0038-075C/00/16503-208–216
Soil Science

March 2000
Vol. 165, No. 3
Printed in U.S.A.

TECHNICAL ARTICLES

SIMULTANEOUS HEAT AND MASS TRANSFER IN SOIL COLUMNS EXPOSED TO FREEZING/THAWING CONDITIONS[1]

I. N. Nassar[2], Robert Horton[3], and G. N. Flerchinger[4]

Soil heat and mass transfer are important processes in nature The effects of soil solution concentration on soil heat and mass transfer have not been investigated thoroughly for freezing/thawing conditions. The objective of this study was to evaluate the SHAW model predictions of heat, water, and chemical transfer in saline and solute-free soils. Heat and mass transfer was studied in closed soil columns. Included were loam soil materials with two salinity levels. Three derivatives of benzoic acid were used as tracers for liquid water movement. Soil was packed into PVC columns that were buried vertically in a field soil profile and exposed to ambient weather conditions. After 72 days, the soil columns were removed from the field and sectioned into 0.02-m increments in order to measure water content, chloride, and benzoic acid tracer distributions. In addition to the observed heat and mass transfer, the SHAW model was used to predict heat and mass transfer in the soil columns. The model described the temperature distributions accurately for both salinized and solute-free soils. Both observed and predicted values of water distribution showed water accumulation in the upper 0.4 m in the solute-free soil. The water diminished slightly in the upper 0.20-m region in the salinized soil columns. Within the salinized soil columns, the final solute distribution did not indicate appreciable net solute movement. The observed and predicted frost depths in the solute-free soil were between 0.45 m and 0.65 m. Freezing was not significant in the salinized soil. The SHAW model should be improved if it is expanded to include the effects of temperature and osmotic potentials on liquid water flow in soil. (Soil Science 2000;165:208–216)

Key words: Frozen soil, soil temperature, coupled heat and water flow in soil, solute redistribution in freezing soil, SHAW model.

A LARGE portion of the world experiences seasons of freezing conditions each year. Soil freezing influences surface hydrology, e.g., infiltration and runoff. Soil freezing also influences vadose zone hydrology. Understanding the mechanisms of heat and mass transfer in soil can lead to better management of erosion, runoff, chemical leaching, and surface and groundwater quality.

Heat, water, and chemical transfer in soil can be affected by salinity, initial water content, and energy and mass boundary conditions. Galinato et al. (1986) reported that vapor flow dominated in dry soil under freezing soil conditions, whereas liquid flow dominated in soil with more than 20% moisture. Eldin et al. (1990) studied the effect of freezing on heat and mass transfer in silty soil. They concluded: (i) increasing the ion concentration in the pore fluid reduced the rate and magnitude of heave, limited frost penetration

[1]Journal Paper No. J-18451 of the Iowa Agric. and Home Econ. Exp. Stn., Ames, Iowa. Projects No. 3262 and 3287, supported, in part, by the Hatch Act and State of Iowa funds.

[2]Alexandria University, Faculty of Agriculture-Damanhoar, Egypt.

[3]Department of Agronomy, Iowa State University, Ames, IA 50011. Dr. Horton is corresponding author. E-mail: rhorton@iastate.edu

[4]USDA-ARS, Northwest Watershed Res. Center, 800 Park Blvd., Suite 105, Boise, ID 83712.

Received June 17, 1999; accepted Oct 22, 1999.

in the soil, reduced moisture transfer to the frozen layer, and kept the soil at a warmer temperature; and (ii) there was an optimum salt treatment for minimum frost heave for each soil. For the soil tested and for the freezing conditions used, that level was 0.5 N.

In similar studies by Cary et al. (1979) and Cary (1987), the presence of solute in the soil decreased frost heave and increased water infiltration. They attributed the decrease of frost heave to reducing water flow to the ice lens.

Hofmann et al. (1990) studied water and solute redistribution under freezing silty clay soil conditions. They reported that water and solute moved to the freezing front causing increases in water and solute concentrations within the soil profile.

