Numerical Simulation of Moisture and Heat Coupled Migration in Seasonal Freeze-thaw Soil Media

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A moisture and heat coupled migration model for one-dimensional vertical frozen-unfrozen soil system under natural conditions was established, and the model solved by Newton-Naphson iteration. The simulated and the tested values shown the model is reasonable. The soil moisture and heat coupled migration characteristics during the seasonal freeze-thaw periods simulated by the model, and the dynamic changes of soil moisture analyzed in the paper. The results show that soil moisture had obvious migration during the freeze-thaw period. During the freezing period, frozen layers developed downward gradually with the accumulation of negative surface temperatures. Soil moisture migrating from the unfrozen layers to the frozen front and the soil moisture content in frozen layers increased while that in the lower unfrozen zone changed little. During the thawing period, some soil moisture evaporated to atmosphere while some migrated downward, so the soil moisture content of the upper layer was less than that in the freezing period. Soil temperature is the primary factor for moisture migration when surface soil freezing. The soil liquid water gradually phases into ice when soil temperature was reduced, so that the soil-water potential of the frozen layer is decreased, which leading to the soil moisture continuous migration to frozen layers. Air temperature has a significant influence on surface soil moisture, and the changes of soil moisture content decreased with the increase of soil depth.

Key words: Freeze-thaw soil, Coupled migration, Soil moisture, Numerical model.

Seasonal frozen soil, which contains ice lens, is a special soil water system. As a significant part of natural water cycle, soil moisture movement plays a major role in agriculture, water resources, and environment and human activities. At present, the characteristics of seasonal frozen soil were discussed by many Chinese and foreign scholars from different angles. During the freezing and thawing process in porous media, the formation of ice crystals and the frost heaving of soil were analyzed (Talamucci, 2003). Based on energy conservation and the principle of orthogonal between mobility and free boundary, moisture and heat coupled migration equation was established to simulate soil freezing and thawing process (Fremond, *et al*., 2000). According to mass, momentum and energy conservation, three-dimensional numerical model for the coupled moisture and heat were given (Goering, *et al*., 2000) and compared[1] the calculated values with the test results. A mathematical model has been built based on the monitoring data (Shoop *et al*., 1997) and researched the unsaturated soil moisture migration during freeze-thaw periods. The heterogeneous soil water movement under isothermal and non-isothermal conditions was simulated successfully adopted soil water, air and heat coupled equations taking the soil matric potential and temperature as variables, (Milly, 1982).

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In China, the researches started relatively late but develop rapidly. Under soil freezing condition, a numerical simulation model of water and heat migration was established and verified through laboratory experiments (Yang, *et al*., 1988). The numerical simulation of moisture and heat migration in channel freezing was conducted (An, *et al*., 1988); the two-dimensional saturated and unsaturated flow mathematical model under the condition of the ridge soil micro-topography was applied to the simulation of the dynamic changes of soil moisture in the winter wheat fields (Wang, *et al*., 2006). The changing and migrating characteristics of soil moisture during the freeze-thaw period were also analyzed by some people (Guo, *et al*., 2002; Yuan, *et al*., 2002; Zheng, *et al*., 2001; Zhu, *et al*., 2004), and the moisture migration of seasonal frozen soil in the Inner Mongolia Hetao irrigation district was analyzed (Zhou, 1994). According to the analyzing results of weather, soil water content within unsaturated zone and soil-water potential, soil moisture migration during the seasonal freeze-thaw period were studied by field observing (Zhang, *et al*., 1996). The one-dimensional numerical model of soil water movement was proposed(Lu, *et al*., 2007), which has been used to calculate the complex surface boundary conditions of soil profile rainfall, irrigation infiltration, surface water, surface runoff, evaporation and transpiration even when these phenomena alternatively occur.

