if conditions under which seepage is occurring change, e.g., infiltration or percolation driving the seepage changes, the size and/or shape of the opening changes, or the evaporative potential exerted by the atmosphere in the tunnel changes. This last condition can be significant when the seepage rate is relatively low and/or when the evaporative potential is expected to change dramatically. Evaporation effects must be carefully considered if (for example) the seepage potential is characterized using data collected in a tunnel ventilated with low-humidity air, and then the estimated seepage potential is used to predict long-term seepage behavior under low percolation and unventilated conditions.

Evaporation from a rock or soil surface is a process that, when coupled with liquid flow in the rock or soil, is difficult and/or computationally expensive to simulate. The EOS4 module of iTOUGH2 describes nonisothermal two-phase flow of water and air with vapor-pressure-lowering effects included, i.e., it is possible to incorporate evaporation from a surface and within the porous medium assuming that vapor diffusion is described by Fick's law. However, this is computationally expensive because liquid, gas, and heat flow are all explicitly simulated. On the other end of the spectrum, the problem could be simplified by estimating the amount of water that is removed from the surface by evaporation and simply include that in a simulation as a mass sink at or near the surface. This approach has the disadvantage of not accounting for boundary condition changes, e.g., temporal changes in the percolation rate driving water toward the seepage face or in the relative humidity in the atmosphere driving the evaporative potential at the surface.

In this paper, we present a method that attempts to compromise between the overly simplified model and the computationally expensive model. The method is an addition to the Richards' equation only approach to simulating unsaturated flow used in the EOS9

¹ Now with LFR Levine•Fricke, 3150 Bristol Street, Suite 250, Costa Mesa, California 92626

module, i.e., that of simulating only an isothermal liquid phase.

THEORY

Evaporation from a surface can be assumed to behave as Fickian-type diffusion of the vapor between the liquid surface and a well-mixed atmosphere with specified relative humidity a certain distance from the liquid surface. In this case, the vapor diffusion rate is calculated from a linear potential gradient over a fixed distance. This can be made analogous to a Richards' equation approach to liquid flow.

In order to use a Richards' equation approach to the problem of evaporation from a rock face, an appropriate capillary pressure must be specified at the atmospheric boundary node. Kelvin's equation relates the relative humidity h [-] to the capillary pressure P_c [Pa]:

$$P_c = \frac{\rho_l RT}{M_w} \ln(h) \quad (1)$$

where M_w [kg mol⁻¹] is molecular weight of water, ρ_l [kg m⁻³] is liquid density, R [J K⁻¹ mol⁻¹] is the universal gas constant, and T [K] is temperature.

A second requirement for using a Richards' equation approach is that the problem must be set up so that the liquid flux corresponds to the "evaporating" mass flux. Liquid-phase flux F_l [kg s⁻¹ m⁻²] can be described by

$$F_l = -k \frac{k_{rl}}{\mu_l} \rho_l (\nabla P_c - \rho_l g) \quad (2)$$

where k [m²] is permeability, k_{rl} [-] is liquid relative permeability, μ_l [Pa·s] is liquid viscosity, and g is gravity.

Similarly, diffusive vapor flux F_v [kg s⁻¹ m⁻²] can be expressed as

$$F_v = -D_{va}^0 \tau \phi S_g \frac{P_0}{P_g} \left(\frac{T}{273.15} \right)^n \nabla C_v \quad (3)$$

where D_{va}^0 [m² s⁻¹] is the strength parameter for diffusive vapor flux at standard conditions ($T = 273.15$ K and $P = 10^5$ Pa), τ [-] is tortuosity, ϕ [-] is porosity, S_g [-] is gas saturation, P_0 [Pa] is standard pressure (10^5 Pa), P_g [Pa] is gas pressure, n [-] is a fitting parameter for the temperature dependence of the diffusion coefficient, and C_v [kg m⁻³] is the vapor concentration.

The vapor concentration C_v can be expressed in terms of relative humidity as follows:

$$C_v = \frac{M_w P_{v,sat} h}{RT} \quad (4)$$

where $P_{v,sat}$ [Pa] is saturated vapor pressure.

If gravity is neglected in Equation 2 and the tortuosity, porosity, and gas saturation product is set to unity in Equation 3, an equivalent permeability, k_{eq} [m²], that allows liquid flux (Eq. 2) to equal diffusive vapor flux (Eq. 3) is

$$k_{eq} = D_{va}^0 \frac{P_0}{P_g} \left(\frac{T}{273.15} \right)^n \frac{\mu_l}{\rho_l} \frac{M_w P_{v,sat}}{RT} \left\{ \frac{\exp \left[\frac{M_w P_{c,F}}{\rho_l RT} \right] - h_A}{P_{c,F} - \ln(h_A) \frac{\rho_l RT}{M_w}} \right\} \quad (5)$$

where h_A [-] is the relative humidity in the well-mixed portion of the atmosphere, and $P_{c,F}$ [Pa] is the capillary pressure at the seepage face. This also assumes that the gradients in Equations 2 and 3 are parallel such that the change in distance cancels from both sides of the equality.