Baker and Osterkamp (1989) studied salt redistribution during freezing of saline sand columns. Their results showed a reduction of salt concentration in the frozen zone compared with the unfrozen zone, indicating a significant amount of salt redistribution during freezing. For downward freezing, the amount of salt rejected near the interface decreased with increasing freezing rate and increased with the salinity of the soil solution in the unfrozen region. Salt rejection from the ice phase in an extended partially frozen region adjacent to the interface and brine drainage from this region seem to be the primary processes responsible for salt redistribution. Baker and Osterkamp (1989) reported also that at a freezing rate of 5 mm/d, there was generally a layer just above the interface where values of the gravimetric water content increased significantly from the initial values. This layer moved with the interface and increased in thickness with time.

Flerchinger (1987) developed a comprehensive model to describe heat and mass transfer under freezing soil conditions (SHAW model). The model includes partial differential equations for water, heat, and chemical transfer. The SHAW model simulates the interrelated heat and water transfer within snow, residue, and soil using estimated or measured weather data. The model was tested under a wide range of conditions (Flerchinger and Saxton 1989; Flerchinger 1991; Flerchinger et al. 1994; and Flerchinger et al. 1996a and b). Flerchinger (1991) used the SHAW model to investigate the effects of typical changes (measurement errors or natural variability) in input parameters on soil freezing.

Simulated frost depth was found to be very sensitive to small changes in air temperature (1° C) and initial snow depth (10 cm). Simulated frost depth was also potentially sensitive to the specified soil temperature for the lower boundary depending on the proximity of frost depth to the bottom of the simulated profile. Site, residue, and soil characteristics (slope, thickness of the residue layer, thermal conductivity of soil particles, soil bulk density, and a surface roughness parameter) had a modest impact on simulated frost. Soil hydraulic parameters had little effect on frost depth, but it had a large impact on water movement toward the zone of freezing and ice content of the frozen soil.

Based on the reported results, solute concentration of soil solution affects heat, water, solute and movement, frost heave, and frost depth. To date, the SHAW model has not been evaluated for a range of soil salinity conditions. Therefore, the objective of this work was to test the SHAW model predictions of heat, water, and chemical transfer in saline and solute-free soils. The predicted values of temperature, water content, and chloride and benzoic acid concentrations were compared with values collected from closed soil columns under field conditions.

MATERIALS AND METHODS

Experiment

Soil materials were collected from the Agronomy and Agricultural Engineering Research Center located in eastern Boone County, Iowa. The soil was classified as a Nicollet soil series, a fine-loamy, mixed, mesic Aquic Hapludoll. The Nicollet soil was derived from calcareous, loamy glacial till. The soil materials were collected by excavation, air-dried, and ground to pass a 2-mm sieve. Soil characteristics, such as hydraulic conductivity, moisture retention curve, particle size distribution, and organic matter content were determined.

The soil materials were moistened either with distilled water (0.247 m^3/m^3) or potassium chloride solution (0.257 m^3/m^3). The initial potassium chloride concentration was 0.78 mol/kg of soil solution (0.169 mol/kg soil) for the salinized soil. Three batches of the solute-free soil were moisturized using either difluorobenzoic acid (DFBA), trifluorobenzoic acid (TFBA) or pentafluorobenzoic acid (PFBA) at initial concentrations of 0.00026, 0.00016, and 0.00018 mol/kg of soil, respectively. Another three batches of salinized soil were prepared using the same initial concentrations of benzoic acids. The moistened soil was covered and stored at 20 °C for more than 10 days. The moistened soil was packed into PVC columns (1.16-m long and 0.052-m I.D.) at an average bulk density of 1.2 Mg/m^3. The soil columns were packed in increments of 0.1 m using an equal mass of soil. Layers of 0.04-m thickness were placed at selected positions from each benzoic acid batch. The DFBA acid layer was positioned at depths of 1.12 to 1.16 m; the PFBA layer was positioned at depths of 0.78 to 0.82 m; and the TFBA layer was located at depths of 0.38 to 0.42 m. Two replicates were used for each treatment (solute-free and salinized soils).

Twelve thermocouples were inserted into each soil column at different depths (0.0, 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.40, 0.50, 0.75, 1.0, and 1.16 m). The soil columns were sealed at both ends using aluminum disks. The soil columns were buried vertically in a field soil profile. The upper column ends were exposed to the ambient weather conditions of Ames, Iowa, from Dec. 6, 1996, until Feb. 17, 1997. The duration of the experiment was 72 days. Temperature was measured bi-hourly and recorded with a CR5 digital recorder (Campbell Scientific, Inc., Logan, UT).

