Numerical Analysis of Coupled Liquid Water, Water Vapor, and Heat Transport in a Sandy Loam Soil

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Abstract
Information on the coupled liquid water, water vapor and heat transport under arable field conditions is still limited, particularly in semi-arid unsaturated soils such as arid southern New Mexico. Hydrus-1D model was applied to evaluate various transport mechanisms associated with temporal variations in soil water content and soil temperature in the unsaturated zone of a sandy loam furrow-irrigated field located at Leyendecker Plant Science Research Center, Las Cruces. The model was calibrated and validated using measured soil water content and soil temperature in the sandy loam soil beds at four depths of 5, 10, 20, and 50 cm for a 19-day period from day of the year (DOY) 85 (26 March 2009) through DOY 103 (April 13 2009) and a 31-day period from DOY 104 (April 14 2009) through DOY 134 (14 May 2009), respectively. Measured soil hydraulic and thermal properties, and daily meteorological data were used in model simulations. Simulated results with the field experiment demonstrated that the model predicted soil water content and soil temperature and their temporal variations at all depths adequately. The total liquid water flux (comprised of isothermal and thermal liquid water) dominated the soil water movement during and early periods of an irrigation event, while the contribution of total water vapor flux (comprised of primarily thermal and much smaller isothermal water vapor) increased with increasing soil drying before and after irrigation. During the progressively soil drying process, the upward isothermal and thermal liquid water fluxes within 15 cm depth also served as potential sources of liquid water, which eventually changed to water vapor near the surface. Water vapor flux was much higher in the layer near soil surface and was approximately 10.4% of the total coupled water flux during the simulation period.

Key-words
Water content, vapor transport, energy balance, unsaturated zone, hydrus, TDR

Introduction
Temporal variations in soil moisture in unsaturated soil zone due to temperature gradients, especially in arid and semiarid agricultural fields, may induce water fluxes in gas and liquid phase, which can play a key role in soil mass and energy transfer near the soil surface. As soil moisture contents near the soil surface are usually low in arid and semiarid regions water vapor movement continues an important part of total water flux and energy balance in unsaturated soils in agricultural and engineering applications (Parlange et al. 1998). The soil water near the soil surface governs the partitioning of precipitation into surface runoff and infiltration, and the partitioning of incoming solar and atmospheric radiation into latent and sensible heat fluxes into the atmosphere (Parlange et al. 1998). Along with solar radiation and soil nutrients, the availability of soil moisture in arable soils is of paramount importance for crop growth and agricultural production. The importance of soil moisture resulted in development of models that simulate water transport both in the liquid and vapor phase. Considering the microscopic structure of a porous medium most of these models is based on theories that account for the coupled energy and mass flow in soil (Philip and De Vries, 1957). Philip and de Vries (1957) developed a moisture migration model (henceforth the PDV model) with inhomogeneous soil temperature profiles to account for the effects of temperature gradients on moisture migration. After almost two decades of discussion, the PDV model still remains the basis for most soil-atmosphere continuum modeling. A considerable attention has been paid to analyzing water transport both in the liquid and vapor phase under field and laboratory conditions (Nassar and Horton, 1992; Cahill and Parlange, 1998). The complexity of the coupled liquid water, water vapor and heat transport in the unsaturated zone and the difficulties associated with field measurements especially near the soil surface necessitate the application of numerical models to analyze these processes. Despite of increasingly interest in numerical model development, information on the movement of liquid water, water vapor and heat under field conditions is still limited, especially under arable soil conditions in Las Cruces. The objective was to model the coupled liquid water, water vapor, and heat transport in the unsaturated zone of a sandy loam onion field in Las Cruces using a numerical code Hydrus-1D.
Materials and Methods

Study Site and Field Measurements

Field experiment was carried out on a furrow-irrigated onion (*Allium Cepa*) field at the Leyendecker Plant Science Research Center (hereafter PSRC), New Mexico State University, New Mexico, USA (Latitude 32\°11.46′ N, Longitude 106\°44.40′ W, with an altitude ranged from 1128 to 1256 m above sea level). At the experiential field the dominant soil was a Harkey, which are characterized as deep, well-drained, formed on flood plains and low stream terraces along the Rio Grande Valley. The average annual temperature and precipitation for the experimental site are 17.7\°C and 29.7 cm, respectively (Gile *et al.* 1981). During a 50-day measurement period from DOY 85 (26 March 2009) to DOY 134 (14 May 2009), field was irrigated 9 times under furrow irrigation systems during DOY 86, DOY 93, DOY 99, DOY 107, DOY 114, DOY 118, DOY 127, DOY 130, and DOY 132.

