NUMERICAL SIMULATION OF WATER CYCLING AND HEAT BALANCE IN AGRICULTURAL ECOSYSTEMS*

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ABSTRACT: In this paper, the authors adopt the model suggested by Lin and et al in [6 — 8] with some improvement in difference schemes. We especially focus on the details of water-heat exchange process in vegetation. For illustration, numerical simulation of the exchange process for wheat in Xu-Chen region in Shandong province is carefully made, the computational results turn out in good agreement with the experimental data.

KEY WORD: agricultural ecosystems, water-heat exchange, numerical simulation

I. INTRODUCTION

The movement and the exchange of water in soil, plant and atmosphere have much to do with agricultural production and living conditions of human beings. In order to utilize water resources more reasonably, enhance the efficiency of plant's water usage and reduce the proportion of water in irrigation, it is necessary to investigate the process of water-heat exchange in SPAC in typical agricultural ecosystems in China.

In recent decades, people came to realize the importance of water-heat exchange in soil, plant and atmosphere continuum. Many works [1 — 3] have showed that various exchange processes occurring at the interface of land and atmosphere are rather complicated. Different structure of vegetation will exert drastic effects on the exchange process and result in a series of changes in climate and environment. Meanwhile some scientists[4] have also noticed that the original ground hydrologic model excluding vegetation effects does not satisfy the ever-growing need for climate and environment study. Hence, it is a great challenge to develop a realistic and feasible ecological model with emphasis on the exchange process including vegetation effects.

It seems that the earliest hydrologic model to calculate transport of water, heat and so on from land to atmosphere have become out of date due to its oversimplicity, Hence, it is indispensable to GCM to propose an appropriate new model. Deardoff[5] suggested a model for predicting temperature, moisture content and so on in surface layer taking vegetation into account and developed a ground hydrologic model with stratified soil, where the changes of the vegetation and soil with space and time and the effects of variation of average properties in surface and deeper layers on exchange process manifest themselves more explicitly.

In this paper, the authors adopt the model suggested by Lin and et al in [6 — 8] with some improvement in difference schemes. We especially focus on the details of water-heat exchange process in canopy. For illustration, numerical simulation of the exchange process for wheat in Yu-Chen region in Shandong province is carefully made, the computational results turn out in good agreement with the experimental data.

II. MATHEMATICAL MODEL

In the whole system of the soil, plant and atmosphere, there are two basic exchange processes: moisture movement and heat transfer. Since evaporation occurs at the expense of energy in the form of latent heat, the above-mentioned two processes are closely related and inseparable.

Because the scale in the vertical direction is much less than that in the horizontal direction, we may assume that the model is one-dimensional. The outline of the model is given in [8]. In SPAC, six important variables in dynamic system are found as follows: volumetric moistures θ_1 in surface layer 1 (of thinness d_1), θ_2 in deep layer 2 (of thickness d_2), mean canopy temperature T_c, bare soil surface temperature T_{gb} and vegetated soil surface temperature T_{gc} in surface layer (of thickness $\overline{d_1}$), and mean temperature $\overline{T}$ in deep soil layer (of thickness $\overline{d_2}$). In addition, the other factors such as evaporation of soil or transpiration of canopy (E_b and E_c) and sensible heat (H_b and H_c) also need to be known. It is noted that the subscripts b and c always indicate bare soil and vegetated surfaces henceforth.
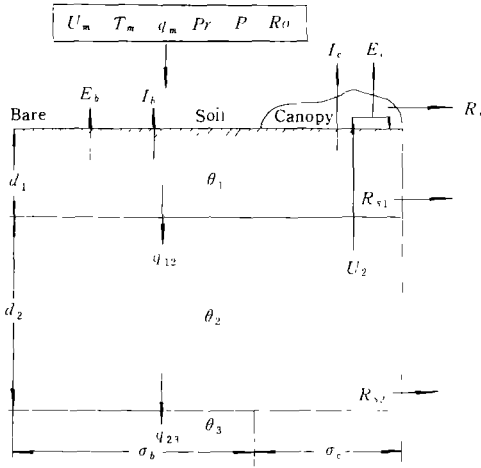

Fig.1   Moisture Movement

Fig.2   Heat Transport

U_m —— atmospheric wind velocity in PBL (cm/s);
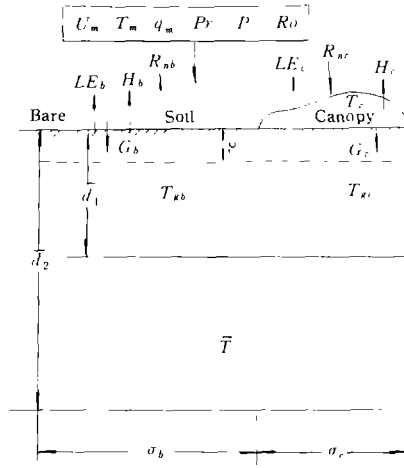q_m —— specific humidity in atmosphere;
P —— atmospheric pressure (mbar);

T_m —— atmospheric temperature (K);
P_r —— precipitation rate (cm/s);
R_n —— net solar radiation (ly/s).

Because the momentum, energy and moisture fluxes heavily depend on the temperature and moisture content in the surface layer, the stratification approach is essential to the study of the problem. In this way, the unsaturated root zone is divided into two layers. Fig.1 shows the process of water movement obeying the governing equations for θ_1 and θ_2:

$$d_1 \frac{d\theta_1}{dt} = \left(I_b - \frac{E_b}{\rho_w}\right)\sigma_b + (I_c - U_1)\sigma_c - q_{12} - R_{s1} \tag{2.1}$$

$$d_2 \frac{d\theta_2}{dt} = q_{12} - q_{23} - U_2\sigma_c - R_{s2} \tag{2.2}$$

where I_b and I_c are infiltration rates into bare soil and vegetated soil, U_1 and U_2 water uptake velocities by roots in the layers 1 and 2, E_b evaporation rate, R_{s1} and R_{s2} are subsurface run-offs in the two layers, q_{12} and q_{23} are moisture fluxes at the interfaces between layers 1 and 2, 2 and 3, $\sigma_c(\sigma_b = 1 - \sigma_c)$ means the percentage of vegetation coverage.

In addition to moisture movement, another factor to be considered is the variation of temperature. According to the way how temperature changes hourly, diurnally or annually, the soil is divided into three layers: the thin surface layer δ, the diurnal temperature change layer $\overline{d_1}$ and the deeper layer $\overline{d_2}$ in thickness. And then following equations (2.3) — (2.6) for the Force-Restore method are derived:

$$h_c C_c \frac{dT_c}{dt} = X_m \tag{2.3}$$

$$\alpha \frac{dT_{gb}}{dt} = \frac{2G_b}{C \cdot \overline{d}_1} - \frac{2\pi}{86400}(T_{gb} - \overline{T}) \qquad (2.4)$$

$$\alpha \frac{dT_{gc}}{dt} = \frac{2G_c}{C \cdot \overline{d}_1} - \frac{2\pi}{86400}(T_{gc} - \overline{T}) \qquad (2.5)$$

$$\frac{d\overline{T}}{dt} = \frac{\sigma_c G_c + \sigma_b G_b}{C \cdot \overline{d}_2} \qquad (2.6)$$

where C and C_c are the volumetric heat capacity of soil and that of canopy, respectively, h_c is the height of canopy, X_m the rate of heat energy absorbed or released by canopy layer in unit time, G_b and G_c are net heat fluxes into the bare soil or vegetated soil surfaces. They could be written as:

$$G_b = R_{nb} - H_b - LE_b \qquad (2.7)$$

$$G_c = S_s \exp(-L_c \cdot X_c)(1 - \alpha_{lc}) - H_{cb} - \sigma(T_{gc}^4 - T_c^4) \qquad (2.8)$$

$$X_m = R_{nc} - LE_c - H_c - S_s \exp(-L_c \cdot X_c)(1 - \alpha_{lc}) + H_{cb} + \sigma(T_{gc}^4 - T_c^4) \qquad (2.9)$$

