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

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ABSTRACT

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 under varying atmospheric conditions. 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 data 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.

1. AIMS AND SCOPE

Modeling:

- ✓ Incorporate various phase change formulations into a traditional multiphase flow model developed by Smits et al. [2011]
- ✓ Demonstrate the accuracy of different phase change formulations by comparing COMSOL simulations to experimental evaporation data
- ✓ Calculate fitting coefficients for various phase change formulations using accurate experimental data collected in the laboratory to determine their change and dependence on different land-atmospheric boundary conditions

Experimental:

- ✓ Development of soil tank apparatus equipped with a sensor network for continuous and autonomous monitoring of soil moisture, relative humidity, temperature, and evaporation rates
- ✓ Generation of precision data under different well-controlled atmospheric boundary conditions

2. MATHEMATICAL THEORY

Existing phase change formulations are dependent on fitting parameters called: phenomenological coefficients (L_p , kg K s m⁻⁵), transfer coefficients (k_m , s m⁻²), constant of proportionality (b , s m⁻²), equilibrium time (t_{eq} , s), evaporation coefficients (f_e , m⁻¹), and condensation (f_c , m⁻¹)

2. MATHEMATICAL THEORY (con't)

Formulation 1 [Bénet et al., 2009]:

$$\dot{m} = -\frac{L_p R}{M_w} \ln\left(\frac{p_v}{p_{veq}}\right)$$

\dot{m} (kg m⁻³ s⁻¹): Rate of phase change
 R (Pa m³ K⁻¹ mol⁻¹): Universal gas constant
 M_w (kg mol⁻¹): Molecular weight of water
 p_v (Pa): Vapor pressure in the gas phase
 p_{veq} (Pa): Equilibrium vapor pressure

Formulation 2 [Prat, 2002]:

$$\dot{m} = k_m (p_v - p_{veq})$$

Formulation 3 [Bixler, 1985; Zhang and Datta, 2004]:

$$\dot{m} = \frac{b(\theta_w - \theta_{rw})RT}{M_w} (p_{veq} - p_v)$$

θ_w (m³ m⁻³): Volumetric water content
 θ_{rw} (m³ m⁻³): Residual water content
 T (K): Temperature
 p_v (Pa): Vapor density
 p_{veq} (Pa): Equilibrium vapor density

Formulation 4 [Le et al., 1995; Scarpa and Milano, 2002]:

$$\dot{m} = \frac{(\theta_w - \theta_{rw})}{t_{eq}} (\rho_{veq} - \rho_v)$$

$t_{eq} \approx \frac{l_{por}^2}{D_v}$
 l_{por} (m): Characteristic length of a cylindrical pore
 D_v (m): Effective vapor diffusion coefficient

Formulation 5 (Modified-Hertz Knudson):

$$\dot{m} = \phi \left(\frac{2\pi RT}{M_w}\right)^{0.5} (f_c p_v - f_e \rho_{veq})$$

$$f_e \approx 1 \text{ at high } T$$

$$\dot{m} = \phi \left(\frac{M_w}{2\pi RT}\right)^{0.5} (f_c \rho_v - \rho_{veq})$$

ϕ (m³ m⁻³): Porosity

Liquid water mass balance, water vapor mass balance, and energy conservation are coupled together using the non-equilibrium formulations in a non-isothermal multiphase COMSOL model to predict evaporation rates

Liquid Water Mass Balance [Bear, 1972]

$$\rho_w \frac{\partial \theta_w}{\partial p_c} \frac{\partial p_c}{\partial t} + \theta_w \frac{\partial \rho_w}{\partial t} + \nabla \cdot (\theta_w \rho_w \mathbf{u}_w) = -\dot{m}$$

Water Vapor Mass Balance [Bear, 1972]

$$\frac{\partial \rho_g w_v \theta_g}{\partial t} + \nabla \cdot (\theta_g \rho_g w_v \mathbf{u}_g - D_v \nabla (w_v \rho_g)) = \dot{m}$$

