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Development of the universal and simplified soil model coupling heat and water transport

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It is very important to develop a universal soil model with higher simplicity and more accuracy, which can be widely applied to very general cases such as wet or dry soil, frozen or unfrozen soil and homogeneous or heterogeneous soil. Firstly in this study, based on analysis of both magnitude order and the numerical simulation results, the universal and simplified soil model (USSM) coupling heat and mass transport processes is developed. Secondly, in order to avoid the greater uncertainty caused by the phase change term in numerical iteration process for the model solution obtaining, new version of the universal simplified soil model (NUSSM) is further derived through variables transformation, and accordingly a more efficient numerical scheme for the new version is designed well. The simulation results from the NUSSM agree with the results from more complicated and accurate soil model very well, also reasonably reproduce the observed data under widely real conditions. The new version model, because of its simplicity, will match for the development of land surface model.

universal and simplified soil model, coupled heat and mass transport processes, frozen soil, arid soil, heterogeneous soil

Many sensitive experiments[1−4] conducted by GCM coupling with land surface models have demonstrated that it is crucial to develop a land surface model that can realistically describe various underlying land surfaces. Soil is the most important and most essential underlying surface in the study of land surface models due to its wide distribution and diverse textures with complicated internal physical process as well as continual alternant among wet, arid, freezing and thawing states. It can exert great impact on every part of the earth system on the interannual, interdecadal and even longer time scale. In the development of land surface models, the simulation study of soil part has been focused on, and many advances and improvements for the study have been carried out. However, due to knowledge limitation, there are the following deficiencies in the soil models used by many popular land surface models:

(1) Most of the soil models have a better performance on wet soil than on arid and semi-arid soil because the models employ the isothermal soil scheme[5,6], which does not take the coupling effect of heat and mass transport processes into consideration and also neglects the contribution of heat and water brought by vapor movement. Even though the consideration of freezing-thawing process has been taken in the models, the parameterization scheme to describe the process is simple to some extent and may not be realistic theoretically. For example, SSib and CLM models[6,7] assume that the freezing process of all liquid water in soil will complete at the freezing point T_f=273.15°K; BATS model[8] assumes that the freezing process of liquid water in soil occurs in a small range around the freezing point. However, the real freezing process is continuous with no

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fixed freezing point or range. The quantitative relation among liquid water content, ice content and temperature must be derived from the constitutive hydrological characteristics (could be obtained through experiments) in frozen soil and the freezing-point depression relation hold for the thermodynamic equilibrium system.

(2) The liquid water movement is described with the moisture content gradient rather than the matric potential gradient in most models[9−11], resulting in the unsuitability for estimating water flow in inhomogeneous soils and the difficulty in the study of physical process in frozen soil as well as of unsaturated soil coupling with saturated groundwater flow.

(3) In almost all land surface models used currently, soil temperature and volumetric moisture content are used as the prognostic variables of energy and mass balance equations, respectively. When the frozen process is considered, the rate term of water-ice phase change with great phase change energy release/absorption is explicitly shown in the energy balance equation. It will introduce great error into temperature estimation and increase the iteration times for a convergent numerical solution if there is a small error in the estimation of the phase change rate.

Therefore, in order to well describe the complicated interaction between the land surface and atmosphere, it is very important to develop a universal soil model which can simulate the heat and water transport processes for a variety of soil conditions such as frozen/unfrozen, homogeneous/inhomogeneous, wet/arid and semi-arid condition. Furthermore, the model should be as simple and realistic as possible in order to match the development of land surface model and climate study.

Examining various soil models used currently, it can be found that the models are quite different in the complexity to deal with the heat and water transport processes and in term they have different applicabilities[9−25]. Basically, they can be generally sorted into three categories. The first kind of the models is the complete coupled heat and water transfer model[15], which is composed of 10 equations, including detailed description of all contributions of heat conduction, phase change, liquid flow and vapor gas diffusion to the energy balance and mass balance of volumetric liquid water, ice and vapor content. The second kind of the models[16,17] is relatively simplified through neglecting the rate term of vapor mass change in the vapor mass balance equation, which keeps 5 equations only. The third kind of models is simple soil model and currently often used, in which the contribution of vapor movement and its phase change to both mass and heat balance as well as the contribution of heat brought by liquid water movement to heat balance are all neglected[9,10,18−24]. There is another version of model, the complicity of which takes middle-of-the-road between the second and the third kinds and in which heat brought with liquid water to heat balance is still taken into consideration[18−21,24,25].

According to the above analysis, it is clear that the following questions should be answered: (1) What kind of soil model can describe the coupled heat and water transfer processes occurring in different soils under a wide range of wetness and temperature as well as various meteorological conditions? (2) What kind of soil model can avoid the uncertainty in calculating caused by the error for estimating ice-water phase change rate? (3) How to decide the reasonably thermodynamic relation among volumetric liquid content, temperature and ice content when the freezing-thawing process occurring in various soils? Based on the complicated but complete soil model suitable for the wide range of different soil states, reasonable simplification and mathematical derivation from the complete model will be carried out step by step in this paper which will give a good answer to the above questions. Moreover, it leads to a universal as well as simplified soil model taking coupling effect of heat and water transport into consideration and suitable for the land surface process and climate study.

1 The universal unsaturated soil model of coupling heat and water transport

1.1 The universal, complete but complicated soil model (UCSM)

A universal, complete but complicated soil model (UCSM) was proposed by Zhao et al.[15]. Coupling effect of heat and water transport has been taken into consideration. It includes 10 equations, in which 4 prognostic equations are listed below:

The change of volumetric content of ice, θ_i, is given by

$$\frac{\partial \theta_\mathrm{i}}{\partial t}+\frac{\dot{M}_\mathrm{i,v}+\dot{M}_\mathrm{i,l}}{\rho_\mathrm{i}}=0. \tag{1}$$

The change of volumetric content of water, θ_l, is given by

$$\frac{\partial \theta_l}{\partial t}+\frac{\partial u_l}{\partial Z}+\frac{\dot{M}_{l,v}-\dot{M}_{i,l}}{\rho_l}=0. \quad (2)$$

The volumetric mass content of vapor, $\theta_v\rho_v$, is given by

$$\frac{\partial \theta_v\rho_v}{\partial t}-\dot{M}_{i,v}-\dot{M}_{l,v}=\frac{\partial}{\partial Z}\left[D_{\mathrm{eff}}\frac{\partial \rho_v}{\partial Z}\right]. \quad (3)$$

The energy equation to describe the change of temperature, $T^*(℃)\ (=T(\mathrm{K})-T_f(=273.15\mathrm{K}))$, is given by

$$\frac{\partial C_v T^*}{\partial t}-L_{i,l}\frac{\partial \rho_i\theta_i}{\partial t}+L_{l,v}\frac{\partial \rho_v\theta_v}{\partial t}=$$

$$-\rho_l c_l\frac{\partial u_l T^*}{\partial Z}+L_{l,v}\frac{\partial}{\partial Z}\left(D_{\mathrm{eff}}\frac{\partial \rho_v}{\partial Z}\right)+\frac{\partial}{\partial Z}\left(K_{\mathrm{eff}}\frac{\partial T^*}{\partial Z}\right). \quad (4)$$

And there are five diagnostic equations: the equation of liquid water flow rate u_l described by extended Darcy law:

$$u_l=K_l\left[-\frac{\partial \psi}{\partial Z}+1\right]. \quad (5)$$

The freezing-point depression equation:

$$\psi=\frac{L_{i,l}(T-273.15)}{gT_f}, \quad (6)$$

where ψ is the soil matric potential determined by the liquid water content θ_l and ice content θ_i (here the osmotic potential is neglected). The extended empirical equation[10] is often used for ψ:

$$\psi=\psi_0\left(\frac{\theta_l}{\theta_s}\right)^{-b}\left(1+c_k\theta_i\right)^2. \quad (7)$$

In addition, there are another two equations, including the equation of vapor density ρ_v that is related with the local equilibrium vapor pressure e_v in soil, and the relation of volumetric vapor content θ_v related with θ_i and θ_l [15].

