AIR-TOUGH: A FULLY 3-DIMENSIONAL LINKING OF ATMOSPHERE WITH SOIL USING EDDY DIFFUSIVITY CONCEPT AND V-TOUGH

Parviz Montazer
Multimedia Environmental Technology, Inc.
3990 Westerly Place, Suite 200
Newport Beach, California 92660
(714) 852-9767

ABSTRACT

In arid climates, evapotranspiration is a strongly-coupled thermodynamic process that is controlled by the interaction of the atmospheric boundary layer and the upper soil surface. Simulation of this process requires a fully-coupled thermodynamic multi-phase fluid-flow and energy-transport code. Such a code was developed in a previous investigation using V-TOUGH. The resulting efficient computer code, A-TOUGH, simulates the effect of dynamic atmospheric fluctuations on vapor movement between the soil and the atmosphere and the resulting moisture movement in the soil. However, the coupling between the atmosphere and soil employed eddy diffusivity which was only a function of time and not a function of space. In the present study the code is extended to allow spatial as well as temporal variation of eddy diffusivity.

I. INTRODUCTION

The problem of interfacing the atmosphere with the surface soil layer is that the flow of air in the atmosphere is turbulent even during the calmest days [2,5]. The transport of vapor in the atmospheric boundary layer near the ground surface is very fast and can be simulated with eddy diffusion. Eddy diffusion is the mixing process between adjacent layers of the air stream with different velocities. The mathematical description of the transport of vapor and other compounds across layers of fluid under turbulent conditions has been the subject of studies in chemical engineering for a number of years[1]. Exact mathematical models of such systems require solution of the Navier-Stokes and material/energy balance equations. Solving these equations is a very difficult task even for simple systems. Numerical solutions are implemented in the atmospheric sciences; however, they are not practical for application to simple evaporation from the soil due to extensive computer requirements. The eddy diffusivity simplification has been used instead to describe the mass and energy transfer across the boundary layers in turbulent conditions[1,2,5]. The transport of vapor from the molecular sublayer to the atmosphere is a function of surface roughness, wind shear, and thermal stratification as well as the humidity (or vapor concentration) gradient. Therefore, the rate of vertical vapor transfer (or evaporative flux) is given by:

$$q_{evap} = -D^{*}_{atm} \left. \frac{\partial \rho}{\partial z} \right|_{z_0} \qquad (1)$$

and

$$\rho(z) = \rho^{*}(z) h(z) \qquad (2)$$

where ρ is vapor density, ρ^{*} is saturated-vapor density, and h is humidity. Eqn. 1 is similar to Fick's law except that the molecular diffusion coefficient is replaced with D^{*}_{atm}, the eddy diffusivity. Eddy diffusivity varies with time as temperature and wind speed change with time. Therefore, in order to couple soil processes with atmospheric processes, the eddy diffusivity and the thermal diffusivity parameters must be varied dynamically in addition to the soil boundary conditions.

The principles described above can also be used to approximate transfer of heat across atmospheric layers with turbulent flow[5]:

$$F_{SH}(z) = K_H \rho c_p \frac{\partial T}{\partial z} \qquad (3)$$

where K_H is the eddy diffusion coefficient for heat (which in this case is set equal to D^{*}_{atm}), ρ is the density of air, c_p is the atmospheric specific heat at constant pressure, T is the temperature, and z is the vertical distance above the ground surface. Therefore, thermal conductivity is calculated for the atmospheric layers as:

$$K_{atm} = D^{*}_{atm} \rho c_p \qquad (4)$$

II. DESCRIPTION OF THE MODEL

A-TOUGH (Atmospheric TOUGH) was based on V-TOUGH (the Vectorized-version of TOUGH, Transport Of Unsaturated Ground water and Heat). TOUGH was originally developed by Pruess[4] and vectorized by Nitao[4]. A-TOUGH can simulate the 3-dimensional transport of air, vapor, and heat through an atmospheric media which can be directly coupled with the transport of moisture, an air-vapor mixture, and heat through porous and/or fractured media. However, it is limited in variation of the eddy diffusivity in space. This is an important limitation for application to sites such as Yucca Mountain where mountainous terrain results in substantial spatial variation of eddy diffusivity.