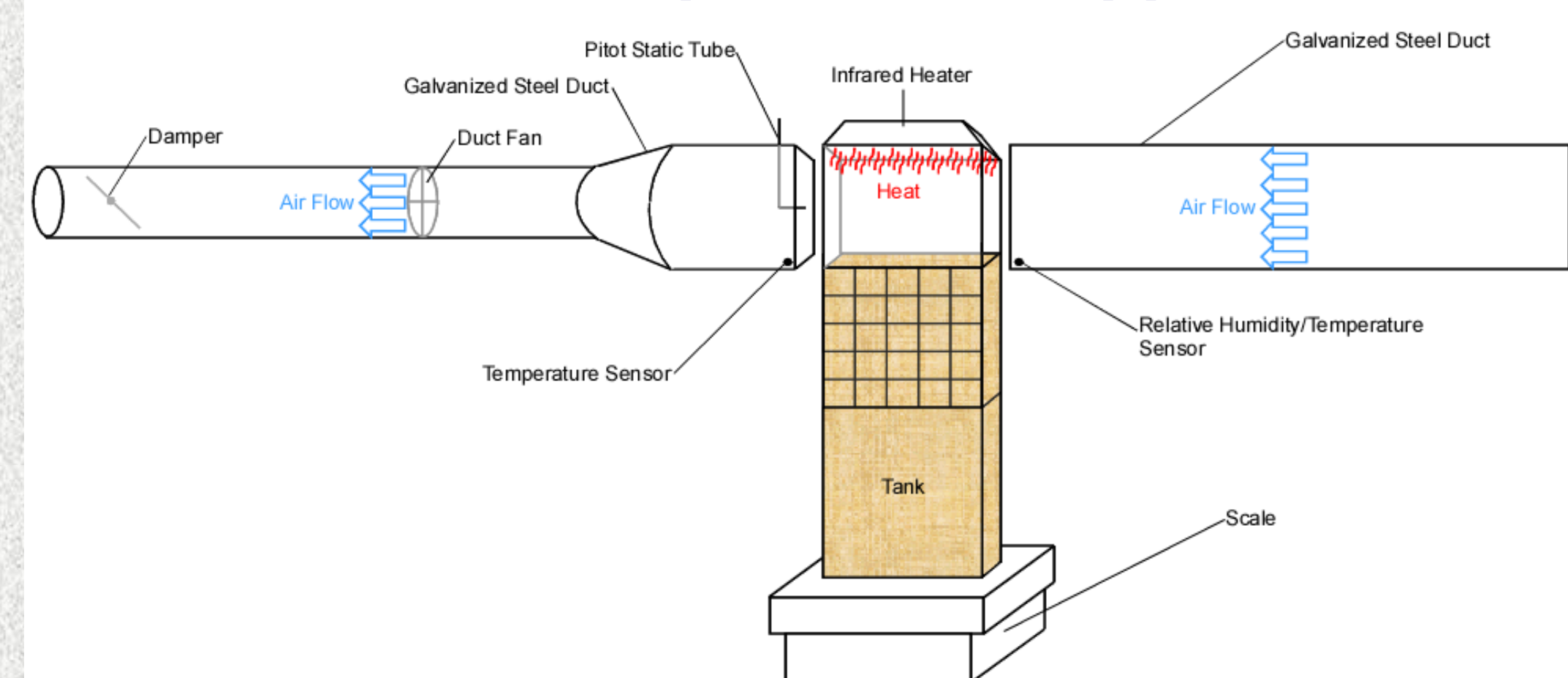
Energy Conservation

$$\nabla \cdot (C_g \rho_g T \mathbf{u}_g \theta_g + C_w \rho_w T \mathbf{u}_w \theta_w - \lambda_T \nabla T) + \frac{\partial \rho_b C_b T}{\partial t} = -LR_{gw} - Q_s$$

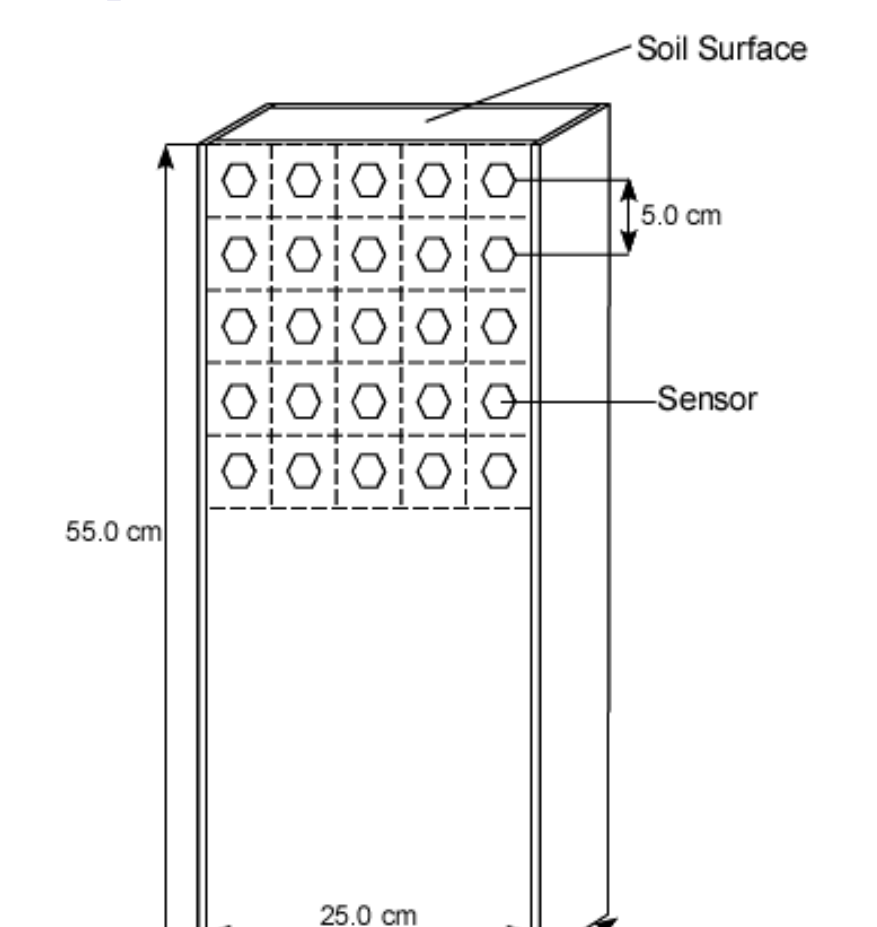
w and g denote the liquid and gaseous phases respectively, θ (m³ m⁻³) is the volumetric fluid content, p_c (Pa) is the capillary pressure, ρ (kg m⁻³) is the density, u (m s⁻¹) is the Darcy velocity, w_v (kg kg⁻¹) is mass fraction of water vapor in gas phase, D_v (m² s⁻¹) is the effective vapor diffusion coefficient, L (J m⁻³) is the latent heat of vaporization, and Q_s (J) is heat loss.

