

Modeling of coupled water and heat fluxes in both unfrozen and frozen soils

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Abstract

Accurate simulation of soil freezing and thawing behavior is critical to understand hydraulic processes in the vadose zone under cold and arid climatic conditions. Using an extended freezing code incorporated in the HYDRUS-1D model, this study was conducted 1) to verify the freezing model using field soil water and temperature data collected in Inner Mongolia grassland, and 2) to investigate the contribution of snowmelt or soil thawing to the seasonal water balance. The results showed that both the freezing model and the snow routine matched well the measured soil water and temperature under unfrozen conditions. However, under frozen conditions, the freezing model reflected the phase change of soil water better and substantially improved the simulation results than the snow routine. The freezing model did not produce surface runoff generated by snowmelt and soil thawing from frozen soil layers. Instead, it overestimated water content and thus underestimated surface runoff after spring snowmelt. We suggest that detailed knowledge of the soil-atmosphere processes is needed to improve the surface runoff algorithm in the frozen soil module.

Key Words

Frozen soil, modeling, water and heat fluxes, Inner Mongolia grassland

Introduction

Coupled water and heat movement in the vadose zone is a central process in many agricultural and engineering issues. In particular, in the cold and arid regions, snowmelt or lateral water movement on frozen soil layers have a non-negligible influence on seasonal water balance. However, although the importance of freezing and thawing processes are recognized widely, the mutual interactions of water and heat flow in frozen soil are limited in laboratory observation and theoretical analysis, and are rarely considered in field applications (Flerchinger and Saxton 1989; Smirnova *et al.* 2000; Hansson *et al.* 2004). This study addresses the field application of the hydrodynamic model HYDRUS-1D (Šimůnek *et al.* 1998). In the current version, an extended freezing code is incorporated, which numerically solves coupled equations governing phase change between water and ice and heat transport using a mass- and energy-conservative method (Hansson *et al.* 2004). Specifically, we will focus on following questions: 1) How well does HYDRUS-1D simulate soil water and temperature with and without the “frozen soil module”? 2) How does the frozen soil module affect soil temperature, soil moisture and runoff simulations?

Materials and Methods

The study was performed on a long-term experimental site of the Inner Mongolia Grassland Ecosystem Research Station (IMGERS, 43°37'50"N, 116°42'18"E). The site was protected from grazing since 1979 (24 ha). Since June 2004, soil moisture and temperature were recorded by a data-logger at 30-min intervals in summer and at 1-h intervals in winter. Soil water content was measured at 5, 20 and 40 cm depth by theta-probes (Type ML2x). When soil is frozen, the measured probe reading refers to the volumetric unfrozen water content. Soil temperature was measured at five soil depths of 2, 8, 20, 40 and 100 cm using Pt-100 probes. Precipitation and other weather variables were recorded by a micrometeorological station. To determine root length density, root samples were taken up to 100 cm soil depth. In addition, soil samples were taken at four depths of 4-8, 18-22, 30-34 and 40-44 cm to determine the water retention characteristics and hydraulic conductivities.

The model of coupled water and heat fluxes was performed with HYDRUS-1D. Variably saturated water flow for above- and sub-zero temperatures is described using the modified Richards equation (e.g., Hansson *et al.* 2004):

$$\frac{\partial \theta_u(h)}{\partial t} + \frac{p_i}{p_w} \frac{\partial \theta_i(T)}{\partial t} = \frac{\partial}{\partial z} \left[K_{Lh} \frac{\partial h}{\partial z} + K_{Lh} + K_{LT} \frac{\partial T}{\partial z} + K_{vh} \frac{\partial h}{\partial z} + K_{vT} \frac{\partial T}{\partial z} \right] - S \quad (1)$$

where θ_u [L^3/L^3] is the volumetric unfrozen water content ($=\theta+\theta_v$; θ and θ_v are the volumetric liquid and vapor water content, respectively), θ_i is the volumetric ice content, p_w and p_i is the density of liquid and ice water, respectively, t is time, z is the soil depth, h is the pressure head, T is the soil temperature, and S is a

