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Modelling of Moisture Transfer in Structures—I. A Description of a Finite-Difference Nodal Model

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The physical, numerical and computational basis of a 1- 2- or 3-D time-dependent finite-difference nodal model for heat and moisture transfer in buildings is described. The model is designed to be very flexible so as to be able to analyse a wide variety of geometries and circumstances. The solution procedure is fully implicit with non-linear processes such as condensation, radiation and convection being described in terms of an effective conductance at each time step. The model is iterated at each time step to arrive at a good estimate of the updated value of these effective conductances. The performance of this model is analysed in a later paper.

NOMENCLATURE

A_{ij}	area of the interface between node i and node j, m^2
c_p	specific heat of air at constant pressure at ambient conditions specifically in units of J m^{-3} $°C^{-1}$
c_i	specific heat of the material making up node i, J kg^{-1} $°C^{-1}$
$\mathscr{C}_i$	concentration of condensate in node i, kg m^{-3}
F^i_{ij}, F^i_{ji}	air change rate from node $i(j)$ to node $j(i)$ referred to volume i, s^{-1}
h	surface coefficient of heat transfer, W m^{-2} $°C^{-1}$
h_c	surface coefficient of mass transfer, kg m^{-2} Pa^{-1}
k_i	thermal conductivity of the material making up node i, W m^{-1} $°C^{-1}$
L	latent heat of evaporation of water, J kg^{-1}
m_i	moisture concentration in node i, kg m^{-3}
mc	moisture content as a % by weight
p_i	water vapour pressure in node i, Pa
q	heat flux W m^{-2}
Q	total heat flow, W
r_{ij}	vapour flow resistance between node i and node j, N s kg^{-1}
R_{ij}	contact resistance between node i and node j, m^2 °C W^{-1}
$\overline{S_iS_j}$	total exchange area, m^2
T_i	temperature of node i, °C
U_{ij}	effective thermal conductance between node i and node j, W m^{-2} $°C^{-1}$
V_i	volume of node i, m^3
δ_{ij}	Kronecker delta
Δt	time step, s
ε	emissivity
κ	a function giving the relationship between vapour pressure and moisture concentration
ϕ	relative humidity, %
ρ_i	density of the material in node i, kg m^{-3} or reflectivity of material at node i
σ	Stefan–Boltzmann constant (5.67×10^{-8} W m^{-2} K^{-4})

BACKGROUND

THE MOISTURE performance of a building structure is a complex 3-D system problem depending upon the interaction between different parts of the structure, for example, the linings, the framing, the cavities, the internal layers and membranes, and a range of transfer mechanisms, in particular air exchange and vapour diffusion. Existing design tools make assumptions on the moisture performance of the structure, which are not always correct. It is widely acknowledged that a better understanding of the moisture performance of structures can be best obtained with suitable mathematical models, see for example [1].

Earlier work by the author, see for example [2], was concerned with modelling the moisture performance of structures analytically. This approach was followed because it leads to a small number of parameters describing the moisture performance of the structure, each with a clear physical meaning, which in turn provide insights into the performance of the structure, and aid the intuition in understanding the interactions that take place between different parts of a complex system. In particular this earlier work gave rise to the key concept of time constants, and how they change as the details of the structure change. An analytical model is also a useful tool in guiding an experimental programme as it highlights key parameters and indicates which of these most sensitively affect the moisture performance of a structure.

However, in order to model a structure's moisture performance analytically, many approximations must be made, some of them quite severe. It is unclear, after these approximations have been made, just how well an analytical model will describe the real performance. A more accurate, if less intuitively helpful, description of the behaviour of a structure requires a numerical model, in which the approximations are kept to the minimum. The existence of such a model should allow closer predictions to be made of the performance, and allow a check on the predictive power of simpler analytical models. There are a number of different geometries for which modelling is deemed to be necessary, e.g. walls,

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attic spaces, flat roofs, sub-floor cavities. The model described here has been designed to be very flexible, so that all these geometries, and any other of interest, can be accommodated.