The resulting code was tested with many simple and some relatively complicated problem sets, including a two-dimensional low-level radioactive waste trench with a layered cap. In addition, the code was verified against the U.S. Geological Surveys code VS2D[3]. The three-dimensional nature of the code could not be tested due to unavailability of data at time of this publication.

III. RESULTS AND CONCLUSIONS

The long-term effect of changes in atmospheric climatological conditions on subsurface hydrological conditions in the unsaturated zone in arid environments is an important factor in determining the performance of a high-level and low-level radioactive waste repositories in geological environment. Computer simulation coupled with paleohydrological studies can be used to understand and quantify the potential impact of future climatological conditions on repository performance. Air-TOUGH efficiently simulates (given current state-of-the-art technology) the physical processes involved in the near-surface atmosphere and its effect on subsurface conditions. This efficiency is due to the numerical techniques used in TOUGH and the efficient computational techniques used in V-TOUGH to solve non-linear thermodynamic equations that govern the flux of vapor and energy within subsurface porous and fractured media and between these media and the atmosphere.

REFERENCES

1. Bird, R.B., Stewart W.E., and E.N. Lightfoot (1965): Transport phenomena; John Wiley & Sons, New York, New York; 780 pp.

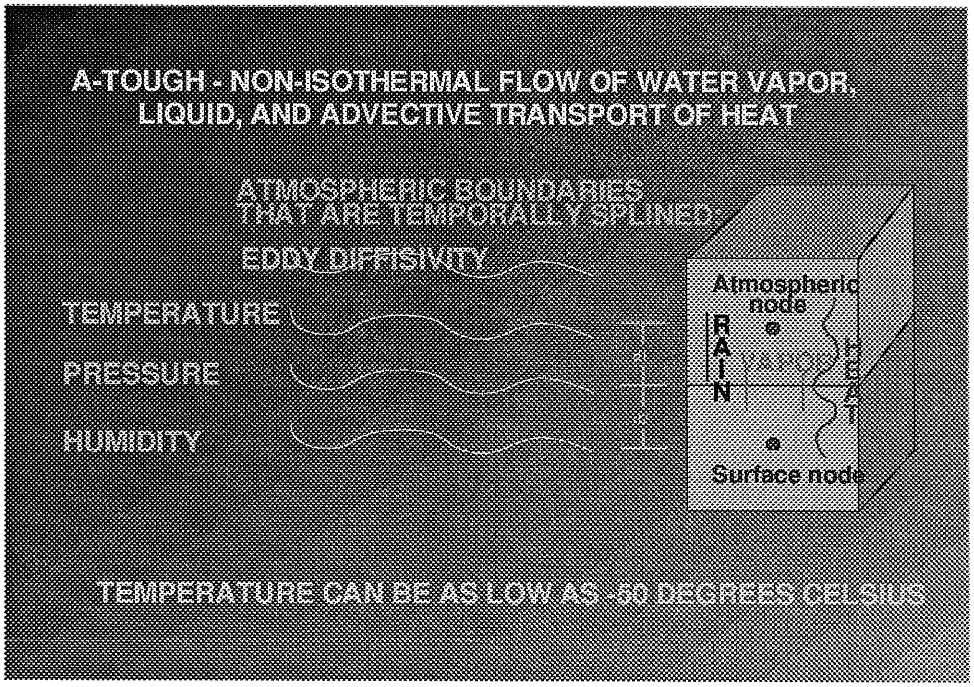
2. Brutsaert, W. H. (1982): Evaporation into the atmosphere: Theory, history, and applications; D. Reidel Publishing Company, London, England; 299 pp.