As indicated above, the study on moisture migration of frozen soil has become a hot international frontier issue. However, it is still inadequate in two aspects. Firstly, researches were mainly on frost heave of engineering, such as West-East project, the construction of Qinghai-Tibet Railway in China, and less on the variation of soil water resources. Second, the moisture and heat migration simulation model for freezing and thawing soil, mostly aimed at the indoor soil column freezing test, whose boundary conditions are so simple that it shows significant discrepancy from the natural moisture migration process. So, it is necessary to further investigate the dynamic changes of soil moisture under natural conditions. Based on the previous research results and soil water movement characteristics, a one-dimensional vertical moisture and heat coupled migration model was established, and the soil moisture and heat coupled migration characteristics were simulated by the model, the dynamic changes of soil moisture was discussed. The results could provide a scientific basis for evaluating and utilizing soil water resources, and preserving soil moisture in the cultivated soil.

Model description

In process of soil freezing and thawing, many factors exert great influence on soil moisture migration, such as the outside air temperature, rainfall (snow), the phase change of soil moisture, and soil physical properties and so on, especially the phase change of soil moisture, which strongly couples the migration of moisture and heat. Therefore, we should carefully handle it when establishing the moisture and heat coupled migration model.

Coupled water and heat migration model

Heat-flow equation

The one-dimensional vertical equation for the latent heat of the phase change in the soil freezing-thawing process is developed with the ignorance of soil evaporation, which is lower during the seasonal freeze-thaw period:

$$\frac{\partial}{\partial z}\left(k_s\frac{\partial T}{\partial z}\right)-\rho_l c_l\frac{\partial (q_l T)}{\partial z}+S=C_s\frac{\partial T}{\partial t}-\rho_i L_f\frac{\partial \theta_i}{\partial t} \quad ...(1)$$

Where z is the depth between calculation points and surface(m); K_s is the thermal conductivity of soil (W/m°C); T is the soil temperature (°C); ρ_l is the density of water (kg/m^3); c_l represents specific heat capacity of water(J/kg·°C); q_l represents downward flux of liquid water (m/s); S is local source (sink) (W/m^3);C_s is the volumetric heat capacity of the soil (W/m °C); t indicates time (s); ρ_i is the density of ice (kg/m^3); L_f is the melting latent heat (kJ/kg); θ_i stands for the ice volume content (m^3/m^3).

For the thermal conductivity of soil (k_s), it is defined as:

$$k_s=\frac{\sum m_j k_j \varpi_j}{\sum m_j \varpi_j} \quad ...(2)$$

Where m_j is the weight factor of the component (in this paper, the weight factors of air, water and minerals are 2.5, 1.0 and 0.2, respectively); k_j stands for the thermal conductivity of the component j when the temperature is 25 $^\circ C$ (the thermal conductivity of air, water and minerals are 0.0256, 0.595 and 2.184 W/m °C respectively); ω_j respects the volume fraction that j accounts for unit volume (m^3/m^3). The volume heat capacity of soil can be computed by the sum of all soil material composition:

$$C_s = \sum \rho_j c_j \omega_j \quad ...(3)$$

Where ρ_j, c_j *and* ω_j represent the density (kg/m^3), the heat capacity (J/kg °C) and the volume fraction (m^3/m^3) of the component j respectively.

Water balance equation

Water balance equation of vertical one-dimension is established:

$$\frac{\partial \theta_l}{\partial t} + \frac{\rho_i}{\rho_l}\frac{\rho \theta_i}{\partial t} = \frac{\partial}{\partial z}\left[K\left(\frac{\partial \psi}{\partial z} + 1\right)\right] + U \quad ...(4)$$

Where K is the hydraulic conductivity of unsaturated soil (m/s); ψ represents the soil matric potential (m); θ_l represents the liquid water content in the frozen soil (m^3/m^3); U is local source (sink) ($m^3\ m^{-3} \cdot s^{-1}$).

In equation (4),

$$\psi = \psi_e \left(\frac{\theta_l}{\theta_s}\right)^{-b} \quad ...(5)$$

$$K = K_s \left(\frac{\psi_e}{\psi}\right)^{n} = K_s \left(\frac{\theta_l}{\theta_s}\right)^{bn} \quad ...(6)$$

Where ψ_e is the air admission potential (m); θ_s describes saturated soil moisture content (m^3/m^3); b is defined as distribution index of pore size; K_s shows the hydraulic conductivity of saturated soil (m/s); n=2+3/b.