Several numerical models for moisture transfer in structures exist of various degrees of sophistication and various domains of application, see for example [3–6]. All but the last of these models are designed for specific geometries while Kohonen's model as described in reference [6] is 1-D. This work describes a very flexible 2- or 3-D finite-difference nodal model for heat and moisture transfer in building structures. In this paper the physical, numerical, and computational aspects of the model are described; comparison between numerical model predictions, analytical model predictions and experimental results are described in a following paper [7].

REQUIREMENTS OF THE MODEL

In designing this model it was decided that the following criteria should be met.

(1) The model should be 1-, 2- or 3-D.

(2) The model should be as flexible as possible so that a wide variety of different circumstances and geometries could be modelled.

(3) The model should be designed in such a way as to allow for easy addition of new features (e.g. phase changes, internal heat and moisture sinks, use at fire temperatures as well as ambient temperatures).

(4) In order to allow easy modification for use at fire temperatures, it was decided that a full view factor treatment of radiation would be used rather than the simpler equivalent network approaches often used at ambient temperatures.

(5) The model should allow more or less lumping of each component of the system according to the state of knowledge of the physics governing the behaviour of that component, or the amount of detailed information required of that part of the system.

(6) It was decided not to model hydrodynamics in detail, so convective processes would have to be modelled using lumped parameters of performance. This is standard practice for these kind of models, see for example [3] and [4].

(7) The solution algorithm should be fully implicit to avoid numerical difficulties with the wide range of nodal sizes allowable, and the wide range of time constants of the subprocesses involved, and to allow these subprocesses to be viewed or averaged out as required, simply by changing the model timestep.

These requirements dictate the details of the model outlined in the next section.

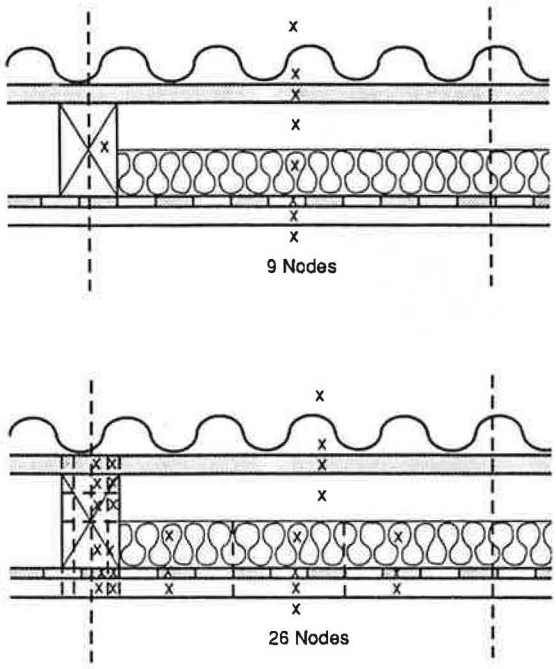

Fig. 1. Identical building structures showing differing possible nodal arrangements.

PHYSICAL BASIS OF THE MODEL

The structure of interest is divided up into a number of nodes, the size, location and number of which is governed by the state of knowledge of the physics governing the behaviour of that component, or the amount of detailed information required of that part of the system. Figure 1 shows two different ways of allocating nodes to the same roof system. Note that in both cases, the cavity is allocated one node, consistent with the limitation that the detailed hydrodynamics of convection is not modelled here.

Moisture movement within a structure is assumed to be by air-borne convection and by vapour diffusion. Moisture movement within solids is very complex, with vapour diffusion, capillary forces, and evaporation-condensation mechanisms operating. The full driving potential will be a complex function of at least moisture concentration and temperature, but in the model the use of vapour pressure as the driving potential is found to be a suitable approximation, particularly below the fibre-saturation point for organic materials or in the hygroscopic region for inorganic materials, and if the temperature gradients are not too large. The argument in favour of the use of vapour pressure as an excellent approximate driving potential becomes compelling when one considers the large amount of data available on vapour diffusion coefficients in solids, see for example [8], and the paucity of data available for any other postulated driving potential [9].

