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TEMPERATURE EFFECTS OF VARYING PHASE COMPOSITION
DURING THE STEADY VERTICAL FLOW OF MOISTURE
IN UNSATURATED STRATIFIED SEDIMENTS

by

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This report is preliminary and has not been reviewed for conformity with U.S. Geological Survey editorial standards and stratigraphic nomenclature.

A. The simple model

Consider the simple model of Figure 1a in which water is flowing downward in unsaturated sediments at the steady rate w (gm/cm² sec). For convenience, we illustrate only one stratum in an otherwise homogeneous section. As the medium is unsaturated, the mass flux is generally divided between a contribution from transport in the liquid state, w_l , and one from transport in the vapor state, w_g . As the flow passes through the stratum with contrasting capillary properties, we expect that the relative contributions of each phase will generally be different. (How different they might be depends upon the dynamics of flow which we shall not address.) As we have assumed steady-state conditions, however, the total mass flux, w , will be the same in each medium, i.e.,

$$w = w_g + w_l \quad (1a)$$

$$= w'_g + w'_l \quad (1b)$$

where primes denote conditions in the stratum. To fix ideas, we suppose that the contrast in properties between the stratum and the enclosing medium is such that a greater proportion of the flow occurs in the liquid state in the stratum, i.e., $w'_l > w_l$. To meet this condition, water vapor must condense near the upper boundary of the stratum at the rate $w'_l - w_l$, and the latent heat of vaporization, L per unit mass, must be liberated there. Hence the upper surface of the stratum must behave as a heat source of strength $\Delta q(\text{top})$

