Geophysical Research Abstracts
Vol. 15, EGU2013-11469, 2013
EGU General Assembly 2013

Evaporation from soils under diurnal boundary conditions: Experimental and modeling investigation to evaluate Non-equilibrium-based approaches

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Evaporation from bare soil is a key component of the hydrologic cycle and the process primarily responsible for governing water and energy exchanges between the land and atmosphere. Despite its importance, there is still a great deal of uncertainty associated with our current understanding of this complex multiphase phenomenon. A common approach when modeling the movement of liquid water, water vapor and heat in the soil immediately below the land-atmosphere interface is to assume that water vapor concentration in air is always in equilibrium with liquid water. However, this equilibrium assumption is called into question by experiments about liquid/gas phase change in porous media suggesting that the equilibrium establishment is not instantaneous; a volatilization or condensation time is observed at the macroscopic scale under certain conditions. Introduction of such a non-equilibrium mass transfer relationship is based on the Hertz-Knudsen equation (HKE) derived from the kinetic theory of gases. Multiple formulations have been presented to represent the rate of phase change between water and vapor, many relying on empirical fitting parameters due to limited experimental data.

The purpose of this work is to perform an unbiased comparison between various conceptual and mathematical formulations for non-equilibrium phase change on evaporation and develop appropriate numerical models to be used in simulations. The key to such a comparison is the availability of accurate data. As such data at the scale of interest is not possible to obtain in field settings, a unique two-dimensional cell apparatus was developed. The test cell was equipped with a network of sensors for automated and continuous monitoring of soil moisture, soil and air temperature and relative humidity, and wind velocity to generate precision data. A fully-coupled numerical model to solve the governing equations for heat, liquid water and water vapor transport in soil was developed. The code implements a non-isothermal solution that accounts for non-equilibrium liquid/gas phase change with gas phase vapor diffusion. Several numerical simulations were performed for different theoretical formulations of phase change, allowing for evaporation/condensation processes to be investigated. The numerical formulations/code, was validated using date generated through a series of experiments conducted in the test cell under varying boundary conditions.

Results from numerical simulations were compared with experimental data. Initial comparisons of various formulations demonstrate the importance of properly including evaporation and condensation behavior in modeling efforts to estimate evaporation. Detailed comparisons are still underway. This knowledge is applicable to many current hydrologic and environmental problems to include climate modeling and the simulation of contaminant transport and volatilization in the shallow subsurface.