The field study was terminated by removing and sectioning the soil columns by 0.02-m increments in order to determine both water content and chloride concentration distributions. Soil water content was determined gravimetrically in each soil section. Chloride concentrations were determined in soil water extracts of 1:2 by using a digital Chloridometer (HAAKE Buchler, Saddle Brook, NJ). The benzoic acid concentrations were determined in water extracts of 1:2 using the high-performance liquid chromatography (HPLC) method (Benson and Bowman 1994).

Model Description

The SHAW model includes governing equations for water, heat, and solute transport in soil.

Water Flow

The following partial differential equation was used to describe water flow:

$$\frac{\partial}{\partial z}\left[K\left(\frac{\partial \psi}{\partial z}+1\right)\right]-\frac{1}{\rho_l}\frac{\partial q_v}{\partial z}+U=\frac{\partial \theta_l}{\partial t}+\frac{\rho_i}{\rho_l}\frac{\partial \theta_i}{\partial t} \tag{1}$$

where K is the unsaturated hydraulic conductivity, m/s; ψ is the matric potential, m; z is the vertical coordinate, m; ρ_l is the density of liquid water, Mg/m^3; ρ_i is the ice density, Mg/m^3; θ_l is the volumetric liquid water content, m^3/m^3; θ_i is the volumetric ice content, m^3/m^3; q_v is the downward water vapor flux, (m/s); U is the source/sink term, m^3/m^3; and t is the time, s. Water moves in liquid phase in response to matric and gravity potential gradients. Water moves in vapor phase in response to temperature, matric potential, and osmotic potential gradients.

Heat Transfer

The following partial differential equation was used to describe transient heat transfer:

$$\frac{\partial}{\partial z}\left(\lambda_s\frac{\partial T}{\partial z}\right)-\rho_l c_l\frac{\partial (q_l T)}{\partial z}+S=C_s\frac{\partial T}{\partial t}-\rho_i L_f\frac{\partial \theta_i}{\partial t}+L_v\left(\frac{\partial \rho_v}{\partial_t}+\frac{\partial q_v}{\partial z}\right) \tag{2}$$

where λ_s is the thermal conductivity of soil, W/m/°C; c_l is the specific heat capacity of water, J/kg/°C; q_l is the downward liquid water flux (m/s); S is the source/sink, W/m^3; T is the temperature, °C; C_s is the volumetric heat capacity of soil, $W/m^3/°C$; L_f is the latent heat of fusion, J/kg; and L_v is the latent heat of vaporization, J/kg. Heat transfer includes conduction, latent heat, and sensible heat mechanisms. Latent heat of fusion is included in the heat flow equation.

Solute Transfer

The following partial differential equation was used to describe solute transfer:

$$\rho_l\frac{\partial}{\partial z}\left[(D_h+D_m)\frac{\partial C}{\partial z}\right]-\rho_l\frac{\partial (q_l C)}{\partial z}+V=\rho_b\frac{\partial S_s}{\partial t} \tag{3}$$

where C is solute concentration, mol/kg of solution; D_h is hydrodynamic dispersion coefficients, m^2/s; D_m is the molecular diffusion coefficient of solute, m^2/s; q_l is the liquid water flow, m/s; V is the source/sink term, $mol/m^3/s$; ρ_b is the bulk density of soil, Mg/m^3; and S_s is the amount of adsorbed solute in solid phase of soil, mol/kg of soil. Solute moves by diffusion-dispersion and convection mechanisms.

Soil Freezing

The temperature at which ice starts to form in the soil depends on the soil matric and osmotic potentials. When ice is present, the total water potential is related to temperature by the Clausius-Clapeyron equation as follows:

$$\phi=\pi+\psi=\frac{L_f}{g}\left(\frac{T}{T+273.16}\right) \tag{4}$$

where ϕ is total water potential, m; π is osmotic potential (m); and g is acceleration of gravity, m s^{-2}. Osmotic potential was computed from

$$\pi = \frac{-CR\,(T + 273.16)}{g} \tag{5}$$

where R is the universal gas constant, J $mole^{-1}$ K^{-1}; matric potential was computed from:

$$\psi = \psi_e \left(\frac{\theta_l}{\theta_s}\right)^{-b} \tag{6}$$

where ψ_e is air entry potential, and b is pore-size distribution index.