Soil bulk density was determined by the core method (Blake and Hartge, 1986), saturated hydraulic conductivity by constant head method (Klute and Dirkson, 1986), soil water retention by pressure chamber method (Klute, 1986) and particle size distribution by the hydrometer method (Gee and Bauder, 1986). Temporal soil water content and soil temperature variations in the onion bed were measured using time domain reflectrometry (TDR) and temperature sensors (Campbell Scientific, Inc., Logan, Utah), respectively. Meteorological variables such as precipitation, solar radiation, air and soil temperatures, wind speed, and relative humidity were obtained from the local weather station. The daily average atmospheric transmission coefficient for solar radiation was estimated for the model input that incorporates transmission coefficients to calculate the daily potential global solar radiation (Campbell, 1985). Soil emissivity was estimated using the relationship given by van Bavel and Hillel (1976). The surface albedo was considered to depend on soil surface wetness according to the simple formulae given by van Bavel and Hillel (1976). When clouds are present the atmospheric emissivity on cloudy days was estimated by adding the energy emitted by the clear portions of the sky to the energy emitted by the clouds (Monteith and Unsworth, 1990), while the clear sky atmospheric emissivity was estimated based on equations given by Idso (1981).

Numerical Modeling

Nonisothermal uniform liquid vapor flow coupled with the heat transport in the unsaturated zone of a sandy loam field for a 50-day period from DOY 85 to 134, 2009 was simulated using the numerical model Hydrus-1D (Saito *et al.* 2006). Root water uptake was not considered.

Results and Discussion

Comparison of Hydrus-1D simulation with measurements

Simulated volumetric water content and soil temperature data are reasonably consistent with the field measurements and soil water content fluctuations predicted by the coupled model indicate that the field measurement is likely to account for both water and vapor flux. Despite a relatively consistent simulation of the temporal variation in soil water contents, Hydrus-1D slightly underpredicted soil water contents at all depths during the validation period. Similarly, there was tendency for simulation to follow the measured temporal soil temperature variation and the model predicted systematically lower soil temperatures at all depths as compared to measured ones, especially during the validation period.

Vertical Profiles of Liquid Water and Water Vapor Flux

The isothermal and thermal liquid water and water vapor fluxes are upward (positive values) almost throughout the entire profile above 15 cm depth at 0000 h of the ‘dry’ day DOY 114 before irrigation (Figure 1). The upward movement of isothermal liquid water and water vapor fluxes within 15 cm was attributed to moisture gradients, while thermal liquid water and water vapor fluxes were upward because of steep temperature gradients. Below a depth of 15 cm, isothermal and thermal liquid water and water vapor fluxes were downward (negative values) when moisture and temperature gradients changed from upward to downward. The isothermal and thermal liquid water fluxes varied from +0.002 to +0.07 cm/d and +0.0003 to +0.04 cm/d throughout the profile above 15 cm, respectively, while the corresponding variation ranges of fluxes were between -0.003 and -0.05 cm/d, and -0.003 and -0.044 cm/d throughout the profile below 15 cm depth.
Simulated vertical distributions of the isothermal and thermal liquid water and water vapor fluxes during a typical 72-h period before and after an irrigation event at 1800 h of DOY 114: (a) at 0000 h of DOY 114 before irrigation, (b) at 0000 h of DOY 115 after irrigation, (c) at 1200 h of DOY 115 (DOY 115.5) after irrigation, and (d) at 0000 h of DOY 116 after irrigation. Positive and negative values of abscissa (x-axis) indicate upward and downward fluxes, respectively.

The increasing upward isothermal and thermal liquid water fluxes above 15 cm indicated that liquid water in deeper layer was drawn to the surface by both moisture and temperature gradients. The variation ranges of the thermal water vapor flux were between +0.0014 and +0.044 cm/d above 15 cm, while the corresponding variation of thermal vapor flux ranged from zero (no flux) to -0.01 below 15 cm. The upward isothermal water vapor fluxes were markedly smaller in magnitude and almost negligible compared with thermal water vapor flux, which fluctuated mostly above 5 cm from zero (no flux) to +0.006 cm/d, while there was no isothermal water vapor flux below 5 cm. Both the upward total liquid water (both isothermal and thermal liquid water) and total vapor flux (mainly thermal water vapor) fluxes within 5 cm are responsible for the water vapor near the soil surface and thus the upward water transport at the experimental field. The total water vapor flux in this unsaturated soil layer of the furrow-irrigated sandy loam onion field contributed approximately 10.4% to total water flux.

Conclusions
Detailed analysis of vertical distributions of liquid water and water vapor fluxes indicated that both isothermal and thermal liquid water and thermal water vapor fluxes due to matric potential gradients associated with soil water content and soil temperature were responsible for water vapor near the soil surface at the experimental field. The liquid water flux dominated the soil water movement during and early periods of an irrigation event, while the contribution of vapor flux increased with increasing soil drying before and after irrigation.

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