$$R_{nb} = S_s(1 - \alpha_{lb}) + S_{lb} \qquad (2.10)$$

$$R_{nc} = S_s(1 - \alpha_{lc}) + S_{lc} \qquad (2.11)$$

where R_{nb}, R_{nc} are the net radiations, S_s is total short wave radiation, S_{lb} and S_{lc} are effective long wave radiations, and α_{lb} (α_{lc}) is the albedo of soil (or canopy). L_c means the leaf area index, X_c the extinction coefficient of radiation, σ is the Boltzmann constant. By reference [8], we know that the temperatures T_{gb} and T_{gc} in δ layer play a decisive role in the whole transportation process. Fig.2 shows the mechanism of variation in the canopy temperature T_c, surface temperature T_{gb} or T_{gc} and deep layer temperature $\overline{T}$. In this paper, we have generalized Lin's result [8] by reasonably assuming $T_g = \varepsilon T(\delta, t) + (1 - \varepsilon)T(0, t)$, then the coefficient α is $1 + 2\varepsilon \frac{\delta}{\overline{d}_1}$, where $0 < \varepsilon < 1$ is weighted factor. If $\varepsilon = \frac{1}{2}$, Lin's original results are obtained. As for the depths $\overline{d}_1$, $\overline{d}_2$, their expressions take the form:

$$\overline{d}_1 = \sqrt{\frac{24\lambda}{\pi C}}, \qquad \overline{d}_2 = \sqrt{365\pi} \cdot \overline{d}_1 \qquad (2.12)$$

the thermal conductivity coefficient λ and volumetric heat capacity C of the soil can be expressed as follows:

$$\left.\begin{array}{l} C = 0.46\theta_{mir} \cdot (1 - \theta) + 0.6\theta_{org} \cdot (1 - \theta) + \theta \\[2mm] \lambda = \sum_{k=1}^{N} \lambda_k \theta_k \end{array}\right\} \qquad (2.13)$$

where θ_{mir} and θ_{org} are volumetric contents of the mineral substance and organic matter in the conductivity of each component, θ is volumetric moisture content, λ_k and θ_k are the heat conductivity and the volumetric fraction of the kth component.

The initial data of the model are determined according to the measurement in situ.

III. DIFFERENCE SCHEMES

In this section, a stable difference scheme is constructed to simulate the above mentioned two exchange processes more effectively.

We prefer the following Euler scheme with the precision of second order for the moisture equations (2.1) (2.2)

$$\left. \begin{aligned} d_1 \frac{\theta_1^n - \theta_1^{n-1}}{\Delta t} &= \left(I_b^{n-\frac{1}{2}} - \frac{E_b^{n-\frac{1}{2}}}{\rho_w} \right) + (I_c^{n-\frac{1}{2}} - U_1^{n-\frac{1}{2}})\sigma_c - q_{12}^{n-\frac{1}{2}} - R_{s1}^{n-\frac{1}{2}} \\ d_2 \frac{\theta_2^n - \theta_1^{n-1}}{\Delta t} &= q_{12}^{n-\frac{1}{2}} - q_{23}^{n-\frac{1}{2}} - U_2^{n-\frac{1}{2}}\sigma_c - R_{s2}^{n-\frac{1}{2}} \end{aligned} \right\} \tag{3.1}$$

where

$$\left. \begin{aligned} f^{n-\frac{1}{2}}(\theta) &= \frac{f^n(\theta) + f^{n-1}(\theta)}{2} \\ f^n(\theta) &= f(\theta^n) \end{aligned} \right\} \tag{3.2}$$

In the meanwhile, we find that if $R_{si}^{n-\frac{1}{2}}(\theta)$ is merely replaced by $R_{si}^{n-1}(\theta)$, the precision of above scheme will decrease by one order. In order to keep the same precision, we need to make a special treatment for R_{si} by extrapolation.

$$\overline{R}_{si}^n = \frac{3}{2} R_{si}^{n-1} - \frac{1}{2} R_{si}^{n-2} \tag{3.3}$$

With R_{si} in (3.1) substituted by $\overline{R}_{si}$, the above scheme is still accurate to the second order. In the computation we are able to prove that the above scheme is both precise and unconditionally stable. As for temperature equations, we have

$$\alpha \frac{dT_{gb(c)}}{dt} = \frac{2G_{b(c)}}{C \cdot \overline{d}_1} - \frac{2\pi}{86400} (T_{gb(c)} - \overline{T}) \tag{3.4}$$

Though Runge-Kutte method is generally adopted for this kind of differential equations, we seek an alternative special method to solve it. For convenience, we take T_{gc} for example:

$$\alpha \frac{T_{gc}^n - T_{gc}^{n-1}}{\Delta t} = \frac{2G_c(T_{gc}^n)}{C \cdot \overline{d}_1} - \frac{2\pi}{86400} (T_{gc}^n - \overline{T}^n) \tag{3.5}$$