IMPLEMENTATION IN iTOUGH2

In order to implement evaporation in the Richards' equation module of iTOUGH2, several specific conditions need to be met.

For connections over which an evaporative flow rate shall be calculated (rather than a standard liquid flow rate according to Richards' equation), the user must assign a connection index value (TOUGH2 variable ISOT) of -16 to -18, instead of the usual 1 to 3.

Effective permeability (Eq. 5) on this connection is internally calculated based on the capillary pressure at the face of the porous medium, the relative humidity in the well-mixed atmosphere, and the temperature and pressure conditions specified (default temperature and pressure conditions are used if none are specified). Relative humidity is specified using the first primary variable (otherwise saturation), and it is converted to capillary pressure by selecting Kelvin's equation (Eq. 1) as the capillary pressure function.

As shown in Figure 1, the connection for evaporation from a porous-medium face is added adjacent to the connection for liquid flow from the face. As discussed above (see Equation (5)), gravity is neglected across evaporative connections.

Time-varying humidity can be specified for the well-mixed atmospheric boundary condition using the first primary variable, liquid saturation, and the TIMBC, USERBC, or RESTART feature of iTOUGH2.

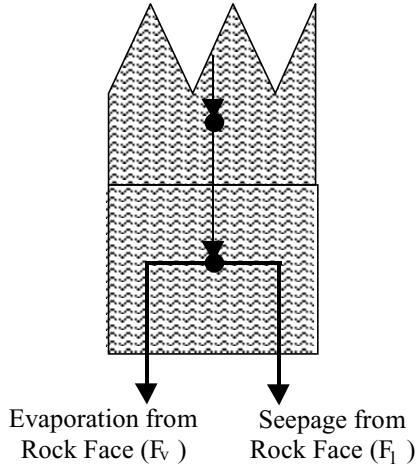


Figure 1. Evaporation and seepage connections from the seepage face.

TESTING

Two simple test cases were used to verify that the approach functioned correctly: first, a variety of capillary pressures (relative humidities) were specified for a two-node system, and the direction and magnitude of the flux were verified analytically by Equation 3; second, expected performance was verified under a range of percolation rates for a fixed evaporative potential.

The range of validity of the approach was also tested by comparing saturation profiles and fluxes between the simplified approach and an EOS4 simulation of the same system. As a byproduct of this comparison, the relative efficiency of the new approach can be evaluated.

First Test Case

A simple test case is used to verify that the coding is correct. Diffusive vapor flux from a seepage face to a well-mixed atmospheric boundary is calculated for a range of capillary pressures at the seepage (rock) face (shown as equivalent relative humidity in Figure 2) and a range of relative humidities at the atmospheric boundary. Figure 2 shows the simulation results, which are verified against a hand calculation of the flux by Equation 2 and found to be correct.

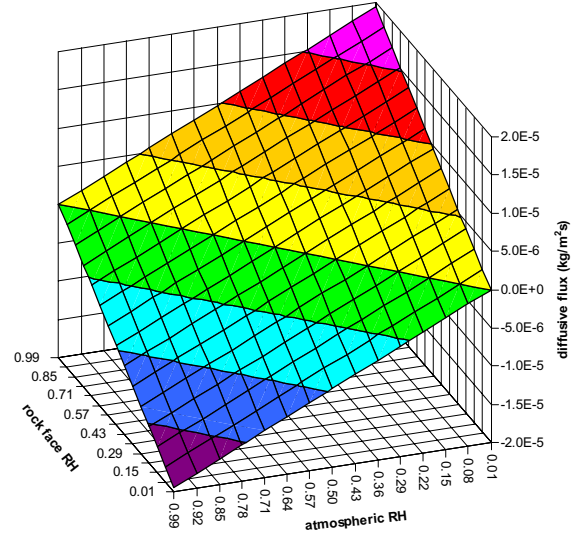


Figure 2. Diffusive vapor flux as a function of relative humidity at the rock face and within the well-mixed atmosphere.

Second Test Case

The capacity of the code to simulate evaporation and seepage simultaneously is verified in a simple vertical column. Water is applied at a constant rate to the top of the column. At the bottom boundary of the column, a seepage boundary condition (with zero capillary pressure) is applied for regular liquid-flow connections. In addition, for evaporation-flow connections, the capillary pressure is set as a function of relative humidity according to Equation (1).