In the above equations, Z and t denote depth in the soil and time; T(K) is the soil temperature; $\dot{M}_{i,v}$, $\dot{M}_{l,v}$ and $\dot{M}_{i,l}$ represent phase change rates; $L_{i,v}$, $L_{l,v}$ and $L_{i,l}$ are specific latent heats of phase change; Subscript *i,v; l,v* and *i,l* represent the directions from ice to vapor, liquid to vapor and ice to liquid, respectively. ρ_l, ρ_i are intrinsic densities of liquid and ice, respectively; C_v is the average volumetric heat capacity; K_l is the hydraulic conductivity; K_{eff} is the effective heat conductivity; D_{eff} is the effective diffusivity of vapor in soil pore; g is the acceleration of gravity; ψ_0 is the saturated soil matric potential; b is the Clapp-Hornberger constant[26]; c_k is a constant. There are 10 unknown variables (θ_i, θ_l, θ_v, ρ_v, T, u_l, ψ, $\dot{M}_{i,v}$, $\dot{M}_{l,v}$, $\dot{M}_{i,l}$) but with 9 equations. Therefore, Zhao et al.[15] and Jordan[27] proposed additional different assumptions to close the equations, whereas the validity of the assumptions has not been proved. It is obvious that this model is not fit for the development of land surface models because it consists of complicated equations and one uncertain assumption.

1.2 Reasonable simplification of the UCSM

With regard to the damping depths of diurnal and annual temperature wave in soil[28,29], it can be proved that the term of $\frac{\partial \theta_v\rho_v}{\partial t}$ in eq. (3) is much less than that of $\frac{\partial}{\partial Z}\left[D_{\mathrm{eff}}\frac{\partial \rho_v}{\partial Z}\right]$ based on the analysis of both magnitude order and the numerical simulation results[1)]. Therefore, neglecting the contribution of the term $\frac{\partial \theta_v\rho_v}{\partial t}$, equation (3) can be rewritten as:

$$\dot{M}_{i,v}-\dot{M}_{l,v}=\frac{\partial}{\partial Z}\left[D_{\mathrm{eff}}\frac{\partial \rho_v}{\partial Z}\right].$$

Using the above equation, mass equations (1)—(2) and energy equation (4) can be simplified to the mass balance equation (8) and equation (9) for the change of temperature, respectively:

$$\rho_l\frac{\partial \theta_l}{\partial t}+\rho_i\frac{\partial \theta_i}{\partial t}=-\rho_l\frac{\partial u_l}{\partial Z}+\frac{\partial}{\partial Z}\left(D_{\mathrm{TV}}\frac{\partial T^*}{\partial Z}+D_{\psi\mathrm{V}}\frac{\partial \psi}{\partial Z}\right), \quad (8)$$

$$\frac{\partial C_v T^*}{\partial t}-L_{i,l}\frac{\partial \rho_i\theta_i}{\partial t}=-\rho_l c_l\frac{\partial u_l T^*}{\partial Z}+$$

$$\frac{\partial}{\partial Z}\left(L_{l,v}D_{\mathrm{TV}}\frac{\partial T^*}{\partial Z}+L_{lv}D_{\psi\mathrm{V}}\frac{\partial \psi}{\partial Z}\right)+\frac{\partial}{\partial Z}\left(K_{\mathrm{eff}}\frac{\partial T^*}{\partial Z}\right), \quad (9)$$

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in which D_{TV} and $D_{\psi V}$ are the vapor diffusive coefficients due to temperature gradient and matric potential gradient, respectively. It is clear that the system of above 10 equations have been primarily simplified to the system of eqs. (5)—(9) without applying the uncertain assumption, and the primarily simplified system is still universal and suitable for simulating different kinds of soil under various conditions. In this paper we call it as the universal primarily simplified soil model (UPSSM).

In order to deduce the UPSSM to simpler one but without losing accuracy and universality, the methodology of magnitude order analysis will be further applied to the primarily simplified system.

Firstly, the magnitude order of various flux terms in the energy and mass balance equations will be compared with each other. In the mass balance equation (8) there are three components of water fluxes:

$$Q_L = -K_1 \frac{\partial \psi}{\partial Z} + K_1,\ Q_{MV} = -D_{\psi V} \frac{\partial \psi}{\partial Z},$$

$$Q_{TV} = -D_{TV} \frac{\partial T^*}{\partial Z};$$

and in the energy balance equation (9) there are three components of heat fluxes too:

$$QH_{\text{conduct}} = -K_{\text{eff}} \frac{\partial T^*}{\partial Z},\ QH_{\text{convect}} = \rho_1 c_1 T^* K_1 \left(1 - \frac{\partial \psi}{\partial Z}\right),$$

$$QH_{\text{vapor}} = -\left(L_{1,v} D_{\psi V} \frac{\partial \psi}{\partial Z} + L_{1,v} D_{TV} \frac{\partial T^*}{\partial Z}\right),$$

where Q_L, Q_{MV} and Q_{TV} are the liquid flux, vapor diffusion fluxes due to matric potential gradient and temperature gradient, respectively, and QH_{conduct}, QH_{convect}, QH_{vapor} represent the heat flux due to thermal conductivity, the heat flux brought by liquid movement and the heat flux from energy released or absorbed by phase change of vapor.

The values of K_1, D_{TV}/ρ_1, $D_{\psi V}/\rho_1$, K_{eff}, $L_{1,v}D_{\psi V}$, $L_{1v}D_{TV}$ and $\rho_1 c_1 K_1 T^*$ for six soil textures (sand, sandy loam, loam, silt loam, sandy clay, and clay) with different soil moisture contents at different temperatures have been calculated in detail, in which the empirical hydraulic relations proposed by Clapp and Hornberger have been used (Table 1 lists all physical parameters).

As examples, only the results of clay and sand are shown in Table 2a, 2b and Table 3a, 3b. While calculating the magnitude order of the water and heat fluxes, the magnitude of two terms, $\frac{\partial T^*}{\partial Z}$ and $\frac{\partial \psi}{\partial Z}$, are involved. Since the most important and most prominent contribution of the two terms are shown near the ground surface, the scales of $\frac{\partial T^*}{\partial Z}$ and $\frac{\partial \psi}{\partial Z}$ near the surface layer are used as their representatives. According to the previous research results[28,29], the temperature variation at the soil surface layer is mainly decided by diurnal temperature wave propagation. The diurnal temperature wave decreases with depth in soil exponentially (exp(–*z*/*d*), *d* indicates the damping depth of around 10cm for most of the soil). Thus, if the amplitude of diurnal temperature wave at the ground surface is $\Delta T \approx O(15-30℃)$, the amplitude of diurnal temperature wave at depth *d* is $O(e^{-1}\Delta T) \approx 5-11℃$. It means that in the surface layer the magnitude of order of $\frac{\partial T^*}{\partial Z}$ is O(10℃/10 cm)= O(100℃/m). As for the $\frac{\partial \psi}{\partial Z}$ at the surface layer, it can be defined by $O\left(\frac{\partial \psi}{\partial \theta_1} \cdot \frac{\partial \theta_1}{\partial Z}\right)$. Generally, $O\left(\frac{\partial \theta_1}{\partial Z}\right) \approx O$(0.1/10 cm) $\approx O$(1/m), thus there is $O\left(\frac{\partial \psi}{\partial Z}\right) \approx O\left(\frac{\partial \psi}{\partial \theta_1}\right)$, which can be derived from the soil hydraulic characteristic relationship.

Table 1 Physical parameters of different soil types

Soil texture	% sand(a)	% clay(b)	θ_s(c)	ψ_S(d)	K_S(e)	b(f)
Sand	92	3	0.339	–0.069	1.07E-06	2.79
Sandy loam	58	10	0.434	–0.141	5.23E-06	4.74
Silt loam	17	13	0.476	–0.759	2.81E-06	5.33
Loam	43	18	0.439	–0.355	3.38E-06	5.25
Sandy clay	52	42	0.406	0.098	7.22E-06	10.73
Clay	22	58	0.468	–0.468	9.74E-07	11.55

(a) Sand proportion; (b) clay proportion; (c) soil porosity; (d) saturated matric potential; (e) saturated hydraulic conductivity; (f) Clapp & Hornberger constant.

Table 2 (a) The values of some terms related to the heat and water fluxes with different soil moisture contents at different temperatures (>0℃) for clay

θ_l (m^3/m^3)	K_l (m/s)	D_{TV}/ρ_l ($m^2K^{-1}s^{-1}$)	$D_{\psi V}/\rho_l$ (m/s)	K_{eff} ($JK^{-1}m^{-1}s^{-1}$)	$L_{lV}D_{\psi V}$ ($Jm^{-2}s^{-1}$)	$L_{l,V}D_{TV}$ ($Jm^{-2}K^{-1}s^{-1}$)	$\rho_l c_l K_l T^*$ ($Jm^{-2}s^{-1}$)	$\frac{\partial\psi}{\partial Z}$
T=0.0℃								
0.05	4.30E-32	0.00E+00	0.00E+00	2.40E-01	0.00E+00	0.00E+00	0.00E+00	1.80E+13
0.2	2.20E-16	7.20E-13	7.80E-16	1.20E+00	2.00E-06	1.80E-03	0.00E+00	5.00E+05
0.46	6.20E-07	4.00E-14	4.60E-17	1.70E+00	1.10E-07	1.00E-04	0.00E+00	1.40E+01
T=10.0℃								
0.05	4.30E-32	0.00E+00	0.00E+00	2.40E-01	0.00E+00	0.00E+00	1.80E-24	1.80E+13
0.2	2.20E-16	1.40E-12	1.60E-15	1.20E+00	4.00E-06	3.50E-03	9.40E-09	5.00E+05
0.46	6.20E-07	7.70E-14	9.10E-17	1.70E+00	2.30E-07	1.90E-04	2.60E+01	1.40E+01
T=30.0℃								
0.05	4.30E-32	0.00E+00	0.00E+00	2.40E-01	0.00E+00	0.00E+00	5.50E-24	1.80E+13
0.2	2.20E-16	4.50E-12	5.70E-15	1.20E+00	1.40E-05	1.10E-02	2.80E-08	5.00E+05
0.46	6.20E-07	2.40E-13	3.10E-16	1.70E+00	7.70E-07	6.00E-04	7.80E+01	1.40E+01

(b) The values of some terms related to the heat and water fluxes with different soil moisture contents at different temperatures (<0℃) for clay

θ_l (m^3/m^3)	θ_i (m^3/m^3)	K_l (m/s)	D_{TV}/ρ_l ($m^2K^{-1}s^{-1}$)	$D_{\psi V}/\rho_l$ (m/s)	K_{eff} ($JK^{-1}m^{-1}s^{-1}$)	$L_{lV}D_{\psi V}$ ($Jm^{-2}s^{-1}$)	$L_{l,V}D_{TV}$ ($Jm^{-1}K^{-1}s^{-1}$)	$\rho_l c_l K_l T^*$ ($Jm^{-2}s^{-1}$)	$\frac{\partial\psi}{\partial Z}$
T=–2.044℃									
0.015	0	2.60E-18	1.40E-12	1.50E-15	5.80E-01	3.90E-06	3.50E-03	–2.20E-11	7.70E+04
0.027	0.1	1.30E-17	1.00E-12	0.00E+00	2.10E+00	0.00E+00	2.60E-03	–1.20E-10	2.60E+04
0.039	0.25	1.80E-18	2.40E-13	0.00E+00	4.40E+00	0.00E+00	6.10E-04	–1.50E-11	1.80E+04
T=–9.98℃									
0.009	0	3.20E-20	7.30E-13	7.80E-16	5.80E-01	1.90E-06	1.80E-03	–1.30E-12	5.30E+05
0.011	0.01	9.90E-20	8.20E-13	0.00E+00	5.50E-01	0.00E+00	2.10E-03	–4.20E-12	3.20E+05
0.02	0.2	3.10E-20	3.10E-13	0.00E+00	3.50E+00	0.00E+00	7.70E-04	–1.30E-12	1.70E+05
T=–20.423℃									
0.007	0	3.70E-21	2.80E-13	2.90E-16	5.80E-01	7.10E-07	7.10E-04	–3.20E-13	1.40E+06
0.015	0.185	4.30E-21	1.40E-13	0.00E+00	3.30E+00	0.00E+00	3.60E-04	–3.70E-13	4.70E+05
0.017	0.25	1.50E-21	7.40E-14	0.00E+00	4.30E+00	0.00E+00	1.90E-04	–1.30E-13	4.10E+05

In order to further analyses and compare the magnitude order of the different water and heat fluxes, a great deal of calculation for the fluxes has been carried out with two observation data sets (the D66 and Rosemount data) by using the UPSSM (eqs. (5)—(9)). Figures 1 and 2, as representatives, only show the typical calculated vertical water and heat fluxes at D66 at different time when the soil site experiencing the unfreezing, freezing and thawing stages.

For the heat fluxes, both the detailed scale analysis and the simulating results show that all values of $\rho_l c_l T^* K_l \frac{\partial\psi}{\partial Z}$ are two more orders of magnitude less than the values of $K_{eff}\frac{\partial T^*}{\partial Z}$, especially when soil is dry or frozen seriously. However, when soil is close to saturated, the magnitude orders of $K_{eff}\frac{\partial T^*}{\partial Z}$ and $\rho_l c_l T^* K_l \frac{\partial\psi}{\partial Z}$ could be the same. With regard to the soil surface layer, the term of heat energy $\rho_l c_l T^* K_l \frac{\partial\psi}{\partial Z}$ means the heat flux brought by the infiltration and its magnitude order is comparable to that of $K_{eff}\frac{\partial T^*}{\partial Z}$ when precipitation rate is larger than 10mm/day. So, the contribution of $QH_{convect}$ from surface infiltration to the energy balance should be reserved. The contribution of QH_{vapor} can be neglected in the energy balance because of its very small contribution under all kinds of soil states.

For the mass fluxes, both the detailed scale analysis and the simulating results show that the magnitude orders of terms $\frac{D_{TV}}{\rho_l}\frac{\partial T^*}{\partial Z}$ and $\frac{D_{\psi V}}{\rho_l}\frac{\partial\psi}{\partial Z}$ do become much

Table 3 (a) The values of some terms related to the heat and water fluxes with different soil moisture contents at different temperatures (>0℃) for sand

θ_l (m^3/m^3)	θ_i (m^3/m^3)	K_l (m/s)	D_{TV}/ρ_l ($m^2K^{-1}s^{-1}$)	$D_{\psi V}/\rho_l$ (m/s)	K_{eff} ($JK^{-1}m^{-1}s^{-1}$)	$L_{lV}D_{\psi V}$ ($Jm^{-2}s^{-1}$)	$L_{l,V}D_{TV}$ ($Jm^{-1}K^{-1}s^{-1}$)	$\rho_l c_l K_l T^*$ ($Jm^{-2}s^{-1}$)	$\frac{\partial\psi}{\partial Z}$
T=0.0℃									
0.05	0	7.90E-14	1.50E-12	1.60E-15	8.30E-01	4.10E-06	3.70E-03	0.00E+00	8.00E+02
0.2	0	1.20E-08	7.00E-13	7.90E-16	2.70E+00	2.00E-06	1.80E-03	0.00E+00	4.20E+00
0.33	0	8.50E-07	4.60E-14	5.10E-17	3.40E+00	1.30E-07	1.10E-04	0.00E+00	6.30E-01
T=10.0℃									
0.05	0	7.90E-14	2.80E-12	3.30E-15	8.30E-01	8.20E-06	6.90E-03	3.30E-06	8.00E+02
0.2	0	1.20E-08	1.30E-12	1.60E-15	2.70E+00	4.00E-06	3.30E-03	4.80E-01	4.20E+00
0.33	0	8.50E-07	8.60E-14	1.00E-16	3.40E+00	2.60E-07	2.20E-04	3.60E+01	6.30E-01
T=30.0℃									
0.05	0	7.90E-14	8.60E-12	1.10E-14	8.30E-01	2.80E-05	2.20E-02	9.90E-06	8.00E+02
0.2	0	1.20E-08	4.10E-12	5.40E-15	2.70E+00	1.30E-05	1.00E-02	1.50E+00	4.20E+00
0.33	0	8.50E-07	2.70E-13	3.50E-16	3.40E+00	8.70E-07	6.70E-04	1.10E+02	6.30E-01

(b) The values of some terms related to the heat and water fluxes with different soil moisture contents at different temperatures (<0℃) for sand

θ_l (m^3/m^3)	θ_i (m^3/m^3)	K_l (m/s)	D_{TV}/ρ_l ($m^2K^{-1}s^{-1}$)	$D_{\psi V}/\rho_l$ (m/s)	K_{eff} ($JK^{-1}m^{-1}s^{-1}$)	$L_{lV}D_{\psi V}$ ($Jm^{-2}s^{-1}$)	$L_{l,V}D_{TV}$ ($Jm^{-1}K^{-1}s^{-1}$)	$\rho_l c_l K_l T^*$ ($Jm^{-2}s^{-1}$)	$\frac{\partial\psi}{\partial Z}$
T=−2.044℃									
0.015	0	2.60E-18	1.40E-12	1.50E-15	5.80E-01	3.90E-06	3.50E-03	−2.20E-11	7.70E+04
0.025	0.075	1.50E-17	1.20E-12	0.00E+00	1.70E+00	0.00E+00	2.90E-03	−1.30E-10	2.80E+04
0.039	0.25	1.80E-18	2.40E-13	0.00E+00	4.40E+00	0.00E+00	6.10E-04	−1.50E-11	1.80E+04
T=−9.98℃									
0.009	0	3.20E-20	7.30E-13	7.80E-16	5.80E-01	1.90E-06	1.80E-03	−1.30E-12	5.30E+05
0.011	0.01	9.90E-20	8.20E-13	0.00E+00	5.50E-01	0.00E+00	2.10E-03	−4.20E-12	3.20E+05
0.02	0.2	3.10E-20	3.10E-13	0.00E+00	3.50E+00	0.00E+00	7.70E-04	−1.30E-12	1.70E+05
T=−20.423℃									
0.007	0	3.70E-21	2.80E-13	2.90E-16	5.80E-01	7.10E-07	7.10E-04	−3.20E-13	1.40E+06
0.01	0.05	1.40E-20	2.90E-13	0.00E+00	1.10E+00	0.00E+00	7.20E-04	−1.20E-12	7.10E+05
0.017	0.25	1.50E-21	7.40E-14	0.00E+00	4.30E+00	0.00E+00	1.90E-04	−1.30E-13	4.10E+05

smaller than the term $K_l\frac{\partial\psi}{\partial Z}$ for unfrozen wet soil. However, when soil is in dry or heavily frozen conditions, the magnitude orders of terms $\frac{D_{TV}}{\rho_l}\frac{\partial T^*}{\partial Z}$ and $\frac{D_{\psi V}}{\rho_l}\frac{\partial\psi}{\partial Z}$ could equal to or greater than that of the term $Q_L = K_l\frac{\partial\psi}{\partial Z}$. It means that the terms $\frac{D_{TV}}{\rho_l}\frac{\partial T^*}{\partial Z}$ and $\frac{D_{\psi V}}{\rho_l}\frac{\partial\psi}{\partial Z}$ should be kept for the model being universal.

It should be noted that the $D_{\psi V}$ and in term $\frac{D_{\psi V}}{\rho_l}\frac{\partial\psi}{\partial Z}$ are zero when freezing because the vapor density of ice in frozen soil is only a function of temperature.

According to the above analysis, a proper simplified version of soil water and heat balance equations can be reduced to:

$$\frac{\partial\theta_l}{\partial t} = -\frac{\rho_i}{\rho_l}\frac{\partial\theta_i}{\partial t} - \frac{\partial}{\partial Z}\left(-K_l\frac{\partial\psi}{\partial Z} + K_l\right) + \frac{1}{\rho_l}\frac{\partial}{\partial Z}\left(D_{TV}\frac{\partial T^*}{\partial Z} + D_{\psi V}\frac{\partial\psi}{\partial Z}\right), \tag{10}$$

$$\frac{\partial C_v T^*}{\partial t} - L_{i,l}\frac{\partial\rho_i\theta_i}{\partial t} = \frac{\partial}{\partial Z}\left(K_{eff}\frac{\partial T^*}{\partial Z}\right) - \rho_l c_l\frac{\partial u_l T^*}{\partial Z}. \tag{11}$$

There are another three equations: (5) (6) and (7) or more general function (12)

$$\psi = \psi(\theta_i, \theta_l). \tag{12}$$

Five equations (10), (11), (5), (6) and (7) or (12) with 5 unknown variables ($\theta_i, \theta_l, T^*, u_l, \psi$) form the universal and simplified soil model (USSM) coupling heat and water transport.

It should be pointed out that in some soil models[9−11] moisture content gradient has been used to describe the liquid water flow $\frac{\partial}{\partial Z}\left(D\frac{\partial\theta_l}{\partial Z}\right)$ where D is the diffusive

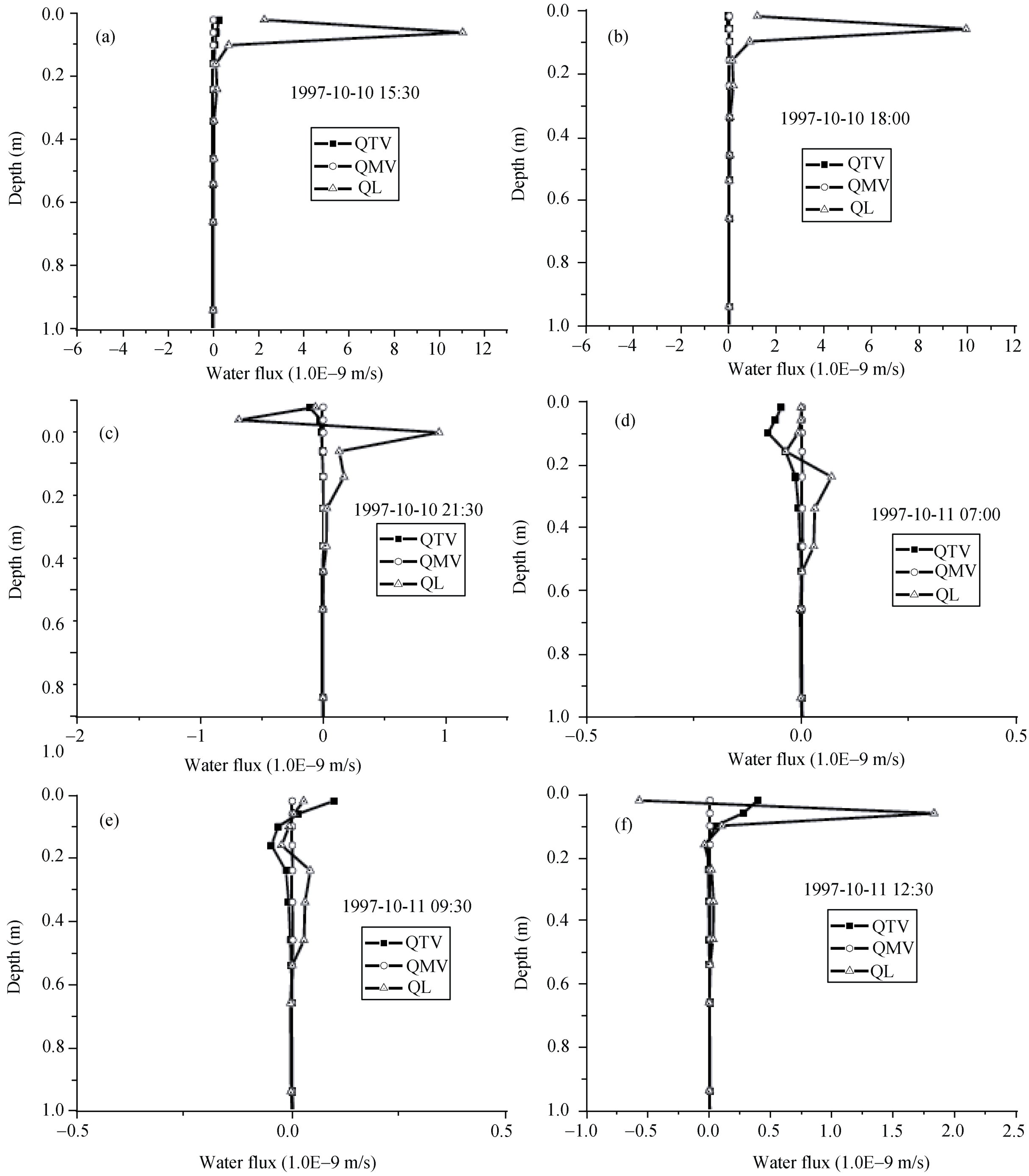

Figure 1 The calculated vertical water fluxes at D66 at different time when the soil site experiencing the unfreezing, freezing and thawing stages. QTV, QMV and QL represent Q_{TV}, Q_{MV} and Q_L (unfreezing stage: (a), (b); freezing stage: (c), (d); thawing stage: (e), (f)).

coefficient (m^2/s) defined by $D = K_1 \dfrac{\partial \psi}{\partial \theta_1}$. It is obvious that the above expression can only apply for the homogeneous soil. However, for the inhomogeneous or frozen soil, due to the discontinuity of soil moisture at the interface between soil layers, the direction of liquid water flow may be opposite to that of decreasing of soil moisture. Thus, the soil moisture content gradient cannot describe the real movement of liquid water. For the frozen soil, the matric potential is not only the function of volumetric liquid water content but also the function of volumetric ice content. It means that while employing the Darcy law, $\dfrac{\partial \psi}{\partial z}$ should be better explained as

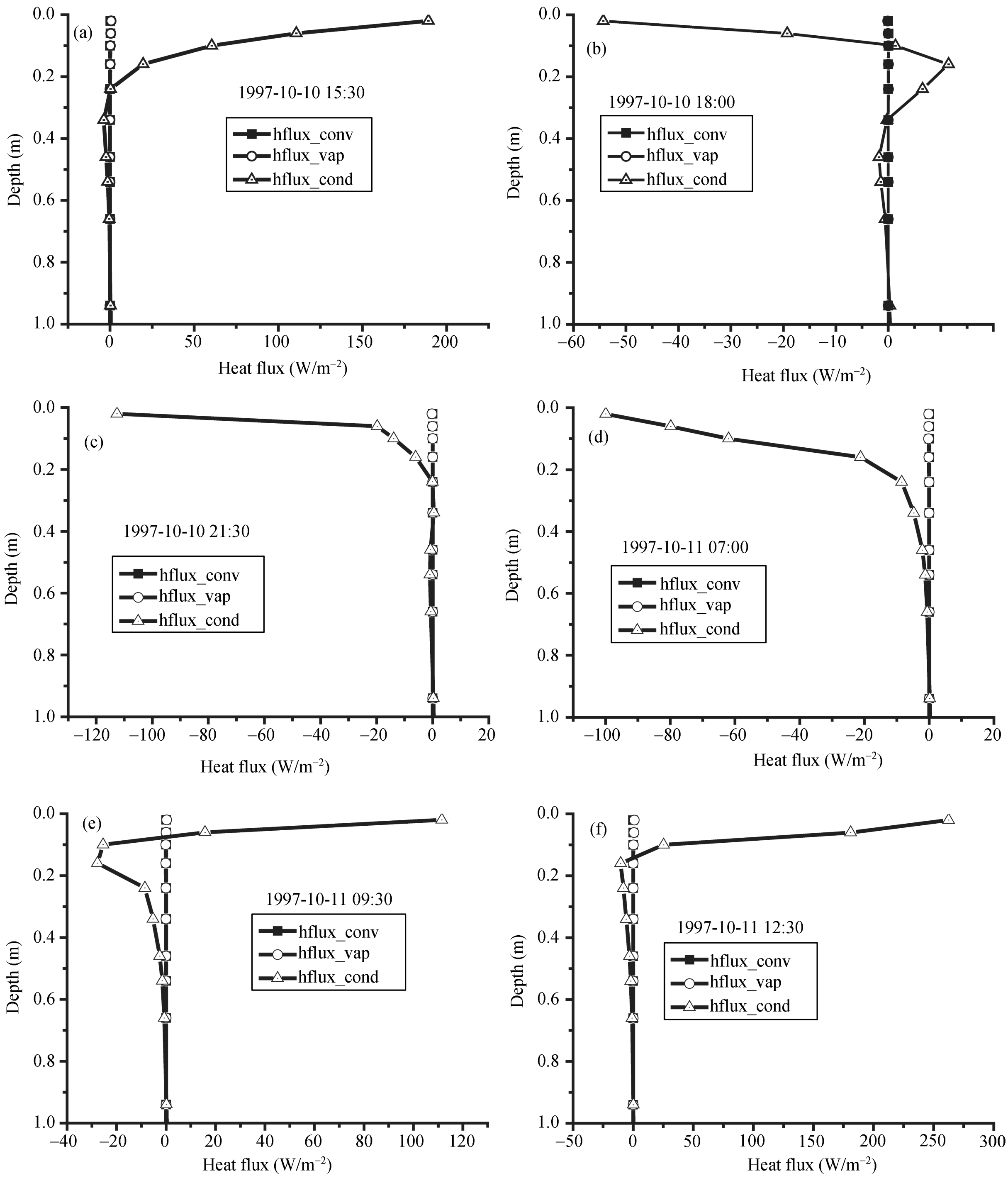

Figure 2 The calculated vertical heat fluxes at D66 at different time when the soil site experiencing the unfreezing, freezing and thawing stages. hflux_conv, hflux_vap and hflux_cond represent QH_{convect}, QH_{vapor} and QH_{condut} (unfreezing stage: (a), (b); freezing stage: (c), (d); thawing stage: (e), (f)).

$\left(\frac{\partial \psi}{\partial \theta_l}\frac{\partial \theta_l}{\partial Z}\right)+\left(\frac{\partial \psi}{\partial \theta_i}\frac{\partial \theta_i}{\partial Z}\right)$ than $\frac{\partial \psi}{\partial \theta_l}\frac{\partial \theta_l}{\partial Z}$. Therefore, if the inhomogeneous and frozen soil will be considered in the universal soil model, it is reasonable to describe the liquid water movement with the matric potential gradient $\left(\frac{\partial}{\partial Z}\left(K_l\frac{\partial \psi}{\partial Z}\right)\right)$.