Because of nonlinearity, $G_c(T_{gc})$ should be linearized, the procedure is carried out as follows:
$\left(\text{notice that } \dfrac{dG_c}{dT_{gc}} = \dfrac{-dH_{cb}}{dT_{gc}}\right)$

$$G_c(T_{gc}^n) = G_c(T_{gc}^{n-1}) + \Delta t \frac{\rho_a C_p}{\gamma_{Hc}} \cdot \frac{T_{gc}^n - T_{gc}^{n-1}}{\Delta t} \tag{3.6}$$

With G_c substituted into (3.6), it is recast into:

$$T_{gc}^n = \frac{T_{gc}^{n-1} + \left[\dfrac{2}{C \cdot \overline{d}_1} G_c(T_{gc}^{n-1}) + \dfrac{\rho_a C_p}{\gamma_{Hc}} T_{gc}^{n-1} + \dfrac{2\pi}{86400} \overline{T}^n \right] \dfrac{\Delta t}{\alpha}}{a + \dfrac{2\pi\Delta t}{86400\alpha}} \tag{3.7}$$

where

$$a = 1 - \Delta t \frac{\rho_a C_p}{\gamma_{Hc}} \cdot \frac{2}{C \cdot \overline{d}_1 \cdot \alpha} \tag{3.8}$$

(3.7) is an explicit expression derived from the implicit scheme.

We use the Euler scheme of the second-order precision for equation (2.3)

$$h_c C_c \frac{T_c^n - T_c^{n-1}}{\Delta t} = \frac{1}{2} [X_m(T_c^n) + X_m(T_c^{n-1})] \tag{3.9}$$

Analogous to the treatment for $G_e(T_{gc})$; we have

$$X_m(T_c^n) = X_m(T_c^{n-1}) + \Delta t \left[\frac{dX_m(T_c^{n-1})}{dT_c} \cdot \frac{dT_c}{dt} + \frac{dX_m(T_{gc}^{n-1})}{dT_{gc}} \cdot \frac{dT_{gc}}{dt} \right] \qquad (3.10)$$

where X_m is seen in (2.9). Because H_c and E_c are functions of T_c and T_{gc}, so we su.. eed

to calculate $\dfrac{dH_c}{dT_c}$, $\dfrac{dH_c}{dT_{gc}}$, $\dfrac{dE_c}{dT_c}$ and $\dfrac{dE_c}{dT_{gc}}$.

IV. NUMERICAL RESULTS AND DISCUSSION

To verify the feasibility of the model, numerical simulation for water and heat cycling in the Yu-Chen region of Shandong province was conducted.

In May 1990, the scientists of the Institute of Mechanics and Institute of Geography, CAS carefully measured water and heat parameters for micrometeorology, soil and canopy in Yu-Chen experimental region. Yu-Chen Observatory is located at 36.57 °N, 116.38 °E with elevation of 23.16 meters ASL. The local soils are made of light clay and silt, and major vegetations consist of wheat and maize. Climate conditions are of continental monsoon type with annual mean temperature of 13.1 °C and annual mean precipitation of 610 millimeters. Since it is not well-distributed seasonally, the shortage of moisture is a severe problem there. For this reason, it is an urgent task to study water cycles and heat exchanges of the land in the region.

In the present paper, wheat is chosen as the vegetation, soil is assumed to be light clay, the period studied is six days from 4th to 9th of May. Because wheat was in its later growing stage, $\sigma_c \approx 1$, i.e., the influences of bare soil are neglected. In this model, parameters are $\theta_{pwp} = 0.06$, $\theta_{fc} = 0.35$, $\theta_s = 0.45$, $z_0 = 3.2$ cm, $h = 60$ cm, $R_{d1} = 0.8$, $R_{d2} = 0.2$. The comparisons between numerical results and experimental data are shown in Fig.3 to Fig.7, where * denotes experimental data, curve denotes its simulation result. The numerical results turn out to agree with the experimental data very well. So the model reflects the essence of physical phenomena and is proved both realistic and feasible.