With this assumption, a heat and mass balance is performed at each node.

Conservation of mass at node i gives:

rate of increase in moisture at node i = net rate

of moisture flow into the node driven by vapour pressure + net rate of moisture flow into the node due to air convection.

Using a discrete time interval Δt and the superscript $'$ for the value of a physical quantity at time $t+\Delta t$ we have for mass conservation at node i in a fully implicit scheme:

$$V_i\left(\frac{m_i'-m_i}{\Delta t}\right)=\sum_j\left(A_{ij}\frac{(p_j'-p_i')}{r_{ij}}+V_i(F_{ji}^i m_j'-F_{ij}^i m_i')\right). \tag{1}$$

Note that $V_iF_{ij}^i = V_jF_{ij}^j$ = volumetric flow rate of air from node i to node j, $m^3\,s^{-1}$.

Similarly, energy is conserved at node i as follows:

rate of gain of heat at node i = net rate of flow of heat into node i by conduction, convection and radiation + rate of latent heat released by condensation of moisture:

$$\rho_i c_i V_i\left(\frac{T_i'-T_i}{\Delta t}\right)=\sum_j(U_{ij}A_{ij}(T_j'-T_i')+c_pV_i(F_{ji}^iT_j'-F_{ij}^iT_i'))+V_iL_i\frac{\Delta\mathscr{C}_i}{\Delta t}. \tag{2}$$

U_{ij} here is an effective conductance whose value is temperature-dependent in the case of convection and radiation (and perhaps also for conduction). The issue of what value to give it is examined below.

In order to solve these equations for the value of the physical quantities at time $t+\Delta t$, given their values at time t, it is necessary to use a common set of variables. This is chosen to be mass concentrations m_i' (rather than vapour pressures p_i'), and temperatures T_i'.

Since $p = p(T, m)$ we put:

$$p=\kappa m \quad \text{where } \kappa=\kappa(T,m)m\leqslant m^{\text{sat}}$$
$$p=p^{\text{sat}} \qquad m>m^{\text{sat}}.$$

The fact that the relationship between vapour pressure and mass concentration changes at saturation means that two different forms of the mass conservation equation must be used. Furthermore, if p reaches p^{sat} then it remains at that value until the moisture concentration falls belows its saturation value. Therefore, provided that the temperature change, or equivalently the time-step Δt, is not too large, there is no need to distinguish between p^{sat} at time t and p^{sat} at time $t+\Delta t$. This leads to two forms of equation (1), viz.

(a) $m_i \leqslant m_i^{\text{sat}}$

$$V_i\left(\frac{m_i'-m_i}{\Delta t}\right)=\sum_{j(p_j\leqslant p_j^{\text{sat}})}A_{ij}\frac{(\kappa_jm_j'-\kappa_im_i')}{r_{ij}}+\sum_{j(p_j>p_j^{\text{sat}})}A_{ij}\frac{(p_j^{\text{sat}}-\kappa_im_i')}{r_{ij}}+\sum_jV_i(F_{ji}^im_j'-F_{ij}^im_i'),$$

i.e.

$$\left(\frac{V_i}{\Delta t}+\sum_j\left(\frac{A_{ij}\kappa_i}{r_{ij}}+V_iF_{ij}^i\right)\right)m_i'-\left(\sum_{j(p_j\leqslant p_j^{\text{sat}})}\frac{A_{ij}\kappa_j}{r_{ij}}+\sum_jV_iF_{ji}^i\right)m_j'=\frac{V_im_i}{\Delta t}+\sum_{j(p_j>p_j^{\text{sat}})}\frac{A_{ij}p_j^{\text{sat}}}{r_{ij}}. \tag{3}$$