Initial and Boundary Conditions

The initial conditions associated with the heat and mass transfer equations, Eq. (1), (2), and (3), are:

$$\begin{aligned} &T\,(z, 0) = T_i, && \theta\,(z, 0) = \theta_i, \\ &C\,(z, 0) = C_i, && (0 < z < L) \end{aligned} \tag{7}$$

where L is soil column length, m.

The temperature boundary conditions at both ends [T(0,t) and T(L,t)] were measured.

The boundary conditions for water and solute are given in terms of net mass fluxes by

$$q_v\,(0, t) + q_l\,(0, t) = 0, \quad n_c\,(0, t) = 0 \quad t > 0 \tag{8}$$

$$q_v\,(L, t) + q_l\,(L, t) = 0, \quad n_c\,(L, t) = 0 \quad t > 0 \tag{9}$$

where n_c is the solute flux, mol/m²/s.

Numerical Solutions

The SHAW model was used to solve Eqs. (1), (2), and (3). In order to simulate the closed soil columns, the SHAW model was modified to force an observed soil surface temperature and no evaporative water flux for the upper boundary. From knowledge of the boundary conditions (measured boundary temperature and zero water and chemical fluxes described by Eqs. (8) and (9)), initial conditions (water content, temperature, and solute concentration) and the soil transport parameters, the model predicts temperature, soil water content, ice content, and solute concentration. Flerchinger (1987) and Flerchinger and Saxton (1989) present a description of the model and the transport parameters.

The model was initialized with an observed soil temperature profile and a uniform water content for the salinized and saline-free columns to represent conditions on December 6. Model calculations were performed to simulate a period

RESULTS AND DISCUSSIONS

Observed and predicted values of temperature, water content, chloride and benzoic acid distributions are reported. The SHAW model was used to predict the simultaneous heat and mass transfer in the closed soil columns.

Figure 1 shows predicted and observed soil temperature after 18 and 72 days for solute-free soil. The predicted and measured temperatures were similar at 18 days. The predicted temperature values responded to conduction, advection, latent heat of fusion and latent heat of evaporation as the major mechanisms of soil heat transfer. After 18 days, the temperature gradient was 25 °C/m in the upper 0.30-m region and 2.6 °C/m in the lower 0.86-m. Low temperature values indicated that freezing was occurring in the column at this time. Also, movement of water toward the soil surface was expected for this large temperature gradient (note Fig. 3). The temperature gradient on Day 72 was 1 °C/m within the soil column.

Figure 3 shows temperature distributions for salinized soil at 18 and 72 days. After 18 days, the temperature gradient was 25 °C/m in the upper 0.30 m region and 3.5 °C/m in the lower 0.86 m. This large gradient could drive water flow toward the soil surface over time. The temperature for salinized soil on Day 72 was not low enough for freezing to occur (note results of Fig. 4 for water distribution). In general, the salinized and solute-free soil columns had similar soil temperature distributions on Days 18 and 72.

Figure 2 shows the predicted and observed water distributions for solute-free soil after 72 days. The upper 0.40-m zone showed water accumulation. At depths of 0.05, 0.20, and 0.40 m, the water contents were greater than the water contents of the adjacent depths. The distribution of water reflected the cycles of freezing and thawing during the course of the experiment (see Fig. 5). The SHAW model predicted significant freezing in the upper 0.45 m of soil. During sectioning of the solute-free soil columns, freezing to depth 0.45 m was observed as well. The predicted amount of ice using the SHAW model decreased as the depth increased (soil temperature increases). Similar results were reported by Pikul and Zuzel (1990). Their results showed that the amount of surface cover reduced the incidence of soil freezing and that the degree of soil wetness at the time of freezing influenced the amount of water that migrated to the freezing