The comparison between numerical results and experimental data for ground surface temperature is illustrated in Fig.3. We find that they fit fairly well and the ground surface temperature varies diurally. The observation and measurement were conducted from six in the morning to
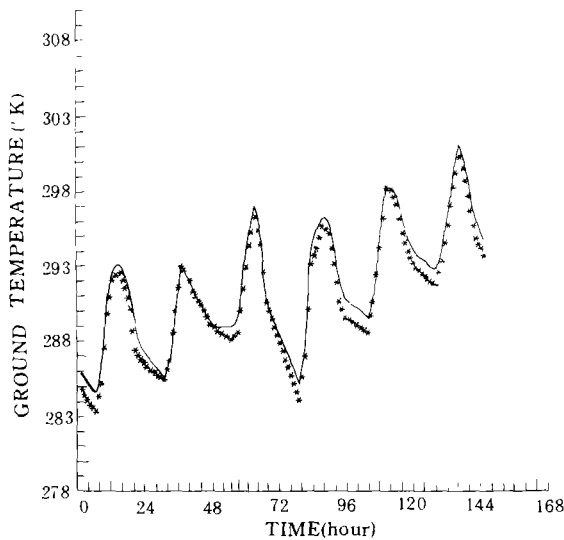

Fig.3 Surface temperature

(* —— experimental data   curve —— numerical results)

ten in the evening with two hour interval. However, the data in the night were obtained merely by extrapolation. It accounts for the fact that the simulation results in daytime are better than those in the night.

The comparison of numerical results with experimental data for temperature deep in 60cm is shown in Fig.4. Simulation results appear very close to experimental data. Since the temperature in deep layer should vary seasonally, whereas 60cm is still not deep enough to eliminate diurnal variation, so the result changes slowly with slight oscillation every day. The results accord with the above facts indeed.

Fig.5 and 6 are the comparison of numerical results with experimental data for volumetric moisture in the soil of 10cm and 60cm deep layers. Because of the sunshine in daytime, much moisture in soil is evaporated, so the volumetric moisture gradually goes down; however, with dew and less evaporation of water at night, the volumetric moisture in soil adds up. It also conforms with the real situation.
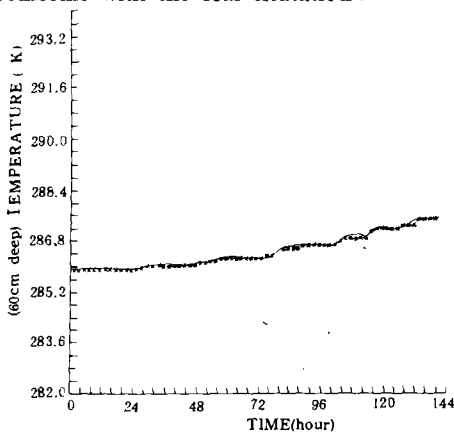
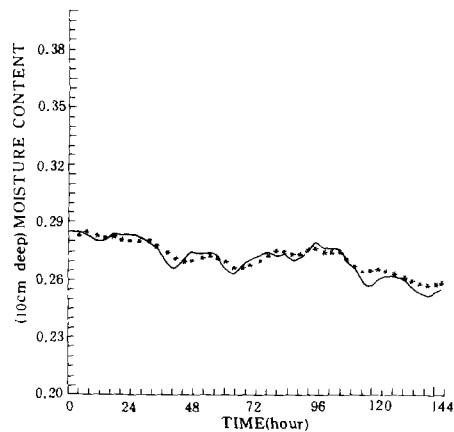Fig.4   60cm deep temperature variance

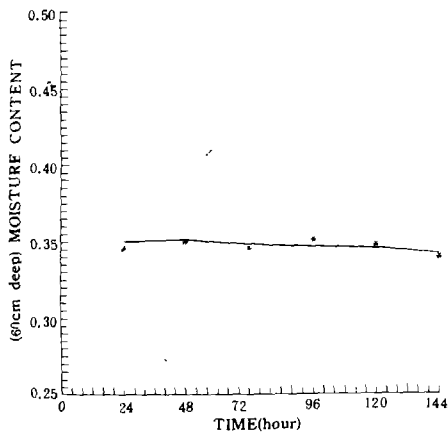Fig.5   10cm deep moisture variance
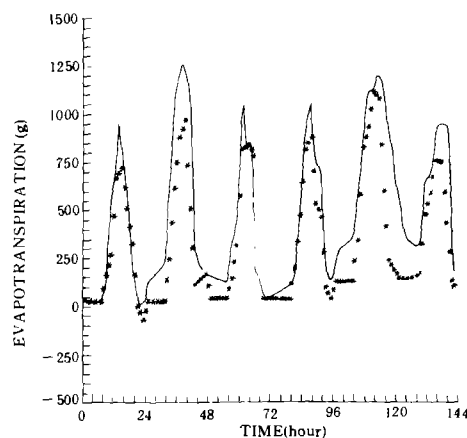
Fig.6   60cm deep moisture variance

