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MASS TRANSFER BETWEEN PHASES AND WATER TRANSPIRATION IN A MEDIUM HAVING DOUBLE POROSITY

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UDC 532.546

Two limiting models are proposed for exchange involving porous granules containing water in the condensed and vapor states. The water uptake rate by plants can be related to the water content.

A model exists for water transport in soil that incorporates plant root transpiration, which leads to a quasilinear parabolic equation for the water content, but it involves major empirical elements and far from always correctly reflects the actual processes [1]. This is due in part to the transport mechanisms assumed and in part to the description of the plant water uptake. The first aspect has been discussed in [2], where water filling was considered for a two-pore medium that simulated a granulated soil. The second amounts to determining the transpiration rate as a function of soil water content.

Various forms of that relationship have been proposed [3-6]. It is usually approximated as a kinked line consisting of several straight sections, with the coefficients taken as certain universal parameters completely determined by root mass density and plant physiology. In fact, that approach is essentially incorrect because the transpiration rate is dependent not only on the water content in the soil but also on the transport rate directly to the roots. The latter varies with the soil structure. Therefore, for a given water content, the transpiration rates for given plants will be dependent on the water transport in the soil, i.e., one cannot consider the process as universal.

1. We represent the soil as consisting of contacting porous granules [2], which for simplicity we take as identical spheres. The plant roots usually lie in the gaps between the granules and absorb water vapor [3]. We assume that condensed water occurs only within the granules, and the water enters the space between them by evaporation and transport in the granules. The rates are usually much less than the mixing rates in the intergranules space on scales of the order of the characteristic microstructure length, so the vapor concentration c can be taken as homogeneous. It is realistic to assume that the rate-limiting step in transpiration is water absorption at the root-surfaces, not transport in the gas. One then represents the uptake as a first-order reaction, and the mass of water absorbed in unit volume of soil in unit time is kc, where k is the product of the specific area of the active root-system surface and the rate constant for the reaction, which may be considered as known.

Several physical mechanisms are involved in water transport within the granules [1, 7, 8]. Heuristically, one can distinguish transport in the condensed state by capillary impregnation, the motion of thin liquid films diffusion in sorbed layers, and so on, as well as diffusion of the evaporating water in the pore space not filled by liquid.

The simultaneous description of those processes is exceptionally complicated, as is familiar from drying theory [8]; to consider the essence, we discuss only simple models, which correspond essentially to different transport rates in the condensed and vapor states subject to some simplifying assumptions.

2. Let the condensed-water transport rate be much less than the vapor rate in the gas. Then we get a model for the evaporation front $r = R(t)$ in each granule, which separates the region $r < R$, in which part κ of the pore space is filled by condensed water, from the part containing water only as vapor [9]. The front as a zero-thickness surface is an idealization, because there are size differences in the capillaries and pores, and saturation pressure differences over the corresponding menisci, together with transport of condensed or sorbed water, so the front is diffuse and there is a finite-thickness inhomogeneous zone. However, the model with a step change in water content a the front is acceptable if that thickness is much less than the granule radius R_0.

Gor'kii Urals University, Sverdlovsk. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 58, No. 3, pp. 470-477, March, 1990. Original article submitted October 18, 1988.

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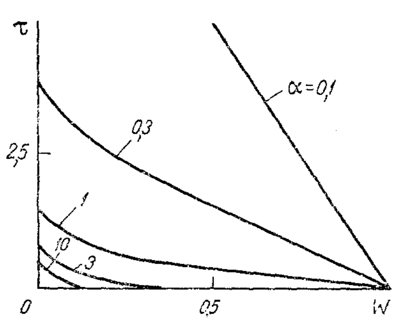

Fig. 1

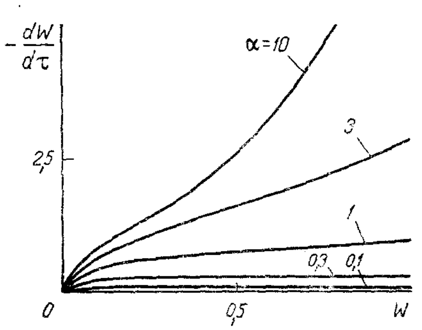

Fig. 2

Fig. 1. Granule water-content dynamics.

Fig. 2. Water-content dependent of transpiration rate.