$$\Delta q(\text{top}) = (w'_l - w_l)L \quad (2a)$$

$$= \lambda wL \quad (2b)$$

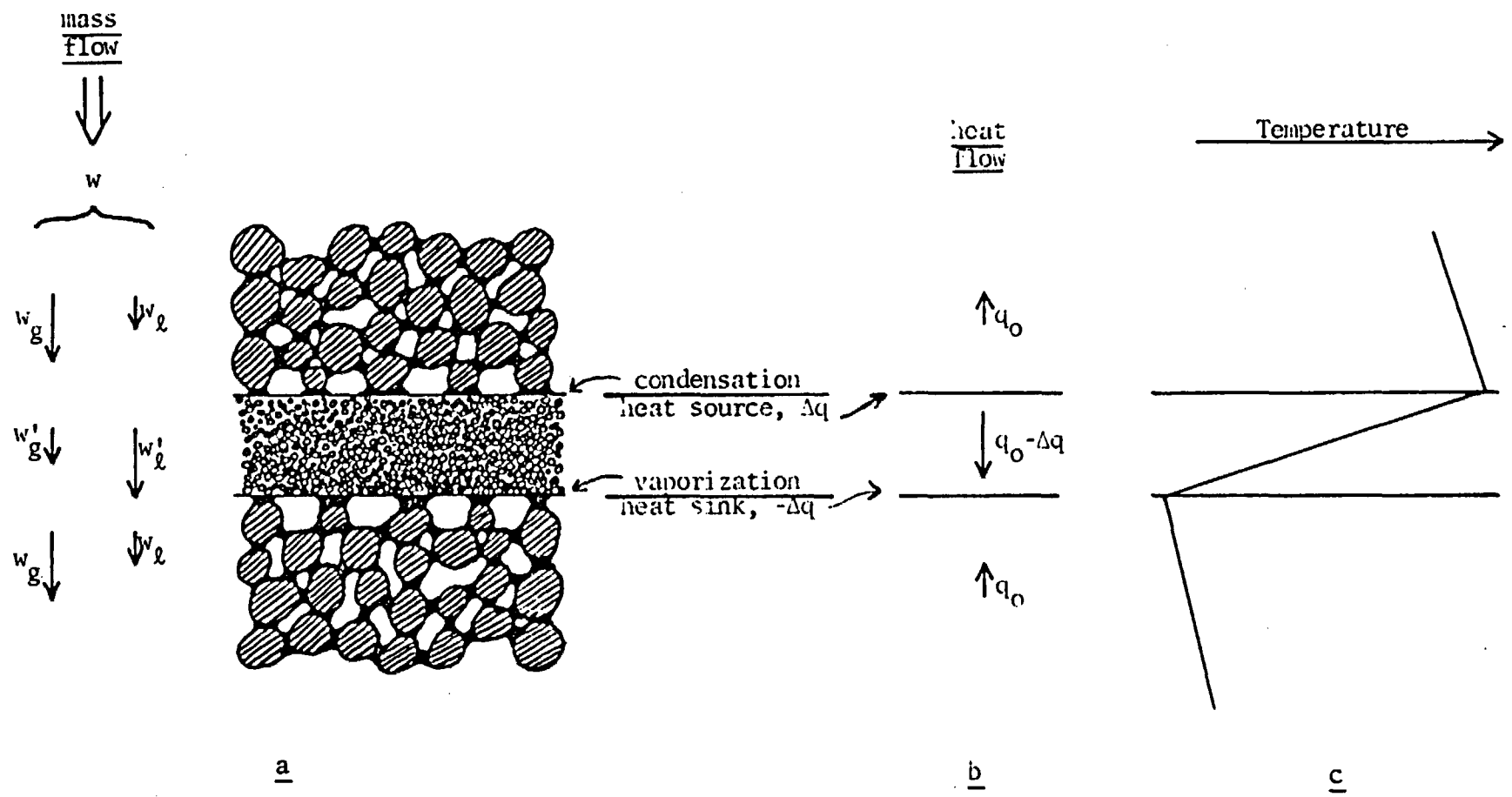


Figure 1

where λ is the increase in the fraction of mass flux carried by the liquid phase when the boundary is crossed, i.e.,

$$\lambda = \frac{w'_\ell - w_\ell}{w} \quad (2c)$$

Similarly as the flow passes through the lower boundary of the stratum vaporization must take place at the rate $w'_\ell - w_\ell$ resulting in a steady heat sink there of strength

$$\Delta q(\text{bottom}) = -\lambda w L \quad (3)$$

Suppose the geothermal flux results in a steady input of heat at the rate q_0 into the bottom of the stratum (Figure 1b). As this flow crosses into the stratum, the sink (equation 3) will reduce its value to $q_0 - \lambda w L$. When the heat emerges at the top of the stratum, it will be augmented by the source (equation 2) so that, in the domain above, its value will again be q_0 ($= q_0 - \lambda w L + \lambda w L$), (see Figure 1b).

The potential importance of this effect stems from the large magnitude of the quantity L , viz.

$$L \sim 580 \text{ cal/gm} \quad (4)$$

If we express w in $\text{gm/cm}^2 \text{ yr}$ (equivalent to a volume flow rates of liquid water in cm/yr), the source strength (2) is

$$\Delta q \left(\frac{\text{cal}}{\text{cm}^2 \text{ yr}} \right) \sim 580 \lambda w (\text{gm/cm}^2 \text{ yr}) \quad (5a)$$

or expressed in heat-flow units ($1 \text{ HFU} = 10^{-6} \text{ cal/cm}^2 \text{ sec}$)

$$\Delta q(\text{HFU}) \sim 18 \lambda w(\text{gm/cm}^2 \text{ yr}) \quad (5b)$$

The background geothermal gradient in continental regions (including NTS) is determined by a regional geothermal flux q_0 of $\sim 1-2$ HFU. Thus it is seen that the source (or sink) associated with condensation (or vaporization) of vertical water flux of only $1 \text{ gm/cm}^2 \text{ yr}$ (i.e., 1 cm/yr seepage velocity) is a full order of magnitude greater than the background heat flow. Consequently, the gradient changes associated with such sources and sinks would be an order of magnitude greater than the background gradient (see Figure 1c). Thus changes from vapor transport to liquid transport for flow rates of only 1 mm/yr could produce anomalies of 100% in the background geothermal gradient. In general, an anomalous negative temperature gradient of the type illustrated (in Figure 1c) should be characteristic of strata favoring transporting the liquid phase in regions of slow downward unsaturated flow. In regions of slow upward flow, the roles of source and sink would be reversed and so would the sign of the temperature-gradient anomaly across such strata. If the anomalous stratum favored vapor flow (instead of liquid flow), the opposite rules would apply (negative gradient anomaly for upflow; positive for downflow). Hence the direction (up or down) of very small steady unsaturated flows might be determined from a superficial examination of the temperature profile and core. The rate of steady flow can be calculated from the magnitude of the gradient anomaly and an estimate of λ ; a lower limit is obtained by setting $\lambda = 1$.

It is important to emphasize that we do not know, at present, whether it is reasonable to expect appreciable changes in phase composition in steady unsaturated flows in bedded tuffs. However, temperature profiles in unsaturated sediments at the Nevada Test Site show steady-state gradient reversals and other anomalies that might be explained by their effects. The applicability of the model to these data is under study.