Fig.7   variance of evapotranspiration

By comparing observational and numerical evaporations in Fig.7, we find that they coincide roughly. However, it should be noticed that due to weakness in all existing formulae for evaluating evaporation, especially in the cases with less wind velocity, the error will occur. Generally speaking, numerical results are larger than experimental data. Another fact to account for the larger numerical results is the formation of dew in the night. The occurrence of negative point in Fig.7 is very likely due to heavy rain that night. The foregoing model, the reliability of which is confirmed satisfactorily, can be expected to be used for other land ecosystems by changing some governing parameters for soil, vegetation, weather and geography. Nevertheless, some aspects in the model need further improving. Especially, the vortex correlation method in

measuring fluxes of various kinds and the coupled model of multi-layered canopy accounting for atmospheric turbulent structure are expected to be used in the near future.

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APPENDIX

1. Evaporations E_b and transpiration E_c

By using the parameters in PBL suggested by Deardroff, such as momentum and energy exchange coefficients C_u and C_q, friction coefficients C_{ub} and C_{uc}, E_b and E_c can be calculated as follows:

and

$$E_b = \beta_b E_{pb} \qquad E_c = \beta_c E_u \qquad (A.1)$$

$$E_u = \frac{E_{pc}}{1 + r_{c\min} / r_{ac}} \qquad (A.2)$$

where E_{pb}, E_{pc} are potential evaporation and transpiration, E_u is the transpiration with ample water supply and minimum stomatal resistance, which is around 100s/m for tall canopy or 50s/m for short canopy in the model.

$$E_{pb} = \rho_w (q^*(T_{gb}) - q_m)/r_{ab} \qquad (A.3)$$

$$E_{pc} = \rho_w (q^*(T_{gc}) - q_m)/r_{ac} \qquad (A.4)$$

where ρ_w is the density of water, q^* is saturated specific humidity. The coefficients β_b and β_c could be written as:

$$\left. \begin{array}{l} \beta_b = \dfrac{\theta - \theta_{pwp}}{[\alpha_1 (\theta_{fc} - \theta_{pwp})]^{\alpha_2}} \\[3mm] \beta_c = \left\{ \begin{array}{ll} \dfrac{\theta - \theta_{pwp}}{\theta_t - \theta_{pwp}} & \theta < \theta_t \\[3mm] 1 & \theta > \theta_t \end{array} \right. \end{array} \right\} \qquad (A.5)$$

where θ_{pwp} is the volumetric moisture content at the wilting point, θ_{fc} is the field capacity, θ_t is a parameter depending on the mean volumetric moisture content, and α_1, α_2 are constants as well.

2. Sensible heat flux H_{cb} between canopy and vegetated soil surface

$$\left.\begin{aligned}
H_{cb} &= \frac{\rho_a C_p (T_c - T_{gc})}{\gamma_{Hc}} \\
r_{Hc} &= \frac{1}{C_{Din} \cdot \overline{u}_{Can}} \\
C_{Din} &= 0.2 C_D = 0.027/(\ln 10/z_0)^2 \\
\overline{u}_{Can} &= 0.4 \mu_h = 1.08 \mu_{*c}/\ln\left(\frac{0.3h}{z_0}\right)
\end{aligned}\right\} \qquad \text{(A. 6)}$$

where ρ_a is the density of air, C_p is its heat capacity, γ_{Hc} is the resistance, h is the height of canopy, z_0 is the roughness of canopy.

3. Water uptake velocity U_1, U_2

$$\rho_w U_i = \left(\frac{\theta_i - \theta_{pwp}}{\theta_t - \theta_{pwp}}\right) R_{di} \cdot E_u \qquad (i=1, 2) \qquad \text{(A. 7)}$$

where R_{di} are proportion of root density in the layer i ($i=1, 2$), respectively.