3. EXPERIMENTAL METHODS

Wind Tunnel Experimental Apparatus:



Experimental Tank :



Wind Tunnel Specifications:

- Maintains wind speeds 0.8 – 5 m s⁻¹
- Pitot-static tubes for velocity measurement
- Infrared heater allows surface temperature to be maintained within the range of 30 – 80 °C
- Scale allows evaporation rates to be measured using mass balance methodology

Test Sand:

- Accusand #30/40
- 99.8% quartz
- $d_{50} = 0.53$ mm
- Bulk density = 2.65 g cm⁻³
- $K_s = 0.104$ cm/s

Monitored:

- Soil Moisture
- Relative Humidity
- Temperature
- Column Weight
- Air velocity

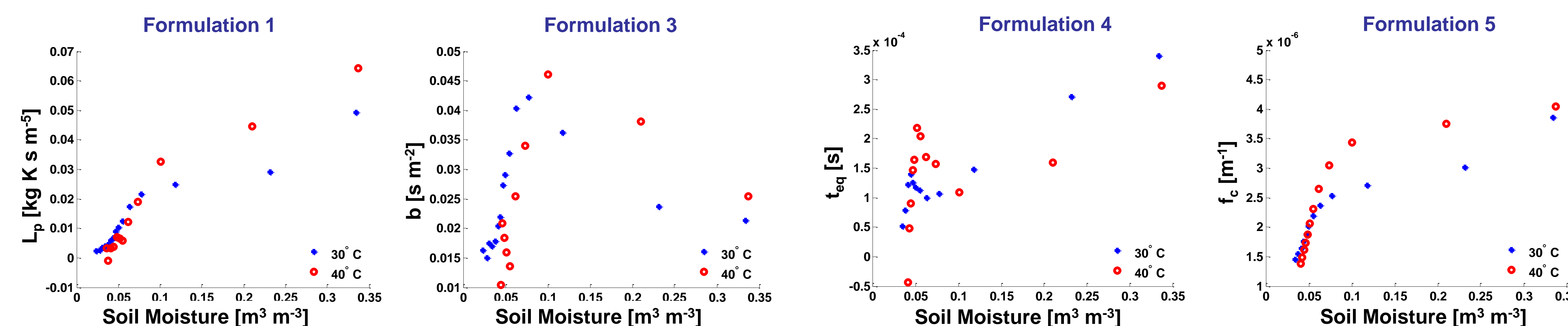
Procedure:

- ✓ Constant air velocity maintained across upper boundary using low velocity open end wind tunnel designed for porous tank experimentation
- ✓ Evaporation induced under strictly drying conditions
- ✓ No flow bottom boundary
- ✓ Experiments run for 10 days