Hydrothermal contact equation

In frozen soil, the liquid water content keeps a dynamic balance with the negative temperature, which reflects the interaction between the water and the thermal motion, the equation can be elaborated with the following expression:

$$\theta_l = \theta_s \left[\frac{L_f T}{g \psi_e (T + 273.16)}\right]^{\frac{1}{b}} \quad ...(7)$$

This equation defines the maximum liquid water content at negative temperature**.** And the soil ice content equals to the total water content minus the liquid water content.

Definite condition

Definite conditions of the soil heat-flow equation

Initial condition is specified as:

$$T\big|_{t=0} = T(z,0)$$

The upper boundary condition of the heat-flow equation on (z=0) is the underlying surface, which is the interface between soil system and atmosphere. Mainly the upper border controls soil moisture and heat characteristics. Moreover, the inputs of system dynamic process include the solar radiation absorbed by the underlying surface, long wave radiation and water heat exchange. With the latent heat of evaporation ignored, heat balance equation of surface soil as shown in following:

$$R_N = H + G + L_f E_f \quad ...(8)$$

Where R_N is the sunshine net radiation (W/m^2); H is the sensible heat of heated air (W/m^2); G represents the heat flux which enters into the soil (W/m^2); L_f indicates the release (or absorption) of energy when the surface soil is freezing (or thawing) (W/m^2).

Here:

$$R_N = R_s(1-\alpha)L_s + R_t \quad ...(9)$$

$$H = \rho_a c_a \frac{(T_s - T_a)}{\gamma_H} \quad ...(10)$$

$$G = -k_s \frac{T_1 - T_S}{Z_1} \quad ...(11)$$

Where R_s is the total solar radiation (W/m^2). α is the reflectivity of surface soil (0.3 and 0.35 for dry and wet soil, respectively). L_s is the net long wave radiation (W/m^2). R_t is the atmospheric long-wave reflection (W/m^2). ρ_α, c_α *and* T_α is the density (kg/m^3), the heat capacity(J/kg·°C) and the air temperature(°C) respectively. Y_H is the aerodynamic drag (s/m). T_1 is the temperature at height Z_1 (°C).

Due the soil matric potential and osmotic potential, there still is unfrozen water in the soil when the temperature falls below 0 °C . The water and ice coexist in the same balance within the freezing temperature. Therefore, the relationship between the ice ratio and temperature of soil must be determined before the calculation of the latent heat of thawing. When ice exists, the vapor pressure of ice is controlled the total soil water potential, the relationship can be derived from the freezing point lower equation.

$$\psi = \frac{L_f}{g}\left(\frac{T}{T_k}\right) \quad \text{... (12)}$$

Where θ is the total water potential (m). T_k is the absolute temperature (°C). g the gravity accelerating rate (m^2/s). When soil temperature T is known, soil matric potential can be determined according to equation (12). Furthermore, liquid water content could be derived from the soil moisture characteristic curve. Following the same argument, if the total water content is given, we can calculate the ice content and the corresponding latent heat.

The bottom boundary condition as shown in following:

$$T\big|_{z=l} = T(l,t)$$

Where l is the soil simulation depth.

Definite conditions of soil water flow equation

The initial condition is:

$$\theta\big|_{t=0} = \theta(z,0)$$

Boundary conditions are:

$$\theta\big|_{z=0} = \theta(0,t)$$

$$\theta\big|_{z=l} = \theta(l,t)$$

Model solution

Instead of the analytical method or semi-analytical method, Newton-Naphson iterative method was adopted to solve the model because the complexity of the initial boundary conditions and the nonlinearity of the moisture and heat coupled migration equations when the soil freezing. It requires inputting factors that weather conditions of the upper boundary, initial soil temperature of the bottom boundary and profile distribution of soil water content. The latter two factors are given by the tested data. Soil temperature and moisture content within each time step acquired by linear interpolation of inputting data in different observation period.