4. Surface run-off R_0 (cm/s)

$$R_0 = \max\left(\frac{Pr}{\rho_w} - \sigma_b I_b - \sigma_c I_c, \ 0\right) \qquad \text{(A. 8)}$$

where Pr is the precipitation.

5. Subsurface run-off R_{si} ($i=1, 2$)

$$\left.\begin{aligned}
R_{si} &= 0 && \text{when } \theta < \theta_{fc} \\
R_{si} &= d_i \cdot (\theta_i - \theta_{fc}) \cdot r /3600 && \text{when } \theta > \theta_{fc} \\
r &= \frac{(\theta_i - \theta_{fc})}{\theta_s - \theta_{fc}} && (i=1, 2)
\end{aligned}\right\} \qquad \text{(A. 9)}$$

where θ_s indicates the saturated soil moisture content.

6. Infiltration rate $I_b (I_c)$

If neglecting the surface retention, infiltration rate $I_b (I_c)$ is given as follows:

$$I_b (I_c) = \min\left[K(\theta_s) \cdot \left(1 + \frac{s}{L_j}\right), \ \frac{Pr}{\rho_w}\right] \qquad \text{(A. 10)}$$

where s is the suction head and L_j the distance of moisture front moving downward below the ground surface.

7. Moisture fluxes q_{12}, q_{23}

$$q_{ij} = -D(\theta)\frac{\partial \theta}{\partial z}\bigg|_j^i + K(\theta)\big|_j^j \qquad (i=1, 2; \ j=2, 3) \qquad \text{(A. 11)}$$

Integration of (A.11), gives

$$\frac{1}{d_{ij}}\int_{z_i}^{z_j} q_{ij}\,dz = -\frac{1}{d_{ij}}\int_{z_i}^{z_j} D(\theta)\frac{\partial \theta}{\partial z}\,dz + \frac{1}{d_{ij}}\int_{z_i}^{z_j} K(\theta)\,dz \qquad \text{(A. 12)}$$

Simplification of (A.12) leads to:

$$\bar{q}_{ij} = \frac{\bar{D}_{ij}(\theta_j - \theta_i)}{d_{ij}} + \bar{K}_{ij} \tag{A.13}$$

where

$$\left.\begin{aligned}
\bar{D}_{ij} &= \frac{1}{(\theta_j - \theta_i)} \int_{\theta_i}^{\theta_j} D(\theta)d\theta \\[2mm]
\bar{K}_{ij} &= \frac{1}{(\theta_j - \theta_i)} \int_{\theta_i}^{\theta_j} K(\theta)d\theta
\end{aligned}\right\} \tag{A.14}$$

In which the depth d_{ij} depend on the moisture profiles in soil, there are two cases altogether:

(i) For monotonous cases, i.e., when $\theta_1 > \theta_2 > \theta_3$ or $\theta_3 > \theta_2 > \theta_1$, we have:

$$d_{12} = \frac{d_1 + d_2}{2} \qquad\qquad d_{23} = \frac{d_2}{2} \tag{A.15}$$

(ii) For nonmonotonous cases, i.e., $\theta_1 < \theta_2 > \theta_3$, or $\theta_1 > \theta_2 < \theta_3$, we take:

$$d_{12} = 0.25(d_1 + d_2) \qquad\qquad d_{23} = 0.25d_2 \tag{A.16}$$

For conveniences'sake, the relation between $D(\theta)$ and $K(\theta)$ can be given as:

$$\left.\begin{aligned}
K(\theta) &= a_1 \exp[a_2(\theta - a_3)] \\
D(\theta) &= b_1 \exp[b_2(\theta - b_3)]
\end{aligned}\right\} \tag{A.17}$$

where a_1, a_2, a_3, b_1, b_2 and b_3 are constants depending on the soil texture and moisture content.

8. The adjustment of the vegetation percentage σ_c according to time and space

Generally speaking, the vegetation percentage σ_c varies with time and space. Such as for wheat, σ_c is small in the early growing stage, and σ_c approaches to 1 in its later stage, thus, if considering the whole growing process, we need to decide its growing period and $\sigma_{c\,min}$. Then an approximate treatment is made by interpolation. In this paper, we carry out calculation in wheat's later growing stage, so we assume $\sigma_c = 1$.