The system is allowed to develop until steady state conditions are reached. The steady-state evaporation rate, seepage rate, and saturation at the seepage face are recorded. The simulation is repeated over a range of percolation rates from zero to more than the evaporative capacity at the lower boundary. Figure 3 shows that, as expected, at the point where the percolation rate exceeds the evaporative capacity at the lower boundary, saturation at the seepage face reaches 100%, the evaporation rate reaches a maximum, and seepage is initiated. At percolation rates greater than the evaporative capacity, all excess flux results in seepage.

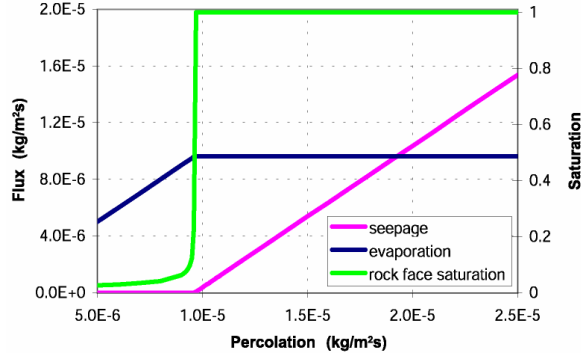


Figure 3. Liquid flux (seepage) and vapor flux (evaporation) in a horizontal column toward an evaporative boundary simulated with EOS4.

Range of Validity of Approach

Because this approach is used to simulate only the diffusion of water vapor from a rock or soil surface, it should be applied in a narrow range of circumstances. Of course, where advective vapor flux in or from the porous medium is an important component of overall mass flux, modules such as EOS3 (for nonisothermal two-phase flow of air and water) or EOS4 (same as EOS3 with vapor-pressure-lowering effects included) should be used. Similarly, where diffusive vapor flux in the porous medium is a significant contributor to the overall mass flux, this approach is unlikely to give reasonable results.

A simple problem is set up to demonstrate under which conditions reasonable results can be expected from this approach. A horizontal column is initiated with a saturation of 90%. At one end of the column, an evaporative boundary condition is specified, i.e., the only mechanism for mass transfer across the boundary is vapor diffusion. All other boundaries are no flow. Conditions in the column are simulated with the EOS4 module and the EOS9 module with the evaporative boundary condition modification.

Figures 4 and 5 show the saturation profiles within the column at increasing times. Note that the evaporative condition is applied at the boundary at 0 m, and the total length of the column is 10 m. The figures only show one meter of the column, adjacent to the evaporative boundary. At early times, when the saturation is high throughout the column, the profiles generated by the modified EOS9 and EOS4 are indistinguishable from each other. At later times, when the saturation near the evaporative boundary is reduced, the modified EOS9 underestimates the amount of saturation reduction, because evaporative vapor flow is only applied across the last connection between the column and the boundary, but not within the porous medium itself. If saturation is sufficiently reduced, liquid relative permeabilities and thus liquid

flow rates are very small. Under these conditions, diffusive vapor flow within the porous medium becomes significant, an effect correctly captured by the EOS4 module. This is particularly evident at the latest time shown, where the EOS4 simulation creates a drying front extending approximately 0.3 m into the porous medium. Note that the saturation value at the porous medium face at late times is approaching the value where the capillary pressure at the face is equivalent to the relative humidity boundary condition (as expressed in Equation 1). Beyond the drying front in the porous medium, however, the saturation profiles approach each other within a short distance; one meter into the porous medium at the latest time, the saturation values are nearly the same.

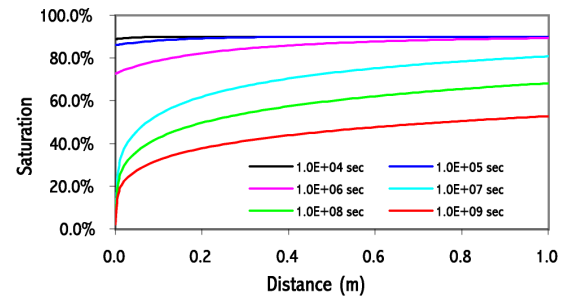


Figure 4. Saturation profile in a horizontal column with flow toward an evaporative boundary simulated with modified EOS9.