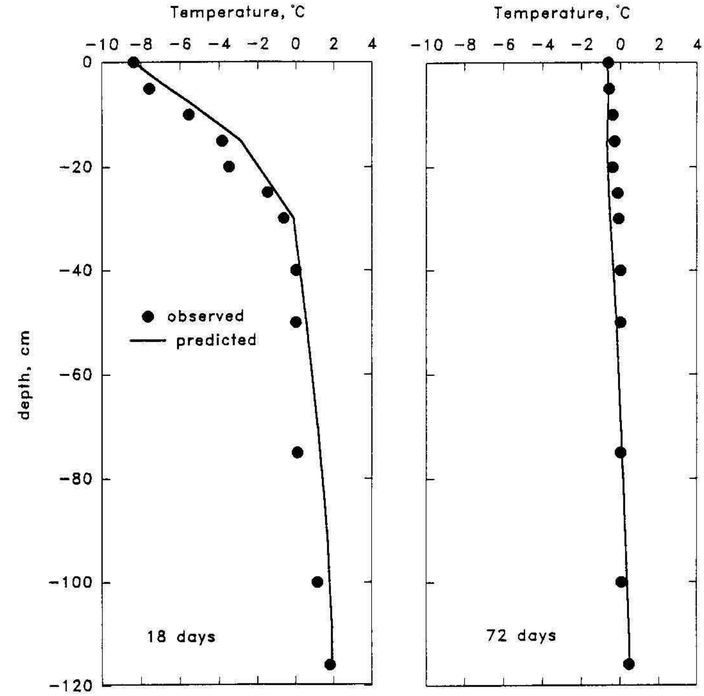

Fig. 1. Observed and predicted soil temperature distributions for solute-free soil after 18 and 72 d.

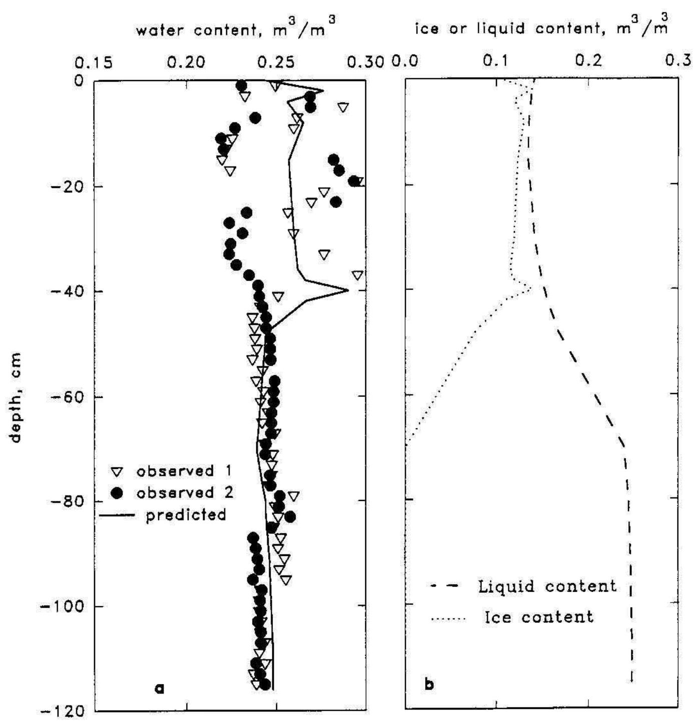

Fig. 2. Observed and predicted total water content (a) and predicted ice content and liquid water content (b) for solute-free soil at an initial water content of 0.247 m³/m³ after 72 days.

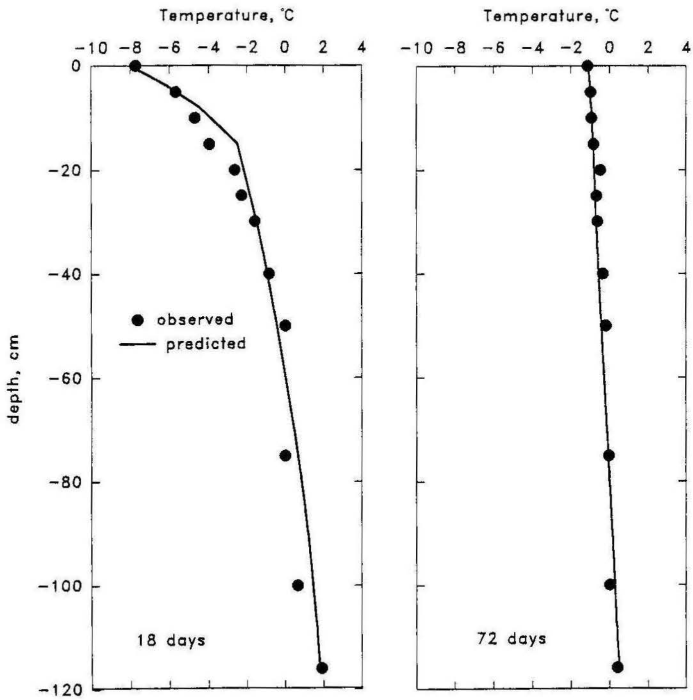

Fig. 3. Observed and Predicted soil temperature distributions for salinized soil after 18 and 72 days.