Table 1. Experimental Conditions

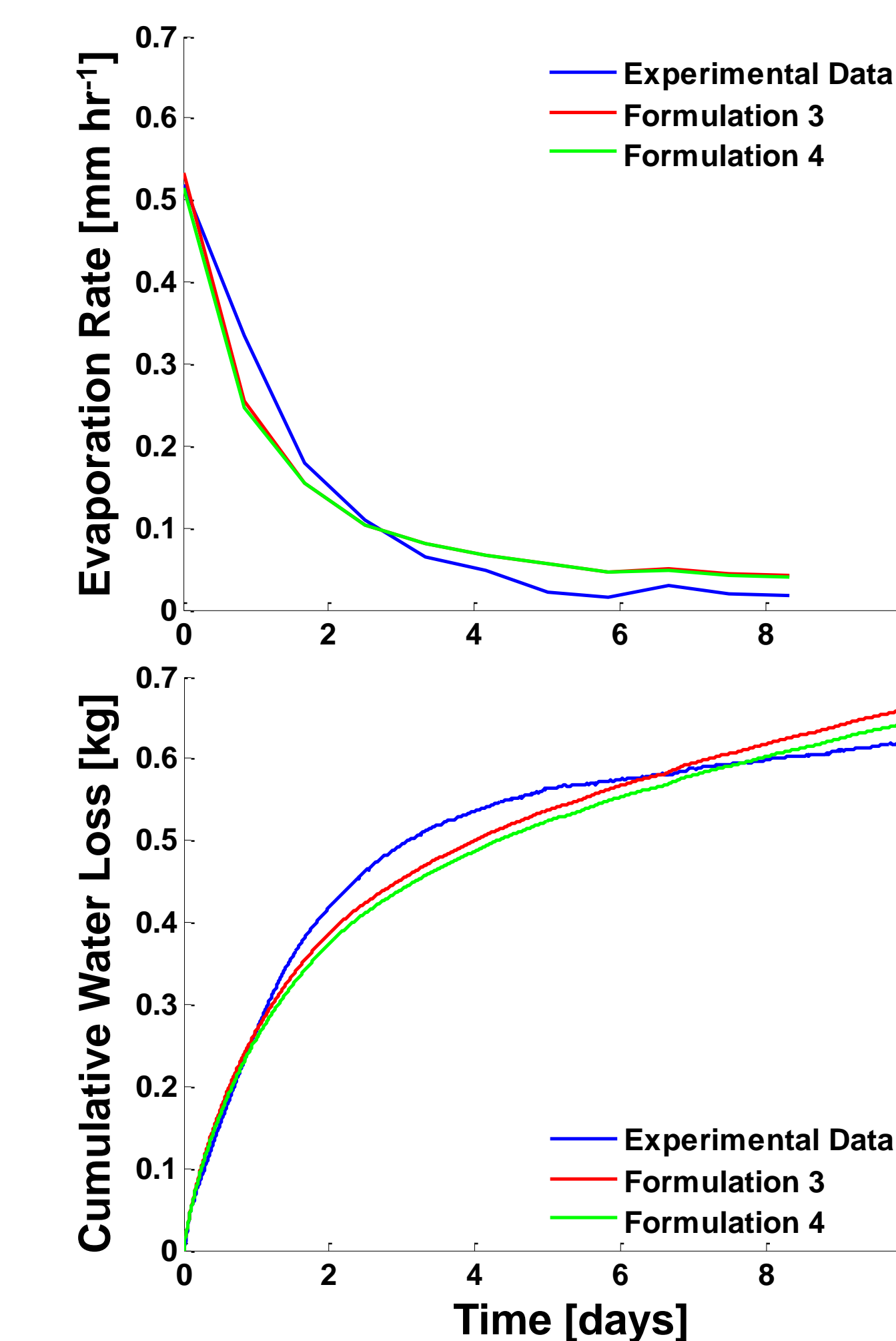
	Surface Temperature (°C)	Initial Water Table Depth (cm bgs)	Porosity (m ³ m ⁻³)
Experiment 1	30	0	0.340
Experiment 2	40	0	0.336
Experiment 3	30	18.5	
Experiment 4	Diurnal Fluctuations	0	

4. Preliminary Experimental Results – Effect of Temperature and Soil Moisture on Phase Change



RESULTS: Fitting parameters decrease with soil moisture. The values of many fitting parameters decrease with temperature.

5. Preliminary Modeling – Comparison of Phase Change Formulations



RESULTS: Formulations 3 and 4 predict nearly equivalent evaporation rates. Stage 1 evaporation is underestimated whereas Stage 2 evaporation (diffusion limited) is over predicted. The overestimation of Stage 1 evaporation by both formulations leads to an overestimation of the cumulative water loss.

6. CONCLUSIONS

- Dependency of fitting parameters on soil moisture and temperature.
- Fitting parameter values decrease with soil moisture.
- Numerical modeling show that use of t_{eq} or b yield nearly identical evaporation rates.
- Experimentation still underway.
- Currently testing the impact of different surface and water table boundary conditions on phase change formulations.
- Future work will focus on the upscaling of the five phase change formulations presented
- Phase change formulations independent of fitting parameters need to be developed

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