1.3 The freezing-thawing scheme in the USSM

Eqs. (6) and (7) or (12) describe two essential relations in soil model from which the quantitative relation among soil temperature, volumetric liquid content and volumetric ice content in frozen soil can be derived. Eq. (12) is the hydraulic characteristics of the soil defining the relation of matric potential with volumetric liquid moisture content (and ice content), which is the fundamental constitutive relationship for the unsaturated frozen soil that even though can only be obtained by experiments until now. Eq. (6) is another fundamental relationship in the freezing-thawing soil derived from the phase-equilibrium relationships among ice, liquid water and vapor under the thermodynamic equilibrium state in soil. If the assumption that the system is under thermodynamic equilibrium state is accepted in frozen soil, the phase change equilibrium relationship among θ_i, θ_l and T, which must be held, could be derived from (12) and (6):

$$\theta_{\mathrm{i}} = \theta_{\mathrm{i}}(\theta_{\mathrm{l}}, T) \quad \text{or} \quad \theta_{\mathrm{l}} = \theta_{\mathrm{l}}(\theta_{\mathrm{i}}, T). \tag{13}$$

The above equation describing the relationship among soil temperature, volumetric liquid content and volumetric ice content under the freezing-thawing state for different soil textures, can be called as the unsaturated soil freezing-melting scheme. Since eq. (12) is empirical, eq. (13) is also semi-empirical somewhat on the basis of the thermodynamics. On the assumption of thermodynamic equilibrium, only one relation, either eq. (12) or (13), could be defined independently and the other one must be derived from the defined independent relation and the relation (6). In some research work, however, the soil freezing-melting schemes different from the derived eq. (13) have been proposed and the constitutive relationship eq. (7) or (12) has also been used together. Doing so should be very cautious because it may be contrary to the fundamental relationship eq. (6) with strictly physical base. The reasonable and universal freezing-melting scheme should follow the basic physical relation eq. (6).

The relation of hydraulic characteristics such as eq. (7) or (12) seems to be more universal and more acknowledged by soil physical scientists[26,30]. Faruoki indicated that the ice has influence on the soil matric potential[31]. Therefore, the empirical hydraulic characteristic equation (7) considering the effect of ice has been used to study the frozen and unfrozen soil. Combining eqs. (7) and (6) can get

$$\theta_{\mathrm{l}} = \theta_{\mathrm{s}} \cdot \left[\frac{L_{\mathrm{i,l}} \cdot T^*}{g\psi_{\mathrm{o}} T_{\mathrm{f}}} \left(1 + c_k \theta_{\mathrm{i}}\right)^{-2} \right]^{-1/b}, \tag{14}$$

in which b, ψ_o and θ_s are the parameters depending on the soil texture.

It can be seen from eq. (14) that: (1) The freezing or melting process in the unsaturated soil is continuous and there is no fixed point or range of freezing temperature where the soil water will be frozen completely. Liquid water will always exist in the unsaturated frozen soil no matter how low the soil temperature is. What all the mentioned above accords with many observations. Thus, it should be careful in defining the temperature of freezing at 0℃ or around certain range. (2) If assuming the volumetric content of ice is zero (θ_i=0.0), the amount of θ_l calculated from eq. (14) is the maximum holding capacity of liquid water which will not freeze at temperature T^* below 0℃. It means that the liquid water in soil with temperature T^* will freeze only when the volumetric liquid water content θ_l is greater than the maximum holding capacity. Eq. (14) can also be changed to

$$T^* = \frac{g\psi_0 T_{\mathrm{f}}}{L_{\mathrm{i,l}}} \left(\frac{\theta_{\mathrm{l}}}{\theta_{\mathrm{s}}} \right)^{-b} \left(1 + c_k \theta_{\mathrm{i}}\right)^2. \tag{15}$$

Assuming θ_{i} =0.0, the critical temperature T^*_{crit} for freezing in soil can be got:

$$T^*_{\mathrm{crit}} = \frac{g\psi_0 T_{\mathrm{f}}}{L_{\mathrm{i,l}}} \left(\frac{\theta_T}{\theta_{\mathrm{s}}} \right)^{-b}. \tag{15a}$$

The above equation indicates that if the soil temperature is below T^*_{crit}, the soil begins to freeze, otherwise, it begins to thaw. And it is clear that T^*_{crit} is lower than 0℃. (3) Because different soil textures have different ψ_0 and θ_{s} and thus different maximum holding capacities of liquid water. Figure 3 displays various curves under different temperatures for different soil textures. From Figure 3, it can be found that for all six soil textures, the variation of liquid water with temperature is the most prominent at the range of 0—−2℃. As for the sand, most of liquid water can become ice at −2℃, whereas there is greater amount of liquid water will not freeze when the temperature drop down to −2℃ for other soils. For example, the maximal volumetric liquid water content would be 0.22 for the clay even when the soil temperature is around −20 ℃.

Therefore, the freezing-thawing scheme (14) can describe the freezing-thawing process realistically in the USSM.

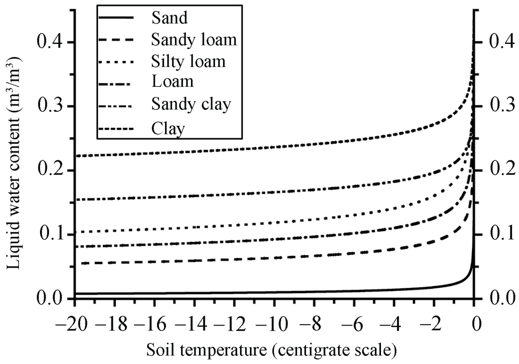

Figure 3 The maximal volumetric liquid water content in different soils with no ice content when the soil temperature is below 0℃.

1.4 The evaporation scheme for dry soil in the USSM

In the dry soil, the equilibrium between liquid water and vapor in the soil pores may not be maintained because the vapor pressure in the soil pore may not be in equilibrium with the local saturated vapor pressure due to the possible large potential evaporation rate at the soil surface. It means that when calculating surface evaporation the assumption of local equilibrium should not be retained[32]. Therefore, in some early researches[14] the evaporation formula had been modified by introducing the concept of soil surface resistance, which favors better understanding and effective description of the soil evaporation process during the drying period. But the function to estimate the soil surface resistance is empirical one of physical properties at soil surface layer, and cannot apply to various soil conditions.

It has been shown from some studies[33] that a dry surface layer (DSL) forms during soil drying, and the vapor to support the vaporization of soil water comes mainly from the bottom of the DSL. Then the concept of DSL or downward shift of evaporation surface has been used to calculate the evaporation flux in dry soil[34,35], which is theoretically clear in the representation of evaporation in dry soil.

The evaporation from dry soil consists of two processes. First, water vapor is transported by molecular diffusion from the DSL to the land surface, and the vapor flux is expressed as

$$E = D_{\text{eff}} \frac{\rho_{\text{a}}}{\rho_{\text{l}}} \frac{hq_e^* - q_s}{z_e},$$

in which q_e^* is the specific humidity of pore air at the depth of the evaporation surface; h is the specific humidity of the air at the soil surface; z_e is the depth of DSL. Second, water vapor is carried from the land surface to the atmosphere, and the flux can be written as

$$E = \frac{\rho_{\text{a}}}{\rho_{\text{l}}} \frac{q_{\text{s}} - q_{\text{a}}}{r_{\text{a}}},$$

where q_{a} represents the specific humidity in the air, and r_{a} is the aerodynamics resistance to the transfer of vapor.

Kondo et al.[36] pointed out that these two fluxes of each process are equal and equal to ground surface evaporation, thus the evaporation can be expressed as

$$E = \frac{\rho_{\text{a}}}{\rho_{\text{l}}} \frac{hq_e^* - q_{\text{a}}}{r_{\text{a}} + z_e / D_{\text{eff}}},$$

where z_e/D_{eff} is equivalent to the surface resistance proposed in earlier studies[14,37], whereas it is not the empirical function of liquid water content at surface layer. Therefore, the above method to calculate the surface evaporation is adopted in the USSM, which can avoid the empirical relationship and suitable for different soil conditions.

2 The new version of the USSM (NUSSM) through variables transformation

It can be found that the governing equations in the USSM are the nonlinear equations, in which the soil temperature and volumetric moisture content are taken as the prognostic variables. It leads that the term of ice-liquid phase change rate, $\frac{\partial \theta_{\text{i}}}{\partial t}$, is explicitly shown in the equations. When soil freezing or thawing, the term of latent heat caused by the water-ice change, $L_{\text{i,l}} \partial \rho_{\text{i}} \theta_{\text{i}} / \partial t$, is included in the energy equation (14). Due to the large quantity of specific latent heat ($L_{\text{i,l}}$=3.336×10^5 J/Kg), this term $L_{\text{i,l}} \partial \rho_{\text{i}} \theta_{\text{i}} / \partial t$ is closely associated with the change of soil temperature. However, the governing equations in the USSM must be solved through iteration. Thus, a small error in the estimation of the phase change rate at the beginning of each iteration step will eventually introduce greater error into the temperature and volumetric moisture calculation that may cause iteration unstable.