(b) $m_i > m_i^{\text{sat}}$

$$V_i\left(\frac{m_i'-m_i}{\Delta t}\right)=\sum_{j(p_j\leqslant p_j^{\text{sat}})}\frac{A_{ij}\kappa_jm_j'}{r_{ij}}-p_i^{\text{sat}}\sum_j\frac{A_{ij}}{r_{ij}}+\sum_{j(p_j>p_j^{\text{sat}})}\frac{A_{ij}p_j^{\text{sat}}}{r_{ij}}+\sum_jV_i(F_{ji}^im_j'-F_{ij}^im_i'),$$

i.e.

$$\left(\frac{V_i}{\Delta t}+\sum_jV_iF_{ij}^i\right)m_i'-\left(\sum_{j(p_j\leqslant p_j^{\text{sat}})}\frac{A_{ij}\kappa_j}{r_{ij}}+\sum_jV_iF_{ji}^i\right)m_j'=\frac{V_im_i}{\Delta t}+\sum_{j(p_j>p^{\text{sat}})}\frac{A_{ij}p_j^{\text{sat}}}{r_{ij}}-p_i^{\text{sat}}\sum_j\frac{A_{ij}}{r_{ij}}. \tag{4}$$

Rearranging equation (2) gives:

$$\left(\frac{\rho_ic_iV_i}{\Delta t}+\sum_j(U_{ij}A_{ij}+V_iF_{ij}^ic_p)\right)T_i'-\sum_j(U_{ij}A_{ij}+V_iF_{ji}^ic_p)T_j'=\frac{\rho_ic_iV_iT_i}{\Delta t}+V_iL_i\frac{\Delta\mathscr{C}_i}{\Delta t} \tag{5}$$

Equations (3)–(5) form a set of equations in the physical quantities of moisture concentration m_i' and temperature T_i' at each node i, which form the basis of the numerical model. It is explained below how these equations are solved.

A number of artifices, loosely based in the underlying physics, are used to handle difficult issues that arise in the modelling of the moisture performance of structures. The issues are: moisture transfer in solids above fibre-saturation or in the region where capillary forces dominate; condensation; and the performance of membranes and impervious layers in the structure.

The issue of moisture transfer in solids above the hygroscopic region is addressed in this model by using a formula for the sorption curve of materials which gives a vapour pressure less than the saturation vapour pressure, even for moisture contents above fibre-saturation or in the non-hygroscopic region. This is in fact physically correct, but there is no claim made that the formula gives the correct values for vapour pressure if the moisture concentration is in this region. This sorption formula allows vapour pressure to be used as the driving potential at all moisture concentrations. Vapour pressure differences are very small for moisture concentrations above the hygroscopic region, so that the diffusion coefficient has to be adjusted accordingly to give the correct moisture transfer rate. Information on moisture transfer above fibre-saturation in organic materials is sketchy, and furthermore, in most cases, framing materials in a building structure will not retain moisture contents at these levels for long periods of time, so it is questionable whether the

search for highly accurate modelling in this region is worth the effort. The formula used is [10]:

$$\ln(mc) = A + B\ln((0.01\phi)^{-c} - 1) \quad (6)$$

where A, B and c are constants characterising the material.

Condensation on surfaces facing into building cavities is handled in this model by introducing a separate node in the cavity close to the surface in question. This node represents the boundary layer that exists between the cavity air and the surface. The thermal and vapour flow resistances between the boundary layer and the surface are set to zero, and between the boundary layer and the cavity to the appropriate convective value (see later). This ensures the correct rate of transfer of moisture to the boundary layer, from both the cavity and the surface. Moisture concentrations in the boundary layer which are greater than the saturation concentration represent, of course, condensation. This is an artifice in that there is no need to represent accurately the thickness of the boundary layer and hence its temperature and moisture gradients.

Alternatively, if condensation is likely to occur at a surface, the boundary layer node can be omitted if the modeller prefers, and an extra node placed inside the solid, close to the surface in question. The model will then show very high moisture concentration at this node, which in quantity will be equivalent to the amount of condensate that would have appeared at a boundary node.