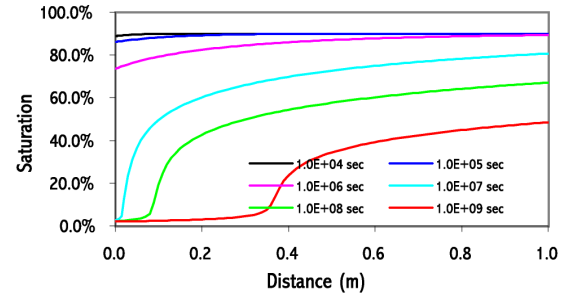


Figure 5. Saturation profile in a horizontal column with flow toward an evaporative boundary simulated with EOS4.

Figures 6 and 7 show the flux profiles in the column at increasing times. At early times, the flux profiles are nearly identical. At later times, the liquid flux, shown in Figure 7 as thin lines, reduces abruptly at the drying front in the EOS4 simulation, while it steadily increases toward the porous medium face in the modified EOS9 simulation. Note that at late times the total flux (liquid plus vapor) simulated with EOS4 is nearly the same as the liquid flux simulated with the modified EOS9.

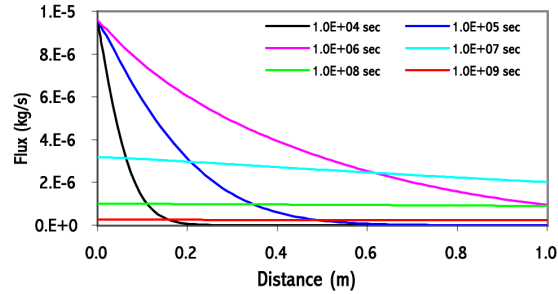


Figure 6. Liquid flux in a horizontal column toward an evaporative boundary simulated with modified EOS9.

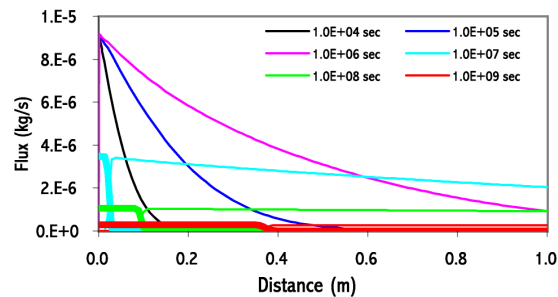


Figure 7. Liquid (thin line) and vapor (thick line) flux in a horizontal column toward an evaporative boundary simulated with EOS4.

Computational Savings of Approach

For simple problems such as those described in the above comparison, execution times were approximately two orders of magnitude faster using the simplified approach described here. For more complex problems, such as those described by Ghezzehei et al. (2003, these proceedings) attempts to estimate the computational savings were unsuccessful because of difficulties in obtaining a complete EOS4 simulation.

CONCLUSION

In order to simulate evaporation from a porous medium face, liquid flux as expressed in Richards' equation is equated with water vapor flux as given by Fickian-type diffusion. An equivalent permeability can be calculated so that the mass flux calculated by Richards' equation will be the same as that calculated

by a Fickian-diffusion type approach. The equivalent permeability is calculated for specific conditions of relative humidity in a well-mixed atmospheric boundary condition and capillary pressure at the porous medium face. Through specific gridding, this approach allows evaporation from a porous medium face to be simultaneously simulated with seepage from the same face. This approach has been incorporated into the EOS9 module of iTOUGH2, so that at each time step the equivalent permeability is recalculated, enabling the effects of a dynamic relative humidity boundary condition to be simulated.

The approach was tested by two relatively simple problems. The first test confirmed that the equivalent permeability has been correctly calculated. The second test showed that the approach with parallel connections for liquid and vapor flow is capable of appropriately simulating simultaneous seepage and evaporation from a porous medium face. Limitations of the approach are encountered when simulating relatively strong evaporation in combination with a small liquid flux in the porous medium. Under these conditions, a dry-out zone develops and propagates into the porous medium, a process more accurately represented by the two-phase module EOS4. Nevertheless, the new approach still provides an adequate solution in the region beyond the drying front.

ACKNOWLEDGMENT

The reviews of Yingqi Zhang and Sonia Salah are greatly appreciated. This work was supported by the Director, Office of Civilian Radioactive Waste Management, U.S. Department of Energy, through Memorandum Purchase Order EA9013MC5X between Bechtel SAIC Company, LLC, and the Ernest Orlando Lawrence Berkeley National Laboratory (Berkeley Lab). The support is provided to Berkeley Lab through the U.S. Department of Energy Contract No. DE-AC03-76SF00098.

REFERENCES

Ghezzehei, T., S. Finsterle, and R. Trautz, Evaluating the Effectiveness of Liquid Diversion around an Underground Opening when Evaporation is Non-negligible, *Proceedings: TOUGH Symposium 2003*, Berkeley, Calif., May 12–14, 2003.