In order to avoid the instability caused by the uncertainty in estimation of water-ice change rate, the soil enthalpy H($H = C_{\text{v}} T^* - L_{\text{i,l}} \rho_{\text{i}} \theta_{\text{i}}$) and total water mass m_a ($m_a = \rho_{\text{i}} \theta_{\text{i}} + \rho_{\text{l}} \theta_{\text{l}}$) are used as the predictive variables instead of the temperature and soil liquid content. Then eqs. (10) and (11) are reduced to

$$\frac{\partial m_a}{\partial t}=-\rho_1\frac{\partial}{\partial Z}\left(-K_1\frac{\partial\psi}{\partial Z}+K_1\right)+\frac{1}{\rho_1}\frac{\partial}{\partial Z}\left(D_{\mathrm{TV}}\frac{\partial T^*}{\partial Z}+D_{\psi\mathrm{V}}\frac{\partial\psi}{\partial Z}\right), \tag{16}$$

$$\frac{\partial H}{\partial t}=\frac{\partial}{\partial Z}\left(K_{\mathrm{eff}}\frac{\partial T^*}{\partial Z}\right)-\rho_1 c_1\frac{\partial u_1 T^*}{\partial Z}. \tag{17}$$

Now volumetric enthalpy H and total water mass m_a in soil can be obtained without estimation of the water-ice phase change rate, and then soil volumetric liquid water content θ_1, volumetric ice content θ_i and soil temperature T^* can be solved by the obtained values of H, m_a and the phase change equilibrium relationship (14). Hereafter, the new version of the USSM is called as the NUSSM for simplicity.

3 The validation of the NUSSM

3.1 Data introduction

Four sets of data will be used to validate the NUSSM, including data from the Rosemount Experiment Station from University of Minnesota, the GAME/Tibet D66 site, the Dunhuang Gobi micrometeorological central station and the HEIFE experiment station. These stations are characteristic by different continental surfaces: The Rosemount Experiment Station is characteristic with seasonal frozen soil; the soil at D66 site is not only permafrost but inhomogeneous vertically; Dunhuang Gobi and HEIFE stations are located in the arid, desert region. Here, only two sets of data will be introduced as following.

(i) The GAME/Tibet D66 data. The D66 site is located in the north of Tibetan Plateau (35°31′N, 93°47′E, 4560 m elevation). Annual precipitation is very little due to the influence of continental plateau climate. The site is flat and rarely sparse grassland. The soil is inhomogeneous permafrost[38] and its type is sandy loam. Automatic Weather Station measured meteorological data at the height of 1.5 m, including the downward solar radiation flux, air temperature, pressure, relative humidity, and wind speed at an interval of 30 minutes. Soil temperature was measured hourly at ten depths, 4, 20, 40, 60, 80, 100, 130, 160, 200, 263 cm. Soil water content was measured hourly with Time Domain Reflectometry at six depths: 4, 20, 60, 100, 160, 225 cm.

(ii) Data from the Dunhuang Gobi micrometeorological central station. The Dunhuang Gobi station is located at 40°10′N, 94°31′E. Its surface elevation is 1150 meters above sea level and the annual precipitation is 40 mm[39] due to the influence of continental climate. The field is flat and the upper soil is mainly pebble, but the bottom is sand. Meteorological data include the direction and speed of wind, temperature as well as humidity at 1, 2, 8, 18 m heights, and the components of radiation measured at 1.5 m height, such as the direct radiation, the total radiation, the reflective radiation, the downward atmosphere radiation and the upward ground radiation. There are three sensors placed on the ground with an angle of 120° to each other. Soil temperature was measured hourly at 6 depths: 5, 10, 20, 40, 80, 180 cm. Soil water content was measured hourly with sensors at four depths: 5, 10, 20, 80 cm. The accuracy of measurements can refer to the reference 40.

3.2 Justification of the simplification for the soil model

Even though eqs. (16) and (17) in the NUSSM are derived strictly based on the analyses of magnitude order and simulating results, in order to further justify the simplification, the comparison of numerical results from the NUSSM (eqs. (16) and (17)) and the UPSSM (eqs. (8) and (9)) both with the completely same parameterization schemes and parameters has been carried out. It should be pointed out that the data at D66 site with vertical heterogeneity could test the performance of the models in simulating the inhomogeneous soil. It can be found that all the results from the NUSSM are almost completely same as those from the UPSSM for four data sets, which justifies the simplification from the UPSSM to the NUSSM. The figures are omitted in the paper.

3.3 Evaluation of the NUSSM

In order to evaluate the behavior of the NUSSM (eqs. (16) and (17)), four data sets are used. As example, only data sets from the D66 site (frozen soil) and Dunhuang Gobi (dry soil) stations have been used to demonstrate the performance of the model under different continental states. Figure 4 shows the comparison of temperature and soil moisture distributions between the simulated results and the observation data at D66 site. Figure 5 displays the comparison of temperature at different depths between the simulated results and the observation