Membranes and impervious layers are handled differently according to their function and importance in the moisture performance of the structure. A highly impermeable layer of minimal thickness placed between other parts of the structure, such as a vapour barrier, is not allocated a separate node of its own but rather is taken into account as a non-zero contact resistance between nodes on either side of the membrane. The model requires a temperature, a moisture concentration, and a vapour pressure to be associated with every node. Materials such as external metal claddings which cannot hold moisture, but whose temperature must be known, are allocated a node, and given an artificial sorption formula so that the requirement for a moisture concentration and vapour pressure value at that node is met with the most minute trace of moisture. Membranes such as building paper which can hold significant quantities of moisture are allocated a separate node and handled in the same way as all other nodes. Their small thicknesses pose no numerical problem because of the fully implicit nature of the model.

EXPRESSIONS FOR EFFECTIVE CONDUCTANCES

Equation (5) contains effective thermal conductances, U_{ij}, between nodes i and j. In this section it is explained how an expression for these conductances is derived for each of the three heat transfer mechanisms of conduction, convection and radiation.

The case of conduction follows straightforwardly from fundamental definitions and gives:

$$\frac{1}{U_{ij}} = \frac{x_{ij}}{k_i} + \frac{x_{ji}}{k_j} + R_{ij}. \quad (7)$$

For convection, the model assumes that convective heat transfer can be expressed in the form:

$$q_{ij} = h_{ij}(T_j - T_i),$$

where:

$$U_{ij} = h_{ij} = aw^b(\Delta T)^c, \quad \Delta T = T_j - T_i$$

a, b, c here are empirically determined coefficients according to the particular convective process taking place. These can be taken as constant at temperatures around ambient.

For example, in the case of free convection across a wall cavity of width w at ambient temperatures [11]:

$$h = 0.68w^{-0.04}(\Delta T)^{0.32}$$

i.e.

$$a = 0.68, \quad b = -0.04, \quad c = 0.32,$$

while the coefficient of convective heat transfer from a horizontal surface can be taken as [12]:

$$h = 1.52(\Delta T)^{0.33},$$

i.e.

$$a = 1.52, \quad b = 0.0, \quad c = 0.33.$$

A similar approach is taken for the transfer of vapour from surfaces. In this case Wee *et al.* [13] have shown that water vapour transfer across cavities is dominated by temperature driven-convection, rather than vapour diffusion, so, for example, the appropriate expression for moisture transfer across a roof cavity under conditions of upwards heat transfer was found to be:

$$h_v = 4.6 \times 10^{-9} w^{-0.181}(2.82\Delta p + \Delta T)^{0.273}.$$

The expressions of Wee *et al.* for convection across cavities are steady-state expressions, and their use in this model is justified because the transient time for shifting from one steady-state convective regime to another will be very short compared to characteristic times for other transfer processes taking place within the structure.

To find an effective conductance between the surface of node i and the surface of node j when the heat transfer mode is radiation requires a knowledge of the geometry of the situation, and the emissivity ε, reflectivity ρ, and temperature of each surface under consideration. In this model a full view factor treatment is given to evaluate this effective conductance.

According to Hottel and Sarofim [14] the net total radiative heat exchange between surface i and j, Q_{ij} (watts), is given by:

$$Q_{ij} = -Q_{ji} = \overline{S_iS_j}(E_j - E_j),$$

where:

$$E_m = \sigma T_m^4,$$

and:

$$\overline{S_iS_j} = \overline{S_jS_i} = -\frac{A_i\varepsilon_i}{\rho_i}\left(\frac{A_j\varepsilon_j}{\rho_j}\frac{D'_{ij}}{D} + \delta_{ij}\varepsilon_j\right).$$