sink/source term normally considered as root water uptake. In Eq. 1, the first five terms on the right-hand side represent liquid flows due to gradient in pressure head (K_{Lh} , [L/T]), gravity, and temperature (K_{LT} , [L²/T/K]), and vapor flows due to gradient in pressure head (K_{vh}) and temperature (K_{vT}), respectively. The hydraulic conductivity of frozen soil is significantly reduced by ice lenses, which is accounted for by an impedance factor, Ω (Lundin 1990), multiplied by Q , as follows:

$$K_{flh} = 10^{-\Omega Q} K_{Lh} \quad (2)$$

the parameter Q is the ratio of the ice content to the total water content.

The governing equation for the movement of energy in soil is given by the following conduction–convection heat flow equation (e.g. Nassar and Horton 1992):

$$\frac{\partial C_p T}{\partial t} - L_f \rho_i \frac{\partial \theta_i}{\partial t} + L_0(T) \frac{\partial \theta_v(T)}{\partial t} = \frac{\partial}{\partial z} \left[\lambda(\theta) \frac{\partial T}{\partial z} \right] - C_w \frac{\partial q_l T}{\partial z} - C_v \frac{\partial q_v T}{\partial z} + L_0(T) \frac{\partial q_v}{\partial z} - C_w S T \quad (3)$$

where L_0 and L_f are the volumetric latent heat of water vaporization and freezing, respectively. C_p is the volumetric heat capacity of the bulk soil, which is determined as the sum of the volumetric heat capacities including solid, organic, liquid (C_w), ice, and vapor (C_v) phase multiplied by their respective volumetric fractions (De Vries 1963). The symbol $\lambda(\theta)$ denotes the apparent thermal conductivity and q the water flux density while T is the soil temperature. The phase change between water and ice is controlled by the generalized Clapeyron equation (e.g., Hansson *et al.* 2004), which defines a relationship between the liquid pressure head and temperature when ice is present in the porous material. Hence, the unfrozen water content can be derived from the liquid pressure head as a function of temperature when ice and pure water co-exist in the soil.

The initial condition was set based on measured water content and temperature. An atmospheric boundary condition and free drainage condition was imposed at the soil surface and bottom boundary of the flow domain, respectively. The soil profile was considered to be 100 cm deep. Root water uptake was simulated using the model of Feddes *et al.* (1978). The current HYDRUS-1D version including soil frozen module (denoted as freezing model) was modified to consider the subsurface soil freezing and thawing processes, as well as the surface energy and water balances. To verify the performance of freezing model, the “normal” version including snow hydrology only without soil frozen module (denoted as snow routine) was also run as a reference.

Results and Discussion

Soil water and heat fluxes are numerically simulated for the whole hydrological year in 2006 (Figure 1). Generally, the simulated and measured soil water contents (SWC) are comparable during the studied period in terms of root mean square error (0.02-0.07 cm³/cm³). Particularly, the freezing model simulates the diurnal water dynamics well which coincides with soil freezing and thawing processes, i.e. soil moisture increases with increasing soil temperature and vice versa (Figure 1b). However, the snow routine only fits soil water contents under unfrozen condition. Under frozen condition, there is a clear disparity between the liquid water content curve simulated by the freezing model and the total water content curve simulated by the snow routine (Figure 1a). This discrepancy is apparently caused by the program of two models, and therefore may be used to approximate the ice content in the soil. For example, the SWC simulated by the freezing model drops shortly after 6th November when the soil is freezing (Figure 1a). However, the SWC simulated by snow routine keeps constant. Hence the difference in water content between two models, i.e., ice content 0.07 cm³/cm³ can be estimated. In late March, due to above 0°C soil temperature, the SWC both measured and simulated by freezing model rise, while the SWC simulated by snow routine keep constant. This again suggests that the freezing model can predict the increase in SWC due to soil thawing well. An increase in SWC in the deep soil layers (20 and 40 cm) due to soil thawing is also clearly predicted (Figure 1). However, there is no indication of vertical water movement since soil water content is low and it can be held by soil.

