

THE SELECTION OF APPROPRIATE FLOW POTENTIALS FOR MOISTURE TRANSPORT MODELS

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ABSTRACT

Central to the formulation of a mathematical model to describe moisture transport through porous building materials is the initial choice of the flow driving potentials. Over the years, a considerable number of different formulations have been proposed involving a variety of potentials. A consequence of this is that, at the present time, there is no commonly accepted model with an associated data base of material properties, which can be applied by the simulation community. This paper identifies the various combinations of potentials which can and have been used by researchers and considers their advantages and disadvantages.

INTRODUCTION

The major difficulty in the formulation of a mathematical model for the movement of moisture through capillary-porous media is the description of the mass flux terms and the determination of the required transport coefficients. Obtaining building material properties can involve extremely long test periods and reproducibility of results is not always possible even for the same kind of material⁽¹⁾. It is clear that the number of coefficients used and the complexity of the experimental procedures required to evaluate them have to be important factors for consideration when developing a simulation model.

Of particular importance in the formulation of the flux equations is the choice of driving potentials. In spite of research stretching back some forty years, there has been no general agreement among researchers as to the fundamental potentials to be used. This has meant that flux equations quoted in literature have widely differing formats and that material transport data obtained by one researcher is of no direct value to a model proposed by another. It is this fact more than any other that has hindered progress towards a comprehensive model which can be passed from the research community into building simulation practice.

This paper gives a brief theoretical approach to the identification of possible driving potentials. Some of the combinations suggested by researchers are given together with comments on their practical and applicational implications. The most appropriate for moisture transport models are then considered.

THEORETICAL TREATMENT

Building materials generally have a broad distribution of pore sizes which result in capillary condensation occurring over a wide range of relative humidities⁽²⁾. This means that, under conditions normally encountered within building materials, water vapour transfer co-exists with liquid transfer⁽³⁾. Therefore, to fully describe the movement of moisture it is necessary to consider the transport of both phases.

Two basic approaches have historically been used in this description. The first, which could be described as mechanistic⁽³⁾, involves the application of linear phenomenological laws, such as D'arcy's law and Fick's law, to the vapour and liquid flows. A more modern approach is to use the method of irreversible thermodynamics⁽⁴⁾⁽⁵⁾. The latter approach will be adopted here.

Application of Irreversible Thermodynamics

The basic assumption in the application of irreversible thermodynamics to mass transport through porous bodies is that the following form of the Gibbs equation is valid for non-equilibrium conditions where interaction rates are sufficiently low⁽⁶⁾

$$TdS = dU - \sum \mu_j dn_j \quad (1)$$

where S is entropy (J/K), U is internal energy (J), μ is chemical potential (J/mol), n is the numbers of moles and T is thermodynamic temperature (K).

The flux rates as defined in irreversible thermodynamics can then be written in terms of the following relation

$$J_j = \sum L_{jk} X_k \quad (2)$$

and the local entropy generation rate (J/Km³s) expressed as

$$\sigma = \sum J_j X_j \quad (3)$$

Here X_j is the driving potential associated with flux J_j and L_{jk} are known as the phenomenological coefficients. Equation (2) implies that the fluxes are coupled i.e. a particular J_j is driven not only by its own conjugate X_j but also by the other potentials involved X_i ; $i \neq j$.

Onsager's reciprocal theory states that where the entropy generation term is of the form of equation (3) the matrix L_{jk} is symmetrical i.e. $L_{jk} = L_{kj}$.

Taking the subscripts 1, 2 and 3 to represent the fluxes of energy (u), vapour (v) and liquid (l) respectively, the general transport equations can be written as

$$J_u = L_{uu} X_u + L_{uv} X_v + L_{ul} X_l \quad (4)$$

$$J_v = L_{vu} X_u + L_{vv} X_v + L_{vl} X_l \quad (5)$$

$$J_l = L_{lu} X_u + L_{lv} X_v + L_{ll} X_l \quad (6)$$

Here J_u is in J/m²s; J_v and J_l are molal fluxes in mol/m²s. The driving forces are ⁽⁶⁾

$$X_u = \nabla \left(\frac{1}{T} \right) = -\frac{1}{T^2} \nabla T \quad (7)$$

$$X_v = \nabla \left(-\frac{\mu_v}{T} \right) \quad (8)$$

$$X_l = \nabla \left(-\frac{\mu_l}{T} \right) \quad (9)$$

To develop the theory further, the assumption of local thermodynamic equilibrium is made ⁽⁵⁾⁽⁷⁾. Then

$$\mu_v = \mu_l; \quad X_v = X_l$$

Now the chemical potential of water vapour in equilibrium with the liquid water in the capillaries may be written as ⁽⁸⁾

$$\mu_v = \mu_v^s + RT \ln \frac{p_v}{p_v^s} = RT \ln \phi \quad (10)$$

where μ_v^s is the chemical potential of vapour in equilibrium with a flat liquid surface, p_v^s is the saturation vapour pressure (N/m²), R is the universal gas constant (J/mol K) and ϕ is the relative humidity.