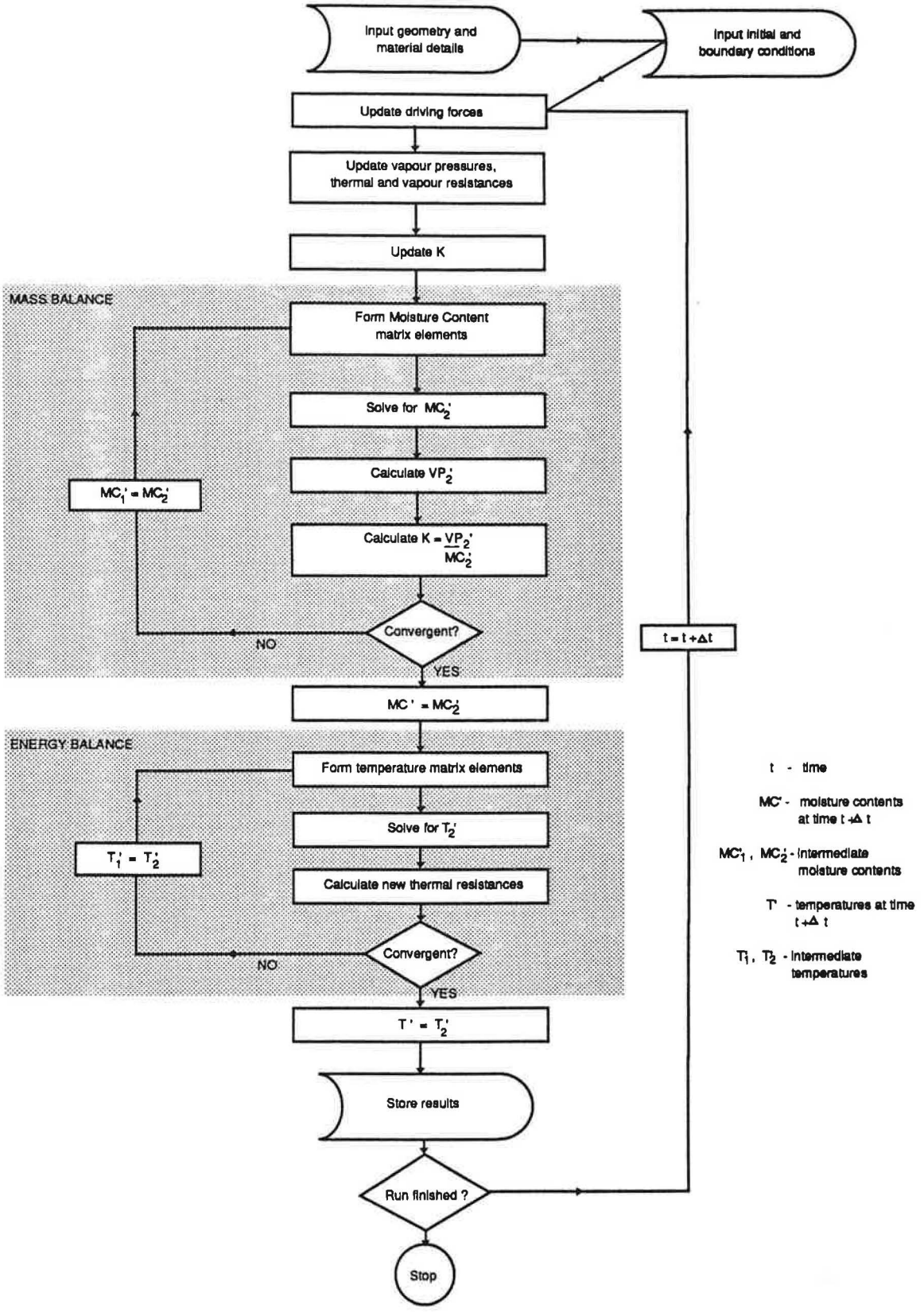

Fig. 2. Flow chart of the numerical model.

$\overline{S_iS_j}$ is known as the total-exchange area (m^2), D is the determinant and D'_{ij} the cofactor of the matrix:

$$[a_{ij}] = A_iF^i_{ij} - \frac{\delta_{ij}A_j}{\rho_j},$$

where, for this formula, F^i_{ij} is the view factor between the surfaces of node i and j.