In contrast to the soil water simulations, soil temperature is simulated well by either the freezing model or the snow routine (Figure 1), except that the freezing model is more accurate to reflect the diurnal dynamics of soil temperature (Figure 1c). This gives evidence of the impact of the frozen soil module on soil temperature simulations. When soil becomes freezing, soil temperature decreases and energy is released to warm up the cold soil. However, given the same total water content, the thermal conductivity of frozen soil is higher than that of unfrozen soil due to the presence of ice. Consequently, the upward soil heat flux is higher when the soil is frozen, thus it tends to cool the soil (Smirnova *et al.* 2000). Certainly, the energy released effect of high thermal conductivity of ice is smaller than that of water phase change. Consequently, the freezing model, that considers the both thermal transport processes, provides a more reasonably and realistic simulation of soil temperature.

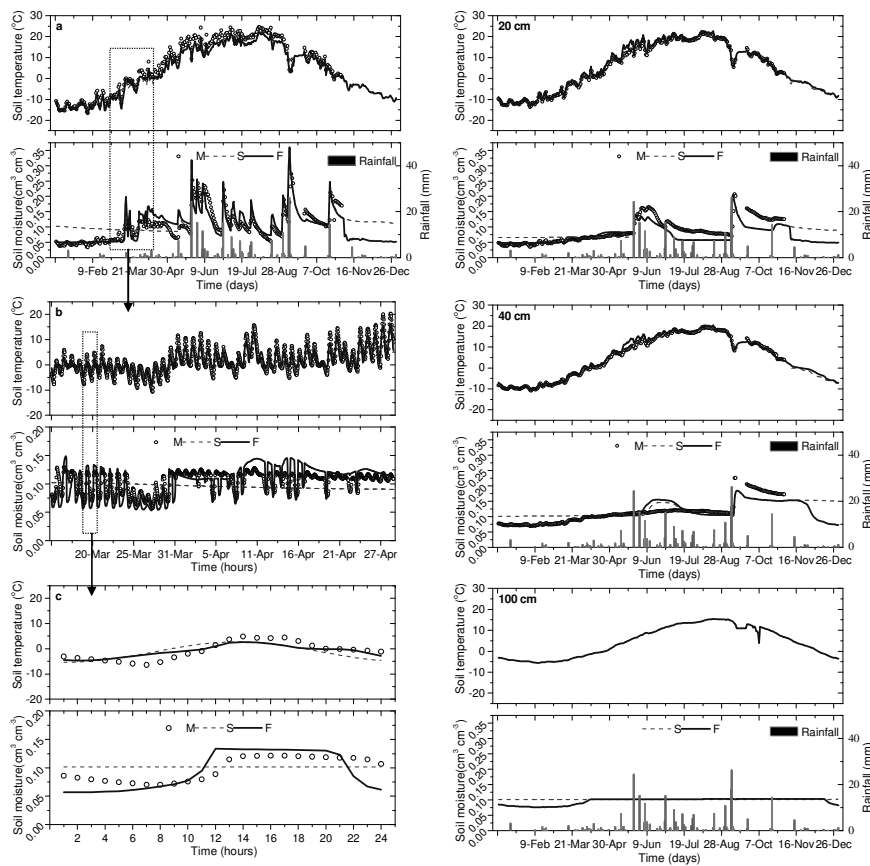


Figure 1. Measured and simulated soil moisture and temperature at 5 (a, b, c), 20, 40, and 100 cm depth during the whole year of 2006 (M: Measured liquid water content; S: Simulated total water content running snow routine; and F: Simulated liquid water content running freezing model).

The snow routine predicts up to 15 mm snow depth (Figure 2a), however, the simulated runoff after air temperature increasing above 0°C is negligible (Figure 2c). This might relate with that the snow routine does not account for surface runoff from the frozen soil layer, but it is likely that surface runoff is generated during snowmelt while soil is fully or at least partially frozen (Figure 2b).

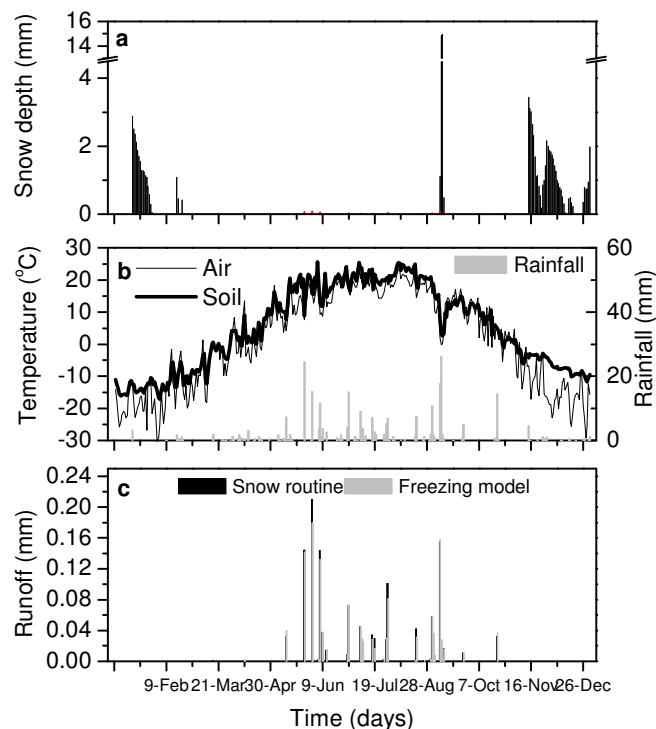


Figure 2. Rainfall, air and soil temperature, snow depth and runoff during the whole year of 2006.

Unexpectedly, the freezing model that can account for the subsurface freezing and thawing processes also does not produce surface runoff during winter (Figure 2c). Instead, we found that the freezing model simulated SWC is higher than the measured ones in the seasonal transition time when soil begins to thaw (Figure 1a). This implies that the freezing model might overestimate water content and thus underestimate surface runoff. Therefore, the freezing model seems still not sensitive enough to estimate surface runoff after spring snowmelt. This might relate to the fact that the freezing model we applied adopts soil surface temperature as the atmospheric boundary condition instead of air temperature, which undoubtedly lags energy transfer (Figure 2b). As a result, the freezing model may incorrectly partition all the snowmelt into infiltration as both soil thawing and snow melting happen simultaneously. Therefore, to solve this model problem, a transferable and double-layered boundary (e.g., one accounting for air temperature and other for soil temperature) is suggested. In addition, the current freezing model is possibly underestimated the reduction in infiltration capacity owing to the blocking effects of ice. Although the current frozen soil module has slight effect on the simulations of surface runoff, we suggest a detailed study on the soil-atmosphere processes and effects of boundary conditions to improve the surface runoff algorithm in the freezing code.

Conclusion

We used an extended frozen soil module of HYDRUS-1D, which solves water and heat transport under both frozen and unfrozen conditions simultaneously. The model was evaluated using field data of soil water and temperature at a long-term experimental site in Inner Mongolia grassland (North China). The results showed that both freezing model and snow routine reflect well the measured soil water and temperature under unfrozen condition, whereas the freezing model substantially improved the simulation results under frozen condition. In addition, the freezing model did not produce surface runoff generated by snowmelt or soil thawing from frozen soil layer. We suggest that seasonal water balance, especially considering rainfall water stored as snow, snow drift and the lateral water flow on frozen soil layers need to be investigated further because of the complicated interactions at the soil-atmosphere interface and thus effects of boundary conditions on the simulation.

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