Model examination and verification

General situation of study area

The experiments were conducted between November, 2004 and March, 2005 at the Taigu Water Balance Experimental Field, which is 60 km away from the south of Taiyuan, Shanxi Province in China. It is locates in the east of Jinzhong basin at approximately 37°262 N, 112°302 E at an altitude of 777 m. The area is characterized by a continental semi–arid climate. The climate is characterized by heavy wind and little rain in spring, rainfall heavily concentrated in summer, continuous rain in autumn, and cold with little snow in winter. Annual average temperature is 9.9 °C. Average annual precipitation is 415 mm, mainly occurring from June to September; annual water surface evaporation potential is 1642 mm; and maximum observed frost depth was 92 cm in 1960. Average relative humidity is 74% and average wind speed is 0.9 m s^{-1} for many years. The annual average frost–free period is about 200 days. During the test period (from September in 2004 to March in 2005), the total solar radiation was 127.2E+04 kJ m^{-2} and the lowest observed total solar radiation was 18.8E+04 kJ m^{-2} in December.

During the experiment, the soil surface is bare and the meteorological data comes from the test station. Soil temperatures were monitored at 8:30 am everyday by thermal resistance. Soil moisture content was determined at 8:30 am everyday by neutron instrument and soil drying method.

Model establishment

As shown in table 1, the information about simulation sites includes gradient, latitude, slope aspect, elevation and surface reflectivity and so on. Meteorological elements consists of the daily maximum temperature (°C), the daily minimum temperature (°C), the dew temperature (°C), wind speed (m/s), rainfall (cm) and the average daily solar radiation (W/m^2). Soil moisture content and initial temperature are measured value. The time step unit is day and the depth of simulation soil is

Table 1. General information of simulated location

Latitude(N)	Gradient	Elevation	Slope aspect	Dry Surface Reflectivity	Wet Surface Reflectivity
37°262	1/4000	777 meters	0 degree	0.3	0.35

1 m. The observation depth of soil temperature and moisture content are 5, 10, 15, 20, 40, 60, 80 and 100 cm below the surface. The soil in test sites is the sandy loam, whose dry bulk density is 1.4 g/cm^3. Saturated hydraulic conductivity was obtained by soil infiltration test during the seasonal freeze-thaw period. It is difficult to measure hydraulic parameters directly such as air admission potential and distribution index of the pore size, so which were calculated according to soil structure, bulk density and particle components.

Model examination

The numerical simulation of soil profiles temperature and moisture content at bare plot were conducted for the model examination and choosing the test period as the examination period. The simulated and the tested soil temperature are shown in Fig.1 and Fig.2

The simulated and the tested soil moisture content are shown in Fig.3 and Fig.4. Simulated values were compared to the tested values using the relative root mean square error (RMSE).

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}\left(Y_i - \hat{Y}_i\right)^2} \quad ...(13)$$

Where Y_i is the tested value, $\hat{Y}_i$ is the simulated value, and N is the number of samples tested

The calculation results were shown that RMSE ranges from 0.5 to 3.0. The value of 0 cm is big, because the surface was impacted by the external factors such as temperature, and soil thermal conductivity changes with the moisture content. However, it still shown that the simulated values are consistent with tested values, which indicates that the model could reflect the actual situation of the study area and parameters selected in the model are reasonable.

Model verification

In order to confirm the reliability of the model, we used the tested data to validate the model further; the regulated soil hydraulic parameters are shown in table 2.