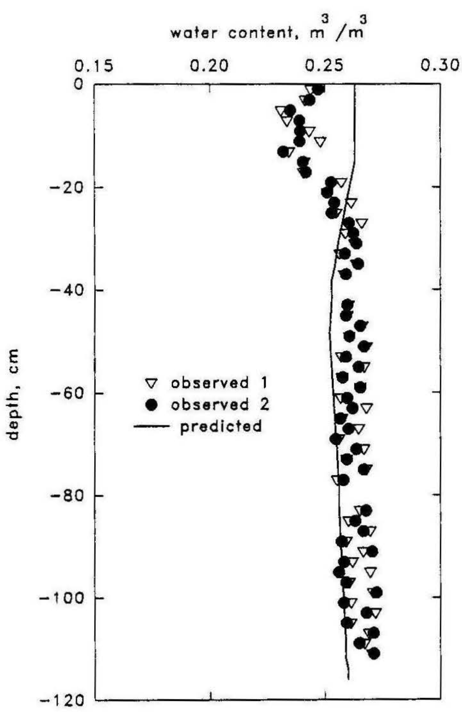

Fig. 4. Observed and predicted total water content for salinized soil at an initial water content of 0.257 m³/m³ after 72 days.

Figure 4 shows the water distributions for the salinized soil columns after 72 days. In general, not much water moved in the salinized soil compared with the solute-free soil. One reason was the presence of solute, which reduced the osmotic potential of soil solution. Freezing in the salinized soil was not as deep or as lengthy as in the solute-free soil. Less freezing resulted in smaller matric potential gradients in the salinized soil than in the solute-free soil and in less upward water movement. After 72 days the net result was

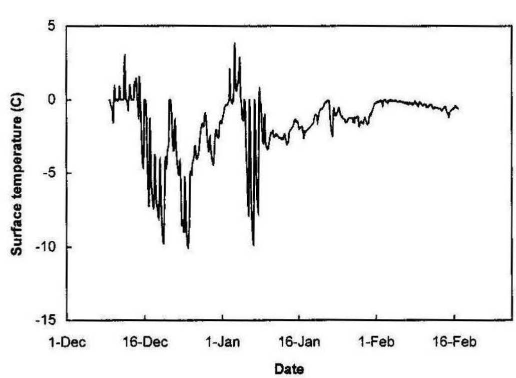

Fig. 5. Observed surface temperature as a function of time for the study period.

that water migrated slightly from the upper 0.20-m region toward the lower region. One reason for the downward water movement was the gravity potential. A second reason was the presence of high solute concentration in the region of 0.20 to 0.25 m (Note Fig. 6). Similar results were reported by Cary (1987), and Hofmann et al. (1990). Cary (1987) found that increasing solutes could decrease frost heaving by reducing water flow to the ice lens. The SHAW model prediction of water content deviated from the observed values. The reason in part for the discrepancies was that the SHAW model did not include the effects of temperature and osmotic potentials on liquid water flow.

Figure 7 shows the predicted and observed relative benzoic acid concentrations in solute-free (Fig. 7a) and salinized soils (Fig. 7b). The predicted values match closely the observed concentrations for both soils. The relative concentration of TFBA that was initially located between depths of 0.38 and 0.42 m was less than the relative concentration of either the PFBA, depths initially between 0.78 and 0.82 m, or DFBA, depths initially between 1.12 and 1.16 m. The results after 72 days indicate more spreading for the TFBA in the 0.0 to 0.40 m region than in the other regions within the soil columns. The surface region was an active region for water movement under temperature and matric potential gradients. The redistributions of the benzoic acid for the salinized (Fig. 7b) and solute-free soil were similar.

Figure 6 shows observed and predicted chloride distributions. The chloride concentration increased at a depth of 0.20 m. Fluxes of chloride were influenced by freezing/thawing cycles. During freezing periods, upward movement of liquid water carried solute from the lower region to the region of 0.20 to 0.25 m. During the thawing periods, the solute was carried by melted water from the upper region (0.0–0.20 m) to the lower region (0.20–0.25 m). The depths below 0.25 m maintained a somewhat uniform solute concentration. This indicates that the diffusive and the convective salt fluxes offset each other.

