

Mathematics of Transport Coefficients for Porous Media Coupled Heat and Mass Flow

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Coupled flows of a volatile liquid and heat in porous media have been represented by various theories and mathematical formulations. The common feature is that fluxes of mass and heat are forced by gradients of potential energy and temperature. A generalized representation is given by one equation for mass transport and one for heat transport. The mass transport flux equation is

$$J_m = AX_m + BX_h \quad (1)$$

and the heat flux equation is

$$J_h = CX_m + DX_h \quad (2)$$

where A , B , C , and D are the transport coefficients. These equations represent the mathematical essence of the mechanistic approach of Philip and de Vries (1957) as well as the irreversible thermodynamic approach of Taylor and Cary (1964) and others.

In equations (1) and (2) X_m and X_h represent the direct driving forces for mass and heat transport, respectively. These are often expressed in terms of the gradient of potential energy, in the case of X_m , and the gradient of temperature, in the case of heat transport. However, we need not be concerned about their exact expression for the present purpose.

The objective here is to examine how the coefficients A through D can be calculated when measured values of the J s and X s are available. Although this question is of great importance, it has received little attention. In many instances the coefficients have been calculated from complex theoretical formulas without regard for direct evaluation through experiment or how the coefficients or the parameters used to calculate them may be interdependent.

Solution of the Equations for the Coefficients

Consider now the linear algebra of equations (1) and (2) in a format more suitable for that purpose. Namely, dependent variables use symbol y rather than J , and lower case is used for both coefficients and independent variables, x .

Suppose two experiments, *I* and *II*, are performed and values of y and x are measured. Results of experiment *I* are

$$y_1 = ax_1 + bx_2 \quad (3)$$

and

$$y_2 = cx_1 + dx_2 \quad (4)$$

while results of experiment *II* are

$$y_3 = ax_3 + bx_4 \quad (5)$$

and

$$y_4 = cx_3 + dx_4 \quad (6)$$

where y_1 and y_3 correspond to mass flux measured values and y_2 and y_4 correspond to heat flux measured values.

These equations may be put in matrix form as

$$\begin{vmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{vmatrix} = \begin{vmatrix} a & b & 0 & 0 \\ c & d & 0 & 0 \\ 0 & 0 & a & b \\ 0 & 0 & c & d \end{vmatrix} \begin{vmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{vmatrix} \quad (7)$$

or as

$$\begin{vmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{vmatrix} = \begin{vmatrix} x_1 & x_2 & 0 & 0 \\ 0 & 0 & x_1 & x_2 \\ x_3 & x_4 & 0 & 0 \\ 0 & 0 & x_3 & x_4 \end{vmatrix} \begin{vmatrix} a \\ b \\ c \\ d \end{vmatrix} \quad (8)$$

where equation (8) is in the form we wish to examine and solve for a , b , c , and d .

In terms of determinants, the solutions are, for a

$$a = \frac{\begin{vmatrix} y_1 & x_2 & 0 & 0 \\ y_2 & 0 & x_1 & x_2 \\ y_3 & x_4 & 0 & 0 \\ y_4 & 0 & x_3 & x_4 \end{vmatrix}}{\begin{vmatrix} x_1 & x_2 & 0 & 0 \\ 0 & 0 & x_1 & x_2 \\ x_3 & x_4 & 0 & 0 \\ 0 & 0 & x_3 & x_4 \end{vmatrix}}, \quad (9)$$

for b

$$b = \frac{\begin{vmatrix} x_1 & y_1 & 0 & 0 \\ 0 & y_2 & x_1 & x_2 \\ x_3 & y_3 & 0 & 0 \\ 0 & y_4 & x_3 & x_4 \end{vmatrix}}{\begin{vmatrix} x_1 & x_2 & 0 & 0 \\ 0 & 0 & x_1 & x_2 \\ x_3 & x_4 & 0 & 0 \\ 0 & 0 & x_3 & x_4 \end{vmatrix}}, \quad (10)$$

and similarly for c and d. These solutions follow Cramer's Rule (Wylie, 1960). There is a unique solution provided that the determinant in the denominator of equations (9), (10), and so forth is nonzero.