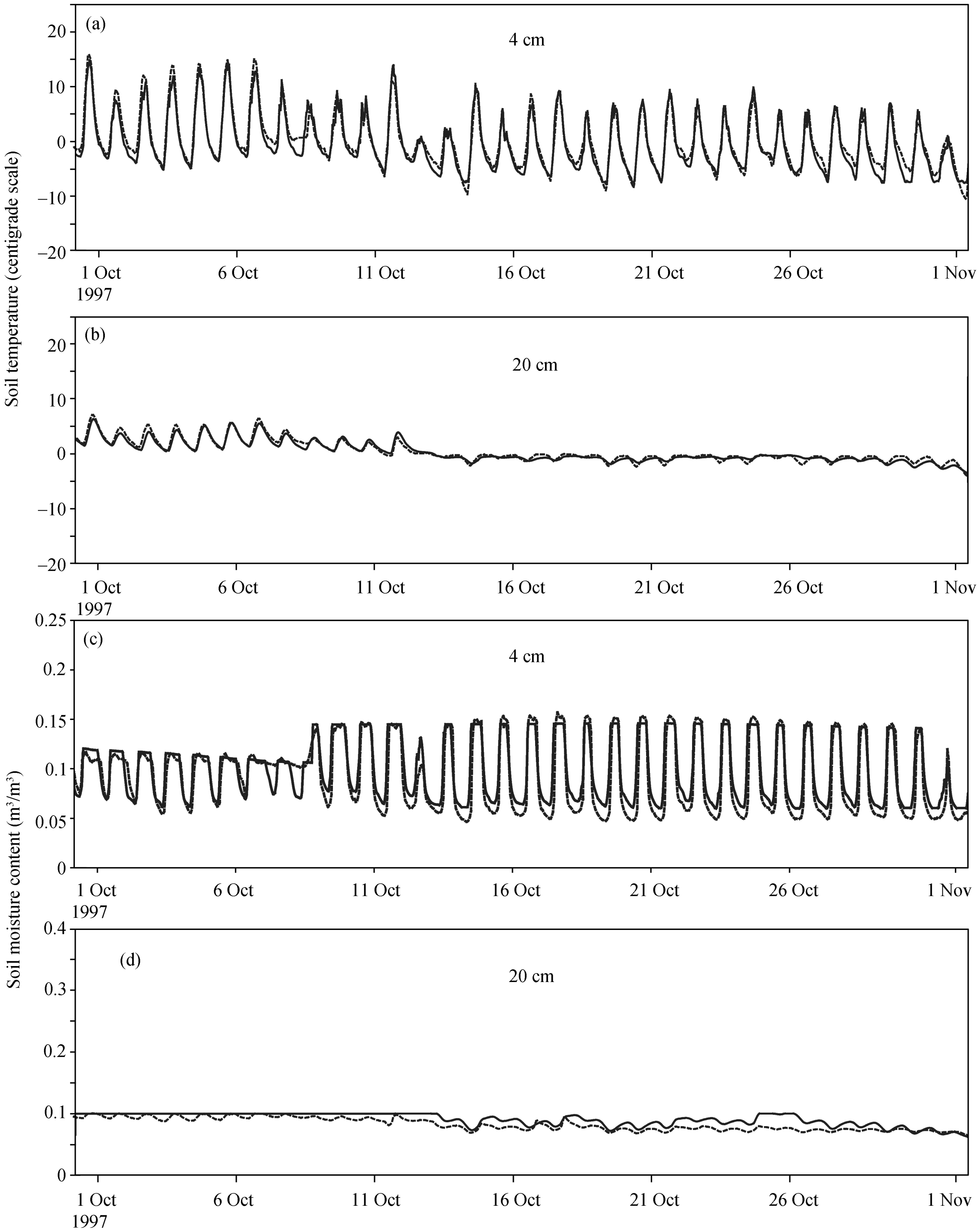

Figure 4 Comparison of soil temperature ((a), (b)), soil moisture content ((c), (d)) at different depths between the results from the NUSSM (solid lines) and the observation data (dashed lines) at D66 site.

data at Dunhuang Gobi station. Due to the arid climate in Dunhuang, soil moisture is very low and the sensible heat flux is much larger than the latent heat flux. And the thermal conductive process dominates the physical process in the soil.

It can be concluded from the above comparisons that the results produced by the NUSSM are in reasonably good agreement with the data sets in either magnitude or variation trend. In addition, the universality of this soil model can be revealed because the above simulating

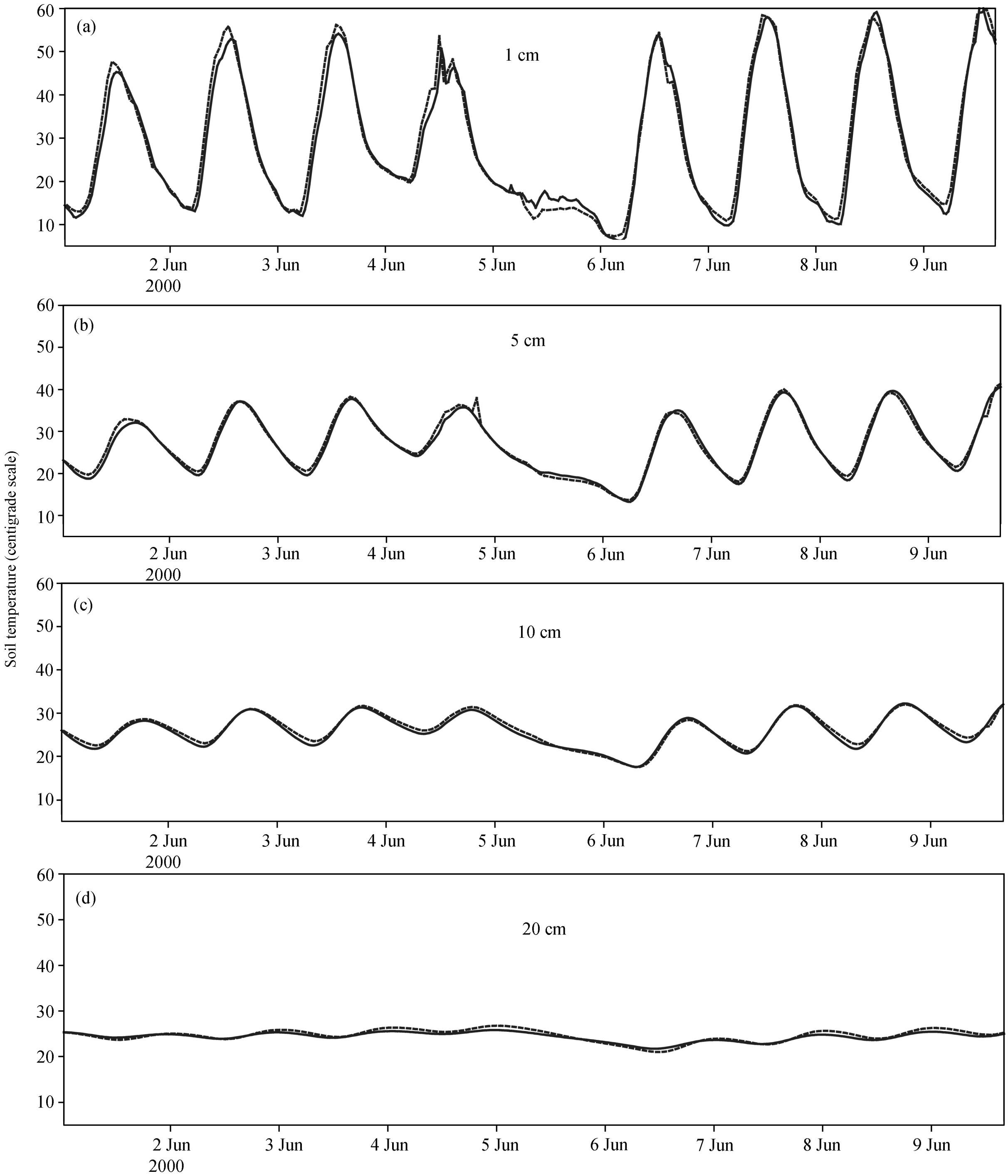

Figure 5 Comparison of soil temperature at different depths between the results from the NUSSM (solid lines) and the observation data (dashed lines) at Dunhuang Gobi station.

examples include the seasonal frozen soil, permafrost and the arid soil. Especially, there is precipitation on 8th, Oct at D66 site, leading to an increase in the soil moisture content, which can be dealt with the wet soil at the soil surface layer. In addition to its good performance, it has also been proved that the NUSSM saves about one-third of computational time compared to the UPSSM. Therefore, the NUSSM not only realistically describes the heat and mass transfer processes occurring in soil but also satisfies the requirement of timesaving in the development of the land surface models as well as the climate models.

4 Conclusions and discussion

The derivation and validation of the new version of universal, simplified soil model (NUSSM) coupling heat and water transfer processes has been explained in this paper. The model can realistically simulate the coupled heat and water transfer processes occurring in the arid, semi-arid and frozen soil, which are defectively described by most common used land surface models.

(1) Firstly, the UCSM coupling heat and water transfer processes was simplified to the USSM based on the analysis of magnitude order. And in order to avoid the uncertainty in calculating caused by dealing with the ice-water phase change rate, the NUSSM is further developed by transforming the USSM through substituting soil enthalpy and total water mass for the soil temperature and volumetric liquid content in the governing equations, respectively.

(2) The NUSSM is suitable for studying both homogeneous and inhomogeneous soil in vertical direction, because the movement of liquid water is described by the matric potential gradient rather than the moisture content gradient.

(3) Assumption of the local equilibrium state at the soil surface has been abandoned when calculating evaporation in arid region and the method of DSL or downward shift of evaporation surface has been adopted instead, which is theoretically clear in the representation of physical process.

(4) The freezing-thawing scheme based on the thermodynamic equilibrium state is applied in the NUSSM for the frozen soil study, leading to its good performance at simulating the freezing-thawing process.

It should be pointed out that this model developed here can also be used for studying the coupled heat and water transfer processes occurring in soil covered with the vegetation, even though the influence of vegetation on the soil water and heat balance has been neglected in this model. In the vegetated region, most of water transported from the ground surface to the atmosphere is dominated by the vegetation, therefore, the extraction through root and the transpiration of vegetation should be included if the vegetation is considered. And other parts in the soil model would be the same as those without the vegetation. Thus, a reasonable soil-vegetation- atmosphere model could be developed based on the realistic NUSSM that can be employed under various soil conditions.

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