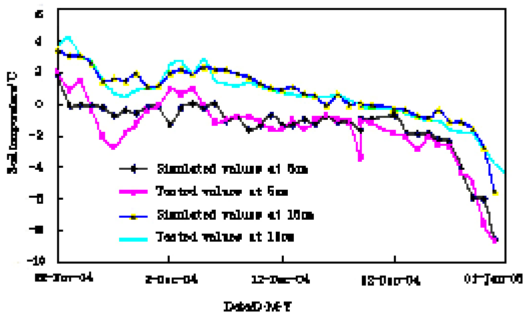

Fig. 1. Comparison between simulated and tested soil temperature at 5cm and 15cm

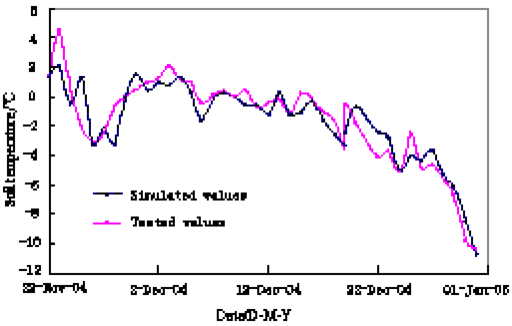

Fig. 2. Comparison between simulated and tested surface soil temperature

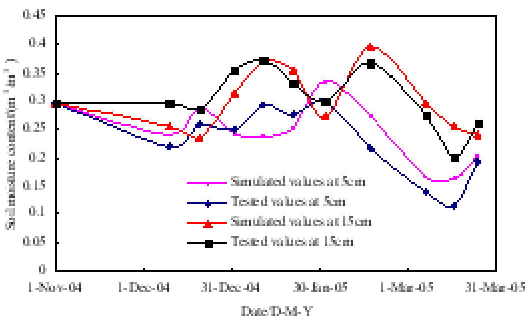

Fig. 3. Comparison between the simulated and tested soil moisture content at 5cm and 15cm

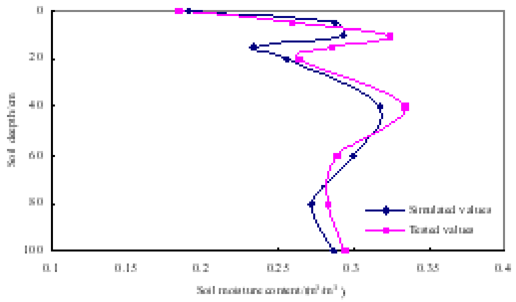

Fig. 4. Comparison between the simulated and tested soil moisture content on December 20, 2004

Table 2. Regulated soil hydraulic parameters

Depth	Distribution index of pore (m)	air admission potential size *b*	Saturated hydraulic ϕ_e(m) (cm/hr)	Saturated volume moisture content conductivity	Soil heat capacity (J/kg·!) (m^3/m^3)
0	4.4	0.04	1.10	0.48	Larger change
5	4.8	0.04	0.73	0.50	Larger change
10	6.1	0.04	0.41	0.52	2.51
15	5.3	0.04	0.55	0.51	2.47
20	4.4	0.04	1.10	0.48	2.403
40	4.4	0.05	1.40	0.48	2.643
60	4.1	0.05	1.30	0.49	2.342
80	4.3	0.05	1.10	0.50	2.342
100	4.6	0.04	0.91	0.50	2.356

The simulated and the tested soil temperature curves at 10 cm and 20 cm demonstrated in Fig.5, and soil moisture content curves at 60 cm and 80 cm are depicted in Fig.6. It turns out that the numerical simulation model could objectively reproduce the characteristics of the process of soil freezing and thawing. This model could be applied to quantitatively simulating the change of soil temperature

Mechanics of moisture and heat coupled migration

The proposed mathematical model is used not only to simulate the dynamic changes of soil moisture under experimental conditions but also to analyze the movement of soil moisture under natural conditions. In order to make a comprehensive analysis of soil moisture variation and explore factors influencing the moisture movement, we selected from November 2005 to March 2006 as the simulation period, and simulated and analyzed the dynamic changes of soil moisture during the freeze-thaw period. Table 3 illustrates temperature and moisture content profile distribution at the bottom boundary.

When soil was frozen during freeze-thaw period, the soil moisture redistributed (shown as the spatial and quantitative change of soil moisture) results from soil moisture migration. This variation happens in both frozen and unfrozen layers. Soil internal freeze-thaw status are transformed due to the influence of soil texture and meteorological factors (solar radiation, air temperature and precipitation), which further affect the soil moisture profile distribution and variation feature. Fig.7 shows the soil moisture content isograms of bare plot in the test area during the seasonal freeze-thaw period.

As illustrated in Fig.7, the temporal and spatial variation of soil moisture content shows different variability at different stages during the freeze-thaw period.

1) Soil at 0-20 cm was thawing during the day and freezing at night at initial freezing stage.