This tells us some things about the nature of the experiments which can lead to determination of coefficients a , b , c , and d . First, if both y_1 and y_3 are zero there is no unique solution and the same applies if y_2 and y_4 are zero. Physically, this means that it is not feasible to find the coefficients by two experiments both of which have either zero mass flux or zero heat flux. To illustrate mathematically, consider what is implied by $y_1 = y_3 = 0$. Clearly, then $x_1/x_2 = x_3/x_4$ or $x_1x_4 = x_2x_3$ and the determinant is evaluated thus

$$\begin{vmatrix} x_1 & x_2 & 0 & 0 \\ 0 & 0 & x_1 & x_2 \\ x_3 & x_4 & 0 & 0 \\ 0 & 0 & x_3 & x_4 \end{vmatrix} = -(x_2x_3 - x_1x_4)^2 = 0. \quad (11)$$

Typical experiments which have been conducted on sealed soil columns by establishing a temperature difference between ends and evaluating the eventual steady state, zero water flux conditions are of the above type. These experiments alone cannot lead to evaluation of the coefficients. An experiment with a nonzero water flux must be included.

Mathematically, all possible experiments can be considered as linear combinations of a zero mass flux and a zero heat flux experiment. The zero mass flux experiment is represented by

$$0 = ax_1 + bx_2 \quad (12)$$

and

$$y_2 = cx_1 + dx_2 \neq 0 \quad (13)$$

while the zero heat flux experiment is represented by

$$y_3 = ax_3 + bx_4 \neq 0 \quad (14)$$

and

$$0 = cx_3 + dx_4 \quad (15)$$

It should be clear that any single experiment can be represented by adding a multiple of equations (12) and (13) to a multiple of equations (14) and (15).

A major theory for the past 50 years with respect to simultaneous transport of water and heat in soil is that proposed by Philip and deVries (1957).

That theory proposes that the coefficients represented by a , b , c , and d are functions, sometimes complex functions, of various soil properties. If we represent these properties symbolically by z_1, z_2, \dots then $a = a(z_1, z_2, \dots)$. Here it is implied that only four of the z_i can be independent.

If the System is 'Isothermal'

One application of equations (1) and (2) is water transport in isothermal soil. The value of X_h is zero for exactly isothermal conditions, so then the above discussion of linear algebra and Cramer's rule solutions is irrelevant. When soil is saturated or in a modestly moist state conditions may in fact be fairly close to isothermal. A great deal of the soil physics of unsaturated flow is based on equation (1) except with $X_h = 0$. In that form it is Darcy's law.

Over the range of conditions where isothermal experiments are feasible the coefficient A of equation (1) can be calculated without concern regarding the determinant of equation (11) being zero. Calculations assuming isothermal conditions in fact predominate. But there could have been temperature differences actually present in many experiments in which it was, however, assumed that they did not exist. In this respect, infiltration experiments producing a wetting front into relatively dry soil but with no measurement of temperature are more common than not. Yet data of Anderson and Linville (1962) indicate a temperature change upon passing of a wetting front. Our recent data indicates similar temperature changes. The magnitude of these temperature changes is from a fraction to several °C.

Which Theory Matches Experiment?

The two primary alternative ways to establish the coefficients of equations (1) and (2) are, as previously indicated, mechanistic and thermodynamic theories. Actually, the thermodynamic theory does not so much prescribe equations to calculate the coefficients as it does to require that certain relationships exist between them. The coefficients, by thermodynamic reasoning, are phenomenological and must generally be measured, but at the same time only three of them may be independent. When equations (1) and (2) are expressed in a form consistent with irreversible thermodynamic theory the coefficients B and C are equal and must also satisfy $B \leq \sqrt{AD}$.

An important task for soil physics should be to design and perform experiments which can adequately compare the theories to actual data. Numerical

models can be used to calculate predicted experimental results under different formulations of the theory, that is, with equations (1) and (2) in different forms as required by the mechanistic and/or thermodynamic theories. It may be difficult to define experiments in which differences of sufficient magnitude will result to confirm which if either theory is more consistent with experimental data. It appears that no such experiments have yet produced a seriously defensible conclusion on this matter.

Conclusion

While I am quite convinced that the above topic is a major one for soil physics, the arguments presented here are as yet in preliminary form. I welcome feedback.

References

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