The model requires the user to calculate the total-exchange areas $\overline{S_iS_j}$ which are taken as input data to the model. The model in turn calculates the equivalent radiation conductances U_{ij} since:

$$Q_{ij} = -Q_{ji} = \overline{S_iS_j}(\sigma T_j^4 - \sigma T_i^4) = \sigma\overline{S_iS_j}(T_i+T_j) \times (T_i^2+T_j^2)(T_j-T_i) = U_{ij}A_{ij}\Delta T.$$

So:

$$U_{ij} = \sigma\overline{S_iS_j}(T_i+T_j)(T_i^2+T_j^2)/A_{ij}.$$

NUMERICAL SOLUTION TECHNIQUE

For the purposes of computation, the physical variables of temperature and moisture concentration are divided into two: non-positive indices are used for the nodes external to the structure, whose value is set according to the external climate at each time-step; and positive indices are used for the internal nodes. This scheme requires the conservation equations (3)–(5), to be rearranged, e.g. equation (5) becomes:

$$\left(\frac{\rho_ic_iV_i}{\Delta t} + \sum_j (U_{ij}A_{ij} + V_iF^i_{ij}c_p)\right)T'_i - \sum_{j>0} (U_{ij}A_{ij} + V_iF^i_{ji}c_p)T'_j = \frac{\rho_ic_iV_iT_i}{\Delta t} + V_iL_i\frac{\Delta\mathscr{C}_i}{\Delta t} + \sum_{j\leqslant 0} (U_{ij}A_{ij} + V_iF^i_{ji}c_p)T'_j.$$

The conservation equations are now seen to be in the form of a pair of matrix equations:

$$[C][T] = [A],$$

$$[D][M] = [B],$$

where $[T]$, $[M]$ are the column matrices:

$$[T] = (T'_1, \ldots, T'_n)^T,$$

and:

$$[M] = (M'_1, \ldots, M'_n)^T.$$

The implied simultaneous equations for T' and m' are then solved by LU decomposition and back-substitution, see for example Press *et al.* [15]. However, the equations are not linear because the coefficients of T' and m' are temperature and mass concentration dependent, in other words the values of κ_i and U_{ij} are not constant from time t to $t+\Delta t$. Hence the values of mass concentration calculated at time $t+\Delta t$ are used iteratively to recalculate values for κ_i, and then the mass concentrations at $t+\Delta t$ are recalculated with these new values of κ_i (but using the values of mass concentration found at time t). This iterative process to refine the κ_i continues until the values for mass concentrations calculated for time $t+\Delta t$ at a given iteration are sufficiently close to the values of mass concentrations for time $t+\Delta t$ calculated at the previous iteration to allow iteration to cease. Usually some three to five iterations are sufficient.

The same iterative process can be carried out over the temperatures, updating U_{ij} between each iteration, but this has not been found necessary, except at fire temperatures where radiation becomes highly non-linear.

COMPUTATIONAL DETAILS

The chief issue facing the user of the model is to specify the geometry of the structure under consideration and to specify the type and details of thermal and hygric transfer between each node. The model has a number of input data structures for this task.

The program is written in FORTRAN-77 and currently runs on a Microvax II. It follows a straightforward flow path as illustrated in the flow chart, Fig. 2. The iterative loop to update the temperature is not used at ambient temperatures.

CONCLUSIONS

A finite difference nodal model for heat and moisture transfer in building structures has been described. The model has been designed to be as flexible as possible, to allow 1-, 2- or 3-D situations to be modelled as well as any conceivable geometry. It has also been designed to allow easy generalisation to other regimes, in particular, fire temperatures; for example, a full view factor treatment of radiation has been given, rather than the equivalent circuit approach often used for ambient temperatures. In this regard the model has been used at steady state with some success at fire temperatures [16]; the major extra factor it will need to handle the non-steady case at these temperatures is a more thorough-going treatment of phase changes of the sort that take place in gypsum plaster board.

Entering the geometrical and material properties of the structure is a large task, and it is proposed in the future that this process will be streamlined through the use of a graphical input front-end to the model.

A later paper [7] describes the first steps in validation of this model under ambient conditions, by comparing its predictions with experimental results and an analytical model developed earlier [2].

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