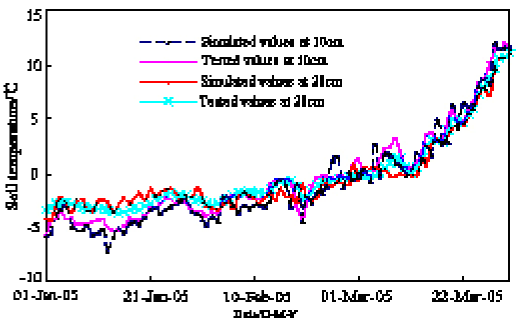

Fig. 5. Comparison between the simulated and tested soil temperature at 10 cm and 20 cm

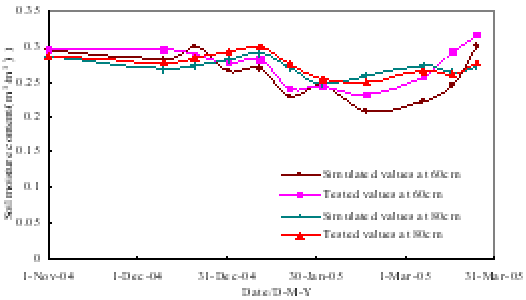

Fig. 6. Comparison between the simulated and tested soil moisture content at 60 cm and 80 cm

With the frozen front developed deeper, soil moisture content within 20 cm increases correspondingly, while that in the subjacent layers only has small changes. With the continuous downward development of the frozen layer, soil moisture content began to rise and achieved the maximum (21%) at 20-50 cm in mid-December.

2) With the enhancement of the freezing effect when frozen layer stable developed downward, the high moisture content zone expands gradually. However, a low moisture content zone (with lowest value of 12%) emerged below 80 cm resulting from the water migration upward to the high moisture content zone.

3) Frozen layer thawed downward from surface and upward from the frozen front during the thawing period. Due to the barrier of frozen layer and the solar radiation, the thawed water migrated to the surface and lost to evaporation, and the surface moisture content reduces to about 10%. The bottom of the frozen layer thawed upwards and the frozen depth was decreasing. Soil moisture redistributed influenced by the soil-water potential gradient during the thawing period, soil moisture of the upper layer migrated to surface and evaporated to atmosphere. While the thawed soil moisture of lower frozen layer drained downward to deep zone and the high moisture content zone disappeared gradually.

The above analysis indicates that temperature is the primary factor that causes the moisture migration when surface soil freezing. Soil freezing makes soil-water potential lower and soil moisture migrate to frozen layers continuously. In the vertical soil profile, the soil of upper layer influenced great by external condition. With the increase of soil depth, the effect of air temperature on soil moisture decreased and the changing range of the soil average moisture content reduced. During the freezing period, soil moisture migrates from the unfrozen layers to the frozen layers and Soil moisture content of each layer rose. However, the change of moisture content under the frozen zone was small. Some of the thawed water from the frozen layer was lost to evaporation and thawed water migrated downward during the thawing period, the soil moisture content of soil profile after thawing smaller than that in freezing period.

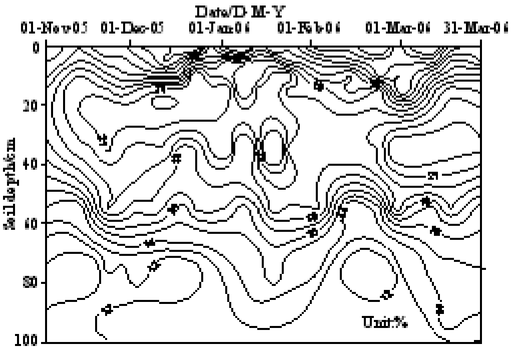

Fig. 7. Soil moisture content isograms of bare plot

CONCLUSION

The moisture and heat migration coupled model was established for one-dimensional vertical frozen-unfrozen soil system, and this model could objectively reflect the real situation of the study area. Besides, soil moisture and heat migration characteristics of one-dimensional frozen and unfrozen soil under natural condition could be quantitatively simulated and predicted. The research provides a better method for the analysis of soil moisture and heat migration characteristics during the seasonal freeze-thaw period. The simulation results can be used for the evaluation and utilization of the soil water resources and provide scientific basis for the agricultural production.

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