B. More general considerations

We consider the steady-state one-dimensional problem of water flowing downward from the surface through unsaturated sediments whose properties vary with depth (z , Figure 2).

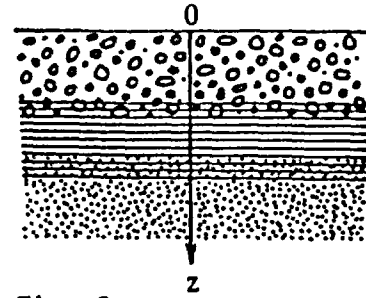


Fig. 2

The total mass-flow rate is a constant w , the sum of contributions from flow in the vapor state w_g and flow in the liquid state w_l , each of which are functions of depth z . The mass-flow rates are the product of a volume-flow rate v and density ρ . Hence

$$w = w_l + w_g, \text{ independent of } z \quad (6a)$$

$$w_l = \rho_l v_l \quad (6b)$$

$$w_g = \rho_g v_g \quad (6c)$$

Differentiation of (6) yields the continuity condition:

$$\frac{dw}{dz} = \frac{dw_l}{dz} + \frac{dw_g}{dz} = 0 \quad (7)$$

The thermal condition of the sediments is a steady-state resulting from a constant temperature on the surface ($z = 0$), a constant geothermal flux q_0 from great depth, and internal sources of heat resulting from steady-state convection and mechanical conversion by the liquid and vapor components of the flow. The energy balance for this condition requires that at any depth

$$\frac{d}{dz} [k \frac{d\theta}{dz}] = \frac{d}{dz} [w_l e_l + w_g e_g] + P \frac{d}{dz} [v_g + v_l] \quad (8)$$

where θ is temperature, k is thermal conductivity, P is pressure, and e_l and e_g are the internal energies per unit mass of water in the liquid and vapor phases respectively.

The term on the left in (8) is the change with depth in conductive heat flow; it is balanced by the local rate of accumulation of heat by convection (first term on the right) and the rate of heat generation associated with reversible volume changes (second term on right). Much of the work of volume change can be incorporated into the first term on the right by replacing the specific internal energy e by the specific enthalpy $h (= e + P/\rho)$.

$$\frac{d}{dz} \left[k \frac{d\theta}{dz} \right] = \frac{d}{dz} [w_l h_l + w_g h_g] - [v_g + v_l] \frac{dP}{dz} \quad (9)$$

We neglect the last term in (9), which is equivalent to assuming that the work of volume change takes place at constant pressure. Now using (2), (3), and the relation

$$\frac{dh}{dz} = c \frac{d\theta}{dz}$$

where c is specific heat at constant pressure, we can express (9) as follows

$$\frac{d}{dz} \left[k \frac{d\theta}{dz} \right] = [w_l c_l + w_g c_g] \frac{d\theta}{dz} - (h_g - h_l) \frac{dw_l}{dz} \quad (10)$$

We define a mean value, \bar{c} , of specific heat of the mass flow by

$$\bar{c} = \frac{w_l c_l + w_g c_g}{w} \quad (11)$$

and denote the conductive flux, positive in the direction of heat flow, by

$$q = k \frac{d\theta}{dz} \quad (12)$$

The latent heat of vaporization L is given by

$$L = h_g - h_l \quad (13)$$

Combining equations (10) through (13) gives a convenient relation between conductive heat flux and conditions of water flow

$$\frac{dq}{dz} = -L \frac{dw_l}{dz} + \frac{\bar{c}}{k} wq \quad (14)$$

The first term on the right shows how, in the steady state, the heat flow changes with depth according to the changing phase composition of the mass flow. The second term on the right is the familiar convection term associated with the transport of thermal capacity.

As the thermal gradient is easier to visualize than the heat flow, it is useful to write (14) for the case of uniform thermal conductivity.

$$\frac{d\Gamma}{dz} = -\frac{L}{k} \frac{dw_l}{dz} + \frac{\bar{c}w}{k} \Gamma \quad (15a)$$

$$\frac{dk}{dz} \equiv 0 \quad (15b)$$

where $\Gamma = d\theta/dz$ denotes thermal gradient. Although (15a) is useful for intuitive purposes, the assumption (15b) usually is not justifiable and the more general form (14) is needed for calculations. In practice, this poses no problem, as the thermal conductivity of the formation is easily determined in the laboratory from core or (if porosity is known) from drill cuttings.

C. The relative importance of the terms in equation (14).

To investigate the role of the second term on the right in (14), consider a medium composed of horizontal strata, each of which has uniform properties

in its interior. Within each stratum, we assume for convenience that the phase composition of the flow will be constant, in which case the first term on the right will vanish, i.e., (14) becomes

$$\frac{dq}{dz} = \frac{\bar{c}}{k} wq \quad (16)$$

Integrating (16) across a stratum of thickness Δz yields

$$\frac{q(\text{top})}{q(\text{bottom})} = e^{-\Delta z/s} \quad (17a)$$

where "top" and "bottom" refer to the stratum boundaries at which q is evaluated and s is a scale length with the sign of w (positive for downward flow)

$$s = \frac{k}{\bar{c}w} \quad (17b)$$

To estimate the expectable range of s we note that the specific heats of liquid and vapor are

$$c_l \cong 1 \text{ cal/gm } ^\circ\text{C} \quad (18a)$$

$$c_g \cong 0.45 \text{ cal/gm } ^\circ\text{C} \quad (18b)$$

and consequently \bar{c} (equation 11) is restricted to a relatively narrow range.

$$\bar{c}[\text{cal/gm } ^\circ\text{C}] \cong \frac{w_l}{w} + 0.45 \frac{w_g}{w} \quad (19a)$$

$$\cong 1, w_g = 0 \quad (19b)$$

$$\cong 0.45, w_l = 0 \quad (19c)$$

Unsaturated sediments normally have thermal conductivities in the range

$$k \sim 0.003 \pm 50\% \text{ cal/cm sec } ^\circ\text{C} \quad (\sim 1.2 \pm 0.6 \text{ W m}^{-1} \text{ K}^{-1}) \quad (20)$$

Using (19b) and (20) in (17b) yields an estimate of scale length s_ℓ for the case where transport is predominantly in the liquid phase

$$s_\ell [\text{km}] \cong \frac{1}{w [\text{gm/cm}^2 \text{ yr}]} \quad (21a)$$

Similarly if the flow is predominantly in the vapor phase, the scale length s_g is

$$s_g [\text{km}] \cong \frac{2.2}{w [\text{gm/cm}^2 \text{ yr}]} \quad (21b)$$

Comparing (21a) and (21b) to (17a), it is seen that for mass flow of constant phase composition at rates on the order of $1 \text{ gm/cm}^2 \text{ yr}$ (Darcian velocities $\sim 1 \text{ cm/yr}$) conductive heat flow across a stratum will be uniform unless its thickness approaches 1 km ; for Darcian liquid flow rates $\sim 1 \text{ m/yr}$ the governing stratum thickness is $\sim 10 \text{ m}$, for $\sim 1 \text{ mm/yr}$ it is 10 km .

Thus for mass flow rates up to $1 \text{ gm/cm}^2 \text{ yr}$, the temperature may be treated by conduction theory ($dq/dz = 0$) in the interior of strata less than a few hundred meters thick if the phase composition of the flow is uniform within such strata.

We now consider the more general case in which the phase composition of flow, and consequently w_ℓ , vary across a layer of thickness δz extending downward from z_1 to z_2 . Using the notation of (17b) in (14) and integrating

over the layer yields

$$\int_{z_1}^{z_2} dq = -L \int_{z_1}^{z_2} dw_{\ell} + \int_{z_1}^{z_2} \frac{1}{s} q dz \quad (22a)$$

$$q(z_1) - q(z_2) \cong L[w_{\ell}(z_2) - w_{\ell}(z_1)] - \bar{q} \frac{\delta z}{s} \quad (22b)$$

where \bar{q} is the mean value of q in the layer, and the relatively small possible variation of s (equations 21) is neglected. The third term will usually be negligible if

$$\frac{\delta z}{s} \ll 1 \quad (23)$$

in which case the variation of heat flow across the layer can be attributed entirely to change in phase composition of the flow, i.e.,

$$[q(z_1) - q(z_2)] \cong 18[w_{\ell}(z_2) - w_{\ell}(z_1)] \quad (24)$$

where q is measured in HFU, and w_{ℓ} is measured in gm/cm² yr. According to (24) if the liquid flow rate increases by 0.1 gm/cm² yr between two depths, the heat flow will decrease by 1.8 HFU between those depths. The form of the depth-dependence of w_{ℓ} in the interval is immaterial; the special case of a discontinuous change in w_{ℓ} (i.e., $\delta z \equiv 0$) is the one discussed originally (equations 2 and 3).