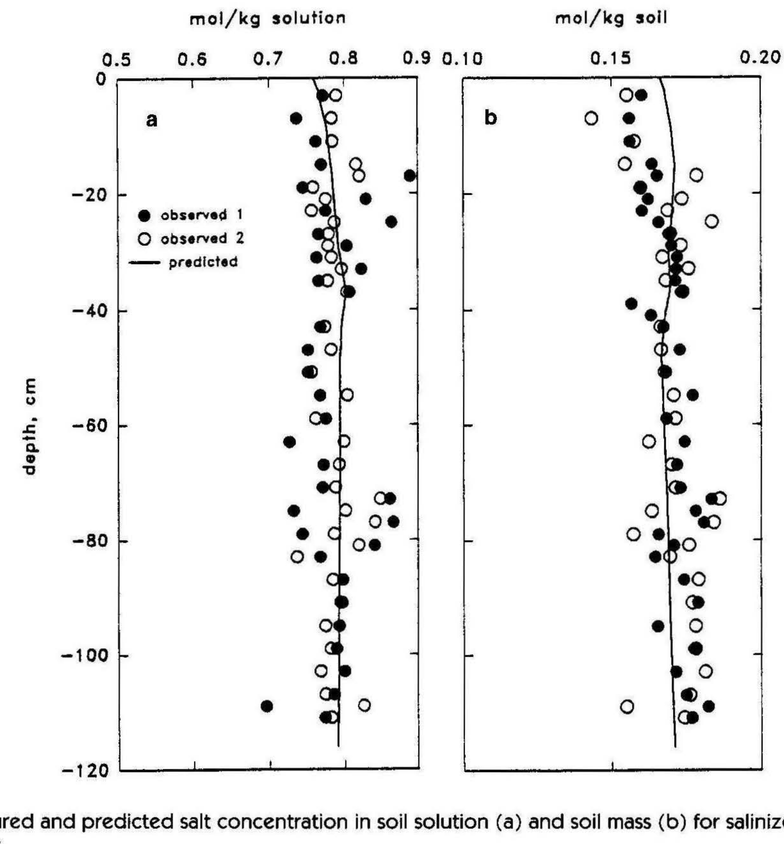

Fig. 6. Measured and predicted salt concentration in soil solution (a) and soil mass (b) for salinized soil columns after 72 days.

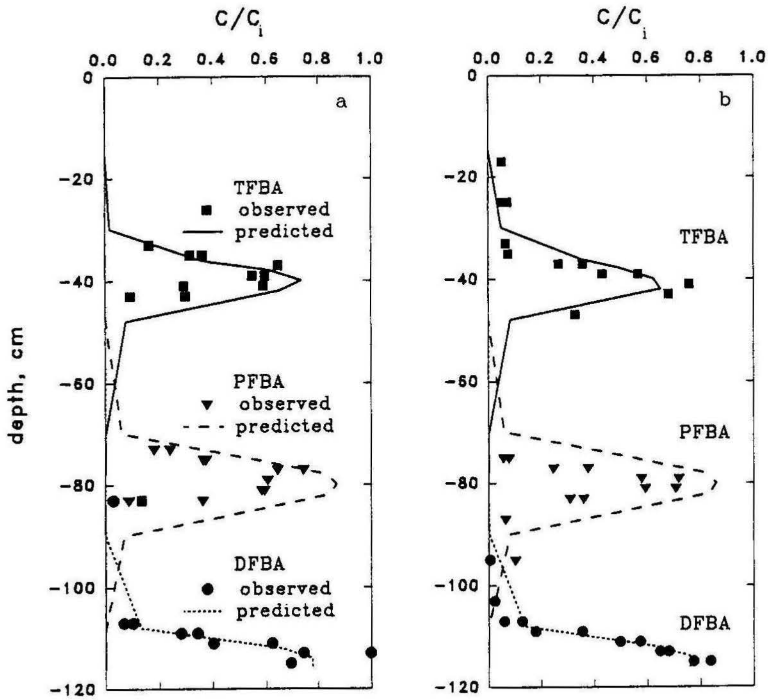

Fig. 7. Measured and predicted benzoic acid concentration in solute-free soil column (a) and in salinized soil column (b).