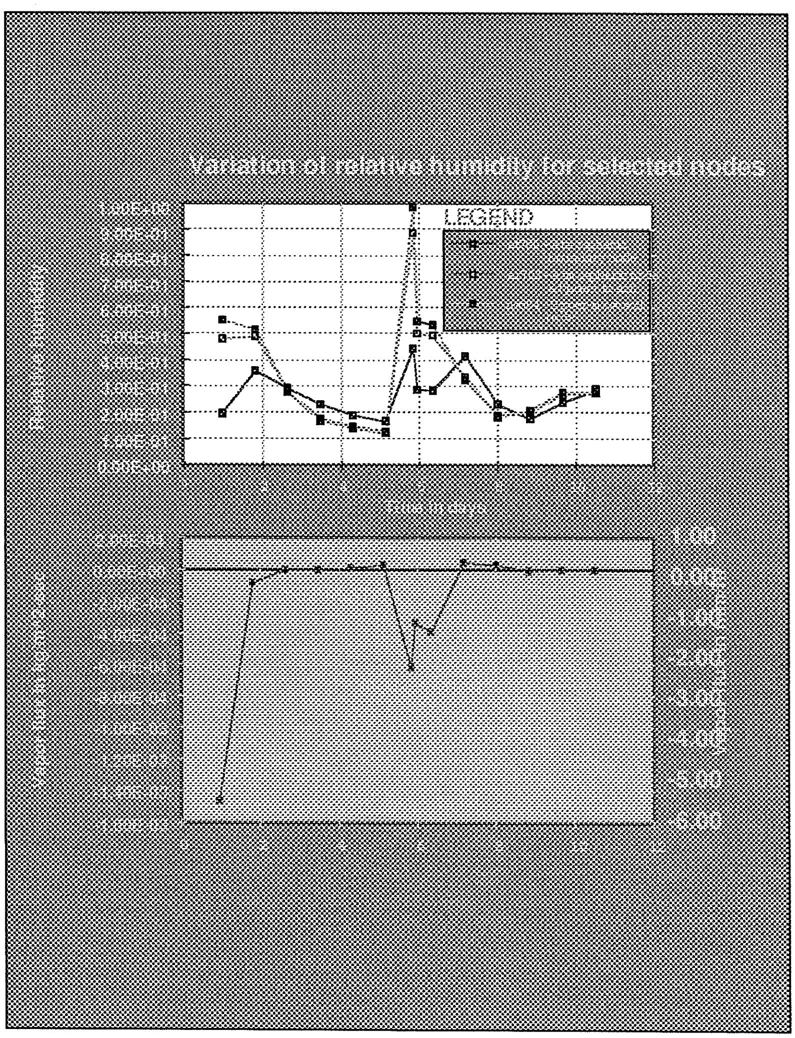
3. Lappala, E.G., Healy, R.W., and E.P. Weeks (1987): Documentation of computer program VS2D to solve the equations of fluid flow in variably saturated porous media; United States Geological Survey - Water Resources Investigation Report 83-4099, Denver, Colorado; 184 pp.

4. Nitao, J. J. (1989): V-TOUGH - An enhanced version of the TOUGH code for the thermal and hydrologic simulation of large-scale problems in nuclear waste isolation; Earth Sciences Department, Lawrence Livermore National Laboratory, Draft 1.1, November 18; 24 pp.

5. Peixoto, J.P. and A.H. Oort (1992): Physics of climate; American Institute of Physics, New York, New York; 520 pp.

6. Pruess, K. (1987): TOUGH user's guide; Earth Sciences Division, Lawrence Berkeley Laboratory, University of California, Berkeley, California, LBL-20700; 78 pp.


A-TOUGH - NON-ISOTHERMAL FLOW OF WATER VAPOR, LIQUID, AND ADVECTIVE TRANSPORT OF HEAT
ATMOSPHERIC BOUNDARIES THAT ARE TEMPORALLY SPLINED:
EDDY DIFFISIVITY
TEMPERATURE
PRESSURE
HUMIDITY
Atmospheric node
R A I N
VAPOR
H E A T
Surface node
TEMPERATURE CAN BE AS LOW AS -50 DEGREES CELSIUS


Variation of relative humidity for selected nodes
LEGEND
1.00
0.00
-1.00
-2.00
-3.00
-4.00
-5.00
-6.00