Noting that μ_v^s is a function only of temperature then ⁽⁵⁾

$$X_v = X_l = -\frac{R}{\phi} \nabla \phi \quad (11)$$

and

$$J_v = -\frac{L_{vu}}{T^2} \nabla T - (L_{vv} + L_{vl}) \frac{R}{\phi} \nabla \phi \quad (12)$$

$$J_l = -\frac{L_{lu}}{T^2} \nabla T - (L_{lv} + L_{ll}) \frac{R}{\phi} \nabla \phi \quad (13)$$

On the basis of equations (11)-(13), relative humidity and temperature can be taken as fundamental driving potentials⁽⁵⁾. However, as an alternative to equation (10), an equally valid approach would be to express μ_v in terms of a perfect gas for which

$$\mu_v = \mu_v^o + RT \ln p_v \quad (14)$$

where μ_v^o is the standard chemical potential, a function only of temperature. From this

$$X_v = X_l = -\frac{R}{p_v} \nabla p_v \quad (15)$$

and

$$J_v = -\frac{L_{vu}}{T^2} \nabla T - (L_{vv} + L_{vl}) \frac{R}{p_v} \nabla p_v \quad (16)$$

$$J_l = -\frac{L_{lu}}{T^2} \nabla T - (L_{lv} + L_{ll}) \frac{R}{p_v} \nabla p_v \quad (17)$$

The form of these equations suggests that vapour pressure and temperature can also be taken as appropriate potentials.

Extension to Other Potentials

From the previous section, temperature in combination with either vapour pressure or relative humidity are identified as appropriate driving potentials. However, by using relationships between thermodynamic properties, other possible potentials can be identified.

(i) The vapour pressure and temperature can be related to the vapour density through the perfect gas law, which gives

$$\rho_v = \frac{p_v}{RT} \quad (18)$$

Vapour density can therefore be considered for use as a potential. The theory developed by Philip and

De Vries⁽³⁾ was based on this choice, as was that of Galbraith⁽⁹⁾.

(ii) The vapour pressure, relative humidity and temperature are related to the liquid capillary pressure through the Kelvin equation⁽¹⁰⁾

$$p_l - p_v = \frac{RT}{v} \ln \phi \quad (19)$$

where v is the liquid molar volume. This introduces capillary pore pressure as a possible potential. The models of Pederson⁽¹¹⁾ and Anderson⁽¹²⁾ incorporated capillary pore pressure as a potential.

(iii) The material moisture content m is related to the relative humidity through the moisture retention curve or sorption isotherm⁽¹³⁾

$$m = m(\phi)$$

and thus gives another possible potential. Philip and DeVries⁽³⁾ and Luikov⁽⁴⁾ used moisture content as a fundamental driving potential.

CHOICE OF POTENTIALS

It is clear from the foregoing that the moisture flux equations can be formulated as a combination of a wide variety of driving potentials. However, it is important to appreciate that while all of these combinations may be acceptable, certain of them may be less suitable in terms of practical applications and the experimental evaluation of the associated transport coefficients. This is particularly so for the case of the 'secondary' potentials identified in the previous section.

A commonly used combination of potentials is material moisture content m and temperature T . This combination was used by Luikov⁽⁴⁾, Philip and DeVries⁽³⁾ and Kohonen⁽¹⁴⁾. Little difficulty is experienced when applying such models to single layers of material or homogeneous media. However when used to model multi-layered structures a problem is encountered, in that the moisture content becomes a discontinuous function at the junction of dissimilar materials. It would seem that, while moisture content has been used as a driving potential, its behaviour is analogous to heat content when considering energy transfer. This must call into question the practicality of using moisture content as a driving potential.

Another approach is given in the models of Anderson⁽¹²⁾ and Pederson⁽¹¹⁾ in which capillary liquid pressure is used as a potential. This approach is also problematic in that there is no direct method for its measurement. It is necessary to calculate values from measurements of vapour pressure and temperature using the Kelvin equation. This causes

problems in the evaluation of the associated transfer coefficient. It could be concluded that, in general, where a potential cannot be directly measured, then its use is of limited application as the determination of transfer coefficients requires secondary calculations.

CONCLUSIONS

The above discussion suggests that practical problems may exist when capillary pressure or moisture content are used as driving potentials, although it is emphasised that such potentials are still widely used. The only remaining couples which could therefore be regarded as suitable are temperature with vapour pressure or relative humidity. The vapour pressure-temperature combination is the one at presently followed by the authors because:

- The potentials are easily measured
- Their functions are continuous through a multi-layered structure.
- The 'single' non-coupled models currently in use⁽¹⁵⁾ incorporate vapour pressure as potential.
- Material performance data is easily obtained using standard measurement techniques, a considerable quantity of which is already available in the form of permeability data.
- Detailed information on moisture content and other such parameters can be calculated from a knowledge of the vapour pressure and temperature fields.

The adoption of a consistent set of potentials by researchers would undoubtedly improve the transferability of data and models. This would increase the pace of development of simulation models and would improve their accessibility to building technologists.

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