CONCLUSION

Experimental and numerical studies of soil heat and mass transfer were performed. The SHAW model was used to predict soil heat and mass transfer within closed soil columns. The model described the temperature distributions well for both salinized and solute-free soil columns. Both observed and predicted values of water distribution showed water accumulation in the upper 0.4 m layer in the solute-free soil. The water depleted slightly in the upper 0.20 m region in the salinized soil columns. The solute did not move in appreciable amounts in the salinized soil. The observed and predicted frost depths in the solute-free soil were between depths of 0.45 m and 0.65 m. Freezing was not observed during sectioning of the salinized soil columns. Increasing the solute concentration lowered the temperature of freezing in the salinized soil in comparison to the solute-free soil. The SHAW model may be further improved by including the effects of temperature and osmotic potentials on liquid water flow in soil.

Heat and mass transfer in soil experiencing freezing/thawing cycles is affected by several interacting mechanisms. Soil water content and soil solution concentration greatly affect frost depth. Research efforts including observations and theory development are needed to further our understanding of these interacting processes.

REFERENCES

Baker, G. C., and T. E. Osterkamp. 1989. Salt redistribution during freezing of saline sand columns at constant rates. Water Resour. Res. 25:1825–1831.

Benson, C. F., and R. S. Bowman. 1994. Tri- and tetrafluorobenzoates as nonreactive tracers in soil and groundwater. Soil Sci. Soc. Am. J. 58:1123–1129.

Cary, J. W., R. I. Papendick, and G. S. Campbell. 1979. Water and salt movement in unsaturated frozen soil: Principles and field observations. Soil Sci. Soc. Am. J. 43:3–8.

Cary, J. W. 1987. A new method for calculating frost heave including solute effects. Water Resour. Res. 23:1620–1624.

Eldin, N. N., L. R. Massie, and N. S. Aggour. 1990. Effect of freezing on mass and heat transfer in porous media. Proceedings of the International Symposium on Frozen Soil Impacts on Agricultural, Range, and Forest Lands. K. R. Cooley (ed.). March 21–22, 1990, Spokane, WA, pp. 177–185. CRREL Special Report 90-1.

Flerchinger, G. N. 1987. Ph.D. dissertation, Washington State University. Simultaneous heat and water model of a snow-residue-soil system.

Flerchinger, G. N. 1991. Sensitivity of soil freezing simulated by the SHAW model. Trans. ASAE 34:2381–2389.

Flerchinger, G. N. and K. E. Saxton. 1989. Simultaneous heat and water model of a freezing snow-residue-soil system I: Theory and development. Trans. ASAE 23:565–571.

Flerchinger, G. N., K. R. Cooley, and Y. Deng. 1994. Impacts of spatially and temporally varying snowmelt on subsurface flow in a mountainous watershed: I. Snowmelt simulation. Hydrol Sci J 39:507–520.

Flerchinger, G. N., J. M. Baker, and E. J. A. Spaans. 1996a. A test of the radiative energy balance of the SHAW model for snowcover. Hydrol Process 10:1359–1367.

Flerchinger, G. N., C. L. Hanson, and J. R. Wight. 1996b. Modeling evapotranspiration and surface energy budgets across a watershed. Water Resour. Res. 32:2539–2548.

Galinato, G. J., J. L. Baker, R. S. Kanwar, and R. Horton. 1986. Soil moisture and nitrate movement under freezing conditions. Paper No. 86–2514. St. Joseph, MI: Am. Soc. Agri. Eng.

Hofmann, L. L., R. E. Knighton, and J. L. Richardson. 1990. Redistribution of soil water and solutes in fine and coarse textured soils after freezing. Proceedings of the International Symposium on Frozen Soil Impacts on Agricultural, Range, and Forest Lands. K. R. Cooley (ed.). March 21–22, 1990, Spokane, WA, pp. 263–270. CRREL Special Report 90–1.

Pikul, J. L., and J. F. Zuzel. 1990. Heat and water flux in a diurnally freezing and thawing soil. Proceedings of the International Symposium on Frozen Soil Impacts on Agricultural, Range, and Forest Lands. K. R. Cooley (ed.). March 21–22, 1990, Spokane, WA, pp. 113–119. CRREL Special Report 90–1.