The vapor diffusion within a granule is described in the quasistationary approximation subject to obvious conditions of the first kind at the front and the outer surface. Then we get expressions for the vapor pattern and mass flux from the front (per granule)

$$c'(r) = c_* - \frac{R_0}{r}\frac{r-R}{R_0-R}(c_* - c),$$
$$q = 4\pi D'\frac{R_0 R}{R_0 - R}(c_* - c), \tag{1}$$

which are dependent on time as a parameter. The masses of water in the regions $r < R$ in the granules and outside them per unit volume of the soil are

$$w_- = w\left(1 + \frac{1-\varkappa}{\varkappa}\frac{c_*}{\rho}\right), \quad w = \varkappa\varepsilon'(1-\varepsilon)\left(\frac{R}{R_0}\right)^3\rho,$$
$$w_+ = \frac{\varepsilon'(1-\varepsilon)}{2}\left\{\left[\frac{R}{R_0}\left(1+\frac{R}{R_0}\right) - 2\left(\frac{R}{R_0}\right)^3\right]c_* + \right. \tag{2}$$
$$\left. + \left[2 - \frac{R}{R_0}\left(1 + \frac{R}{R_0}\right)\right]c\right\},$$

where w means the condensed water content in the soil.

The second expression in (2) is obtained by integrating $c'(r)$ from (1) for the part $R < r < R_0$ of the granule and then multiplying the result by the numerical granule concentration $n = 3(1-\varepsilon)/4\pi P_0^3$. The mass content of vapor in the space between the granules per unit soil volume is εc.

The water mass conservation equations for those regions ar

$$dw_-/dt = -nq, \quad d(\varepsilon c + w_+)/dt = -kc + nq. \tag{3}$$

We introduce the dimensionless quantities

$$W = \frac{w}{\varkappa\varepsilon'(1-\varepsilon)\rho}, \quad C = \frac{c}{c_*}, \quad \tau = \frac{3D'c_*}{\varkappa\varepsilon' R_0^2\rho}t, \tag{4}$$

in which $W = (R/R_0)^3$ is the ratio of the true condensed water content in the granules to that corresponding to uniform saturation of the pore space with a given degree κ; C is the relative vapor pressure in the space between the granules. From (1) and (2), we get for the quantities (4) from (3) that

$$\left(1 + \frac{1-\varkappa}{\varkappa}\frac{c_*}{\rho}\right)\frac{dW}{d\tau} = -\frac{W^{1/3}}{1-W^{1/3}}(1-C),$$
$$\frac{1}{\varkappa\varepsilon'(1-\varepsilon)}\frac{c_*}{\rho}\frac{d}{d\tau}\left\{\varepsilon C + \frac{\varepsilon'(1-\varepsilon)}{2}\left[W^{1/3}(1+W^{1/3}) - 2W + \right.\right. \tag{5}$$

$$+\left(2-W^{1/3}\left(1+W^{1/3}\right)\right)\Big]C\Big\}=-\alpha C+\frac{W^{1/3}}{1-W^{1/3}},$$

$$\alpha=\frac{kR_0^2}{3(1-\varepsilon)D'}.$$

Clearly, c_*/ρ is less than one by many orders of magnitude, and if $c_*/\rho \ll \kappa$, one naturally uses the small-parameter method in solving (5), with W and C as power series. For practical purposes, it is sufficient to take the first terms, and the equations for them follow from (5) with $c_*/\rho = 0$. The second equation gives

$$C=W^{1/3}\left[W^{1/3}+\alpha\left(1-W^{1/3}\right)\right]^{-1}, \tag{6}$$

and the first after substitution from (6) gives

$$\frac{dW}{d\tau}=-\frac{\alpha W^{1/3}}{W^{1/3}+\alpha\left(1-W^{1/3}\right)}. \tag{7}$$

The solution to (7) with initial condition $W(0) = W_0$ is

$$\left(\frac{1}{\alpha}-1\right)(W_0-W)+\frac{3}{2}\left(W_0^{2/3}-W^{2/3}\right)=\tau. \tag{8}$$

An arbitrary initial condition imposed on C in general is not obeyed, as (6) shows, because of the loss of the derivative $dC/d\tau$ in (5) in the small-parameter method. To satisfy that condition we need an additional internal expansion in the solution to (5) in the boundary layer represented by small τ, where we consider (6) and (8) only as an external expansion, and then use an asymptotic link-up procedure [10]. The internal independent variable can readily be shown to be $\tau' \sim (\kappa c_*/\rho)\tau$, i.e., an extent for the boundary layer less by a factor $\kappa c_*/\rho$ than the characteristic time scale for these processes, which means physically that C relaxes from an arbitrary initial value to that defined by (6) much more rapidly than (6) varies. As $c_*/\kappa\rho \ll 1$, that relaxation can be neglected. With $W_0 = 1$, (6) implies $C(0) = 1$, which is a natural initial condition corresponding to a thermodynamic equilibrium state at the start. In that particular case, it is not necessary to construct the internal expansion.

Figures 1 and 2 show the dependence of W on τ and of $-dW/d\tau$ on W for $W_0 = 1$ and various α. The intercepts on the ordinate in Fig. 1 give the dimensionless time for complete granule dehydration, for which part κ of the pore space at the initial instant is completely filled with condensed water, and in particular

$$t^*\approx\frac{\varkappa\varepsilon' R_0^2}{6D'}\,\frac{\rho}{c_*},\quad \alpha\gg 1;\quad t^*\approx\frac{\varkappa\varepsilon'(1-\varepsilon)}{k}\,\frac{\rho}{c_*},\quad \alpha\ll 1, \tag{9}$$

i.e., t^* is determined only by the rate of the rate-limiting process.

Figure 2 shows that the W dependence of $-dW/d\tau$ can vary considerably with α; it represents the transpiration rate up to terms of order $c_*/\kappa\rho$ for $\alpha > 1$, and it increases more rapidly than in proportion to W, while for $\alpha < 1$, it does so more slowly. With $\alpha \gg 1$, the W dependence is very strong, while if $\alpha \ll 1$, $-dW/d\tau$ is approximately constant at α for all water contents, apart from the region $W \lesssim \alpha^3$. This shows why it is fruitless to attempt to formulate a universal dependence of the transpiration rate on the water content unrelated to the soil structure.

3. If the condensed-state transport rate is much higher than the evaporation and diffusion rates in the granules, one naturally assumes that the condensed water is uniformly distributed in the granules at any time, and then the evaporation is simultaneous in all parts of each granule, while the diffusion is described in the quasistationary approximation by

$$D'\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dc'}{dr}\right)+\gamma\left(c_*-c'\right)=0. \tag{10}$$

The diffusion coefficient is of course dependent on the pore space within the granules accessible to the vapor. The assumption made here that D' is constant is approximately true only for relatively small κ. The kinetic coefficient γ and the vapor equilibrium concentration c_* can also vary over time because of changes in the transfer of water molecules from the condensed or adsorbed state to the gas, e.g., as a results of sequential evaporation from the steadily smaller pores and capillaries. Those affects are neglected here for simplicity.

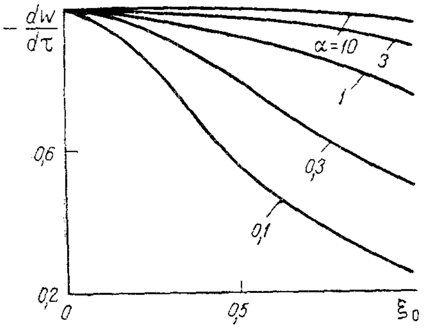

Fig. 3

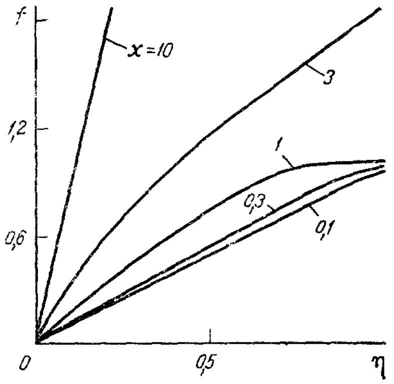

Fig. 4

Fig. 3. Parametric dependence of the transpiration rate.

Fig. 4. Solving the equation for the impregnation depth: $x = \varphi/k$.

There are many discussions such as in [11] on the justification for using phenomenological equations such as (10) to describe diffusion in adsorbent grains, catalysts, and so on. The quasistationary approximation in (10), as in the diffusion equation for a model with a moving evaporation front, is justified because the transpiration is slow, time-scale $\approx \kappa\rho/c_*$. Similar arguments have been put forward previously [12] for transport in a medium with double gas porosity and sorption capacity on the pore walls.

The solution to (10) subject to regularity at $r = 0$ and $c' = c$ at $r = R_0$ is

$$c'(r) = c_* - \frac{\xi_0 \operatorname{sh} \xi}{\xi \operatorname{sh} \xi_0}(c_* - c), \quad \xi = \sqrt{\frac{\gamma}{D'}} R,$$

$$q = 4\pi D' R_0 (\xi_0 \operatorname{cth} \xi_0 - 1)(c_* - c), \quad \xi_0 = \sqrt{\frac{\gamma}{D'}} R_0. \tag{11}$$

The following are the water mass-balance equations in dimensionless form analogous to (5) when terms of order $c_*/\kappa\rho$ are neglected:

$$dW/d\tau = -(1 - C), \quad 1 - C - \beta C = 0. \tag{12}$$

Here W and C are still defined by (4), but

$$\tau = \frac{3D'}{\varkappa \varepsilon' R_0}(\xi_0 \operatorname{cth} \xi_0 - 1)\frac{c_*}{\rho} t,$$

$$\beta = \frac{kR_0^2}{3(1 - \varepsilon) D' (\xi_0 \operatorname{cth} \xi_0 - 1)} = \frac{\alpha}{\xi_0 \operatorname{cth} \xi_0 - 1}, \tag{13}$$

and κ now means the proportion of the pore volume in the granules filled by condensed water at the start.

The solution to (2) is trivial:

$$C = \frac{1}{1 + \beta}, \quad W = W_0 - \frac{\beta}{1 + \beta}\tau \tag{14}$$

(here W cannot be defined as $(R/R_0)^3$, and it decreases as a result of the proportional decrease in the proportion of the volume occupied by the condensed water from the initial value κ). The second initial condition (for C) is not considered for the reasons given above.

The transpiration rate is equal to $-dW/d\tau$ if terms of order $c_*/\kappa\rho$ are neglected, and in the present case is independent of W. However, it is dependent on the kinetic coefficients characterizing the evaporation, diffusion, and uptake by the plants. In the limiting cases of relatively fast and slow evaporation,

$$-\frac{dW}{d\tau} \approx \frac{kR_0}{3(1 - \varepsilon)\sqrt{\gamma D'}}, \quad \xi_0 \gg 1; \tag{15}$$

$$-\frac{dW}{d\tau}\approx\frac{k}{(1-\varepsilon)\gamma},\quad \xi_0\ll 1.$$

In the second case, the transpiration is not dependent at all on the quantities characterizing the diffusion rate. Figure 3 shows the ξ_0 and α dependence of $-dW/d\tau$. The complete dehydration time is

$$t^*=W_0\left(-\frac{dW}{d\tau}\right)^{-1}=\frac{\alpha+\xi_0\,\mathrm{cth}\,\xi_0-1}{\alpha}W_0, \tag{16}$$

and the dependence on ξ_0 and α is the converse of that shown in Fig. 3.

These results are useful not only in describing transpiration trends and using them for particular cases but also because they enable one to judge what conditions must be provided (e.g., how far the soil should be granulated) to provide the desired transpiration rate.

4. The following are simple examples of these results applied to transport. We consider the stationary case of unpressurized irrigation with a constant flow rate from the free surface of the soil, which contains uniformly distributed roots. If the soil is hydrophilic, the unpressurized infiltration occurs in a system of contacting granules, with the gaps between them almost everywhere filled by moist air [2]. The vapor transport in that space is by diffusion, i.e., in the stationary case,

$$Dd^2c/dx^2+nq-kc=0, \tag{17}$$

in which x is the vertical coordinate, which is reckoned downwards from the surface. In the section 2 model, flow is possible in the granule system only at $R = R_0$, so in that case one has to assume that in the wetted soil zone ($x < h$), the granules are uniformly saturated, while outside it, they do not contain any condensed water. The mass flow of vapor from all the granules in unit volume for $\kappa \approx \text{const}$ is

$$nq=\varphi(c_*-c),\quad \varphi=3\delta/R_0,\quad 0<x<h, \tag{18}$$

where δ characterizes the evaporation rate from unit area of the surface of a saturated granule and is roughly speaking proportional to γ. In the section 3 model, instead of (18) we have

$$nq=\varphi(c_*-c),\quad \varphi=\frac{3(1-\varepsilon)D'}{R_0^2}(\xi_0\,\mathrm{cth}\,\xi_0-1),\quad 0<x<h, \tag{19}$$

in which ξ_0 is defined in (11) no matter what the granule filling. For $x > h$, $nq = 0$ in both cases.

We take the vapor flux from the free surface as zero and specify continuity in the concentration and flux at $x = h$ together with bounded values for $x \to \infty$ to get from (17) and (18) or (19) that

$$\begin{gathered}c=\frac{\varphi}{\varphi+k}\left[1-\frac{\mathrm{ch}(\lambda x)}{\mathrm{ch}(\lambda h)+(\lambda/\nu)\,\mathrm{sh}(\lambda h)}\right]c_*,\quad 0<x<h;\\ c=\frac{\varphi}{\varphi+k}\,\frac{\exp[-\nu(x-h)]}{1+(\nu/\lambda)\,\mathrm{cth}(\lambda h)}\,c_*,\quad h<x<\infty,\\ \lambda=\sqrt{\frac{\varphi+k}{D}},\quad \nu=\sqrt{\frac{k}{D}},\end{gathered} \tag{20}$$

which defines also the transpiration rate kc distribution.

This h can be derived from the condition for equality of the total mass of water evaporating in unit time to the given mass flow rate Q at the surface, i.e., from

$$Q=k\int_0^\infty c\,dx=\varphi\int_0^h(c_*-c)\,dx. \tag{21}$$

From (20) we get an equation for $\eta = \lambda h$:

$$f(\eta)=\eta+\frac{\varphi/k}{\lambda/\nu+\mathrm{cth}\,\eta}=\frac{Q}{c_*}\,\frac{(\varphi+k)\lambda}{\varphi k}, \tag{22}$$

whose solution finally determines the (20) concentration distribution for the vapor. Figure 4 shows $f(\eta)$ for various φ/k.

The condensed-water distribution remains in general unknown. to derive it explicitly, one needs to consider a transport model for the condensed state in a granule system on the basis for example of the Buckley-Leverett theory.

A second example is that of establishing thermodynamic equilibrium in a granulated porous medium as a result of gas desorption from the pore walls after the equilibrium has initially been perturbed by sharp reduction in the pressure [12]. Here one naturally uses the section 3 model. We introduce the partial pressure $p = (R_gT/M)$ of the gas capable of sorption and the value p_* corresponding to thermodynamic equilibrium, where the section 3 results give successively

$$\varepsilon \frac{dp}{dt} = \varphi (p_* - p), \quad \ln \frac{p_* - p_0}{p_* - p} = \frac{\varphi}{\varepsilon} t, \tag{23}$$

with φ defined in (19), where the interpretation of that quantity is the new feature by comparison with [12], and $p_0 = p(0)$.

The second formula in (23) is useful for measuring φ from the slope of $\ln(p_* - p)$ against t. If the relaxation terminates with the establishment of a pressure $p^* < p_*$, the sorption capacity is defined by

$$w = (M/R_gT)(p^* - p_0). \tag{24}$$

Similarly, one can consider other more complicated cases, including nonstationary ones, for water or sorbed-gas transport in the presence of internal absorption and phase transitions or sorption and desorption.

NOTATION

c and C, dimensional and dimensionless vapor concentrations; D, diffusion coefficient; h, impregnation depth; k, absorption coefficient; M, molecular mass; n, numerical granule concentration; p pressure; Q, and q, mass fluxes per unit area of free surface on irrigation and from one granule; R and R_0, radii of evaporation front and granule; R_g, gas constant; r, radial coordinate; T, absolute temperature; t, time; w and W, dimensional and dimensionless water contents in the condensed state; x, vertical coordinate; α and β, parameters defined in (5) and (13); γ, δ, and φ, evaporation coefficients; ε, volume fraction of soil accounted for by gaps between granules; ε', porosity of granule material; λ and ν, parameters introduced in (20); κ, volume proportion of pore space in granules occupied by condensed water; η, dimensionless impregnation depth; ξ, dimensionless radial coordinate; ρ, density of liquid; τ, dimensionless time. A prime denotes a quantity within the granules, while a subscript asterisk denotes the equilibrium state, and a raised asterisk a quantity characterizing process termination.

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