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A NUMERICAL SOLUTION OF TWO-DIMENSIONAL PROBLEMS INVOLVING HEAT AND MASS TRANSFER

G. COMINI* and R. W. LEWIS†

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Abstract—The finite element method is used for the solution of two-dimensional heat- and mass-transfer problems in porous media. The formulation is given in general terms and is not restricted to any particular type of element.

It is demonstrated in the paper that the versatility of the technique results in a viable method of solution for new practical applications of the Luikov system of equations.

NOMENCLATURE

A, generalized convective coefficients [see equation (13)];
c_m, moisture capacity [$kg_{moisture}/kg_{dry\ body}\,{}^\circ M$];
c_q, heat capacity [$J/kg \cdot K$];
C, generalized capacities [see equation (12)];
$\mathbf{C}$, capacity matrix;
j_m, specific mass flux [$kg_{moisture}/m^2\,s$];
j_q, specific heat flux [W/m^2];
J, generalized fluxes [see equation (13)];
k_m, moisture conductivity [$kg_{moisture}/m \cdot s \cdot {}^\circ M$];
k_q, thermal conductivity [$W/m \cdot K$];
K, generalized conductivity [see equation (12)];
$\mathbf{K}$, conductivity matrix;
l, reference length [m];
N, shape function;
r, radial co-ordinate [m];
t, temperature [°C];
T, $= t/t_0$, dimensionless temperature;
$\mathbf{T}$, vector of nodal temperature values;
u, mass transfer potential [°M];
U, $= u/u_0$, dimensionless mass-transfer potential;
$\mathbf{U}$, vector of nodal values of mass-transfer potential;
x, y, Cartesian co-ordinates [m];
X, Y, dimensionless co-ordinates ($X = x/l$; $Y = y/l$).

Greek letters

α_m, convective mass-transfer coefficient [$kg_{moisture}/m^2\,s \cdot {}^\circ M$];
α_q, convective heat-transfer coefficient [$W/m^2\,K$];
γ, direction cosines of the outward normal $\mathbf{n}$;
Γ, boundary surface [m^2];
δ, thermo-gradient coefficient [$^\circ M\,K^{-1}$];
ε, ratio of the vapour diffusion coefficient to the coefficient of the total diffusion of moisture;
$\boldsymbol{\phi}$, $= [\mathbf{T}, \mathbf{U}]^T$, vector of potential values at the nodes;
ϑ, time [s];
θ, $= \vartheta/\vartheta_0$, dimensionless time;
λ, heat of phase change [J/kg];
Ω, domain of definition [m^3];
ρ, dry body density [kg/m^3].

Subscripts and superscripts

a, ambient;
e, element;
i, initial;
m, mass;
n, time level;
q, heat;
x, y, in direction of x, y;
w, surface;
δ, thermo-diffusion;
ε, heat sink due to internal evaporation;
0, reference;
*, equivalent.

*Istituto di Fisica Tecnica e Laboratorio per le Tecnica del Freddo del C.N.R., V. Marzolo 9, Padova, Italy.

†Department of Civil Engineering, University of Wales, Singleton Park, Swansea, U.K.

INTRODUCTION

THE INTERRELATION between heat and mass transfer in porous bodies was first established by Luikov [1, 2, 10] who proposed a two term relationship for non-isothermal mass diffusion and also determined experimentally the coefficients of diffusion and thermo-diffusion for a number of moist materials. Later [3], via the use of thermodynamics of irreversible processes, he defined a coupled system of partial differential equations for heat- and mass-transfer potential distributions in porous bodies. Applications in this and other fields such as drying theory, building thermo-physics and heat and moisture migration in soils can be found in [4, 5]. Independently, Krischer [6] and De Vries [7] also proposed systems of differential equations of the Luikov type for temperature and moisture content distributions in porous bodies.

The analytical solution of these types of equations presents great mathematical difficulties, and consequently solutions are given for only the simplest of geometrical configurations and boundary conditions [8]. In any realistic problem resort must be made to numerical techniques. These have usually been based on the finite difference method as proposed in the literature [9]. An alternative technique, based on the finite element method, showed that finite element and analytical solutions correlated to within 1% for the case of one-dimensional problems involving boundary conditions of different kinds [10].

In this paper the finite element method is extended to situations of greater complexity and engineering significance. Results are presented for two typical drying processes and for a problem of heat and moisture transfer through a basement foundation.

Transfer equations

If the total pressure is assumed constant throughout the moist body and a zonal system of calculation is used [8], the heat and mass exchange in porous materials can be described in every zone Ω^e of the entire domain of definition Ω, by the following equations:

$$\begin{aligned}\rho c_q \frac{\partial t}{\partial \vartheta} &= k_q \nabla^2 t + \varepsilon\lambda\rho c_m \frac{\partial u}{\partial \vartheta}\\ \rho c_m \frac{\partial u}{\partial \vartheta} &= k_m \delta \nabla^2 t + k_m \nabla^2 u\end{aligned} \tag{1}$$

where t and u are the heat- and mass-transfer potentials and the coefficients ρ, c_q, c_m, k_q, k_m, ε, λ, δ are taken as constant and equal to their respective mean values in each zone.

A general set of boundary conditions for the system of equations (1) is given by

$$t = t_w \tag{2}$$

on Γ_1, i.e. the portion of the boundary with a constant temperature and

$$k_q \nabla t \mathbf{n} + j_q + \alpha_q(t - t_a) + (1-\varepsilon)\lambda\alpha_m(u - u_a) = 0 \tag{3}$$

on Γ_2, being that part of the boundary subjected to heat flux conditions.

Also, for the mass transfer we have

$$u = u_w \tag{4}$$

on Γ_3, i.e. the portion of the boundary with a constant moisture potential and

$$k_m \nabla u \mathbf{n} + j_m + k_m \delta \nabla t \mathbf{n} + \alpha_m(u - u_a) = 0 \tag{5}$$

on Γ_4, which is that portion of the boundary subjected to a moisture flux. The variables t_w, u_w, t_a, u_a, j_q, j_m, α_q, α_m are all known functions of position and/or time.

The problem defined by equations (1)–(5) can be rewritten in a generalised two dimensional form;

$$\begin{aligned}C_q \frac{\partial T}{\partial \theta} &= K_q\left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2}\right) + K_\varepsilon\left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2}\right)\\ C_m \frac{\partial u}{\partial \theta} &= K_\delta\left(\frac{\partial^2 T}{\partial X^2} + \frac{\partial^2 T}{\partial Y^2}\right) + K_m\left(\frac{\partial^2 U}{\partial X^2} + \frac{\partial^2 U}{\partial Y^2}\right)\end{aligned} \tag{6}$$

with boundary conditions:

$$T = T_w \quad \text{on} \quad \Gamma_1 \tag{7}$$

$$K_q\left(\frac{\partial T}{\partial X}\gamma_x + \frac{\partial T}{\partial Y}\gamma_y\right) + J_q^* = 0 \quad \text{on} \quad \Gamma_2 \tag{8}$$

$$U = U_w \quad \text{on} \quad \Gamma_3 \tag{9}$$

and

$$K_m\left(\frac{\partial U}{\partial X}\gamma_x + \frac{\partial U}{\partial Y}\gamma_y\right) + J_m^* = 0 \quad \text{on} \quad \Gamma_4. \tag{10}$$

In the above, dimensionless variables: $T = t/t_0$, $u = u/u_0$, $\theta = \vartheta/\vartheta_0$, $X = x/l$, $Y = y/l$ are utilised, with $t_0(=t_a)$, $u_0(=u_a)$, θ_0 and l taken as reference values.

Generalized capacities C's, generalized transfer coefficients K's and generalized "equivalent" fluxes J^*'s are also referred to. Boundary conditions (8), (10) are formulated in such a manner as to retain the symmetry of the problem. Also, with a suitable definition of the generalized coefficients, K_ε can always be made equal to K_δ thus making the system of equations (6) symmetric. If, in particular, the following condition is imposed

$$K_\varepsilon = K_\delta = \varepsilon\lambda k_m \delta / k_q \tag{11}$$

from equations (1)–(5) it follows that:

$$\begin{aligned}C_q &= \left(\frac{\rho C_q l^2}{k_q \vartheta_0}\right)\left(\frac{t_0 \delta}{u_0}\right); \quad C_m = \left(\frac{\rho C_m l^2}{k_m \vartheta_0}\right)\left(\frac{\varepsilon\lambda k_m u_0}{k_q t_0}\right);\\ K_q &= \left(\frac{k_q + \varepsilon\lambda k_m \delta}{k_q}\right)\left(\frac{t_0 \delta}{u_0}\right); \quad K_m = \frac{\varepsilon\lambda k_m u_0}{k_q t_0};\end{aligned} \tag{12}$$

and

$$\begin{aligned}J_q^* &= A_q(T - T_a) + A_\varepsilon(U - U_a) + J_q;\\ J_m^* &= A_\delta(T - T_a) + A_m(U - U_a) + J_m;\\ A_q &= \left(\frac{\alpha_q l}{k_q}\right)\left(\frac{k_q + \varepsilon\lambda k_m \delta}{k_q}\right)\left(\frac{t_0 \delta}{u_0}\right);\\ A_m &= \left(\frac{\alpha_m l}{k_m}\right)\left[1 - \left(\frac{1-\varepsilon}{\varepsilon}\right)\left(\frac{\varepsilon\lambda k_m \delta}{k_q}\right)\right]\left(\frac{\varepsilon\lambda k_m u_0}{k_q t_0}\right);\\ A_\varepsilon &= \left(\frac{1-\varepsilon}{\varepsilon}\right)\left(\frac{\alpha_m l}{k_m}\right)\left(\frac{k_q + \varepsilon\lambda k_m \delta}{k_q}\right)\left(\frac{\varepsilon\lambda k_m \delta}{k_q}\right);\\ A_\delta &= -\left(\frac{\varepsilon\lambda k_m \delta}{k_q}\right)\left(\frac{\alpha_q l}{k_q}\right).\end{aligned} \tag{13}$$

FINITE ELEMENT FORMULATION

The variable potentials $\mathbf{T}$ and $\mathbf{U}$ are approximated throughout the solution domain Ω by the relationships:

$$\begin{aligned}T \cong \bar{T} &= \sum_{r=1}^{m} N_r(X, Y) T_r(\theta) = \mathbf{NT}\\ U \cong \bar{U} &= \sum_{r=1}^{m} N_r(X, Y) U_r(\theta) = \mathbf{NU}\end{aligned} \tag{14}$$

where T_r and U_r are the nodal values and N_r are the usual shape functions which represent the potential distributions and are defined piecewise element by element [11].

If the approximations given by equation (14) are substituted into the governing differential equations (6) a residual is obtained which is then minimized using Galerkin's approach. This requires that the weighted errors over the domain must be zero, with the shape functions N_r being utilized as the weighting functions [12]

$$\int_\Omega N_r\left[K_q\left(\frac{\partial^2 \bar{T}}{\partial X^2} + \frac{\partial^2 \bar{T}}{\partial Y^2}\right) + K_\varepsilon\left(\frac{\partial^2 \bar{U}}{\partial X^2} + \frac{\partial^2 \bar{U}}{\partial Y^2}\right) - C_q \frac{\partial \bar{T}}{\partial \theta}\right] d\Omega = 0 \tag{15}$$

$$\int_{\Omega} N_r\left[K_\delta\left(\frac{\partial^2\bar{T}}{\partial X^2}+\frac{\partial^2\bar{T}}{\partial Y^2}\right)+K_m\left(\frac{\partial^2\bar{U}}{\partial X^2}+\frac{\partial^2\bar{U}}{\partial Y^2}\right)-C_m\frac{\partial\bar{U}}{\partial\theta}\right]d\Omega = 0. \quad (16)$$

Applying Green's theorem to the above expressions and rearranging, results in the following system of differential equations [10, 12]

$$\mathbf{K}\boldsymbol{\phi}+\mathbf{C}\dot{\boldsymbol{\phi}}+\mathbf{J} = 0 \quad (17)$$

where **K**, **C** are $2M \times 2M$ symmetric matrices:

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}_q & \mathbf{K}_\varepsilon \\ \mathbf{K}_\delta & \mathbf{K}_m \end{bmatrix}; \quad \mathbf{C} = \begin{bmatrix} \mathbf{C}_q & 0 \\ 0 & C_m \end{bmatrix}. \quad (18)$$

The dot indicates differentiation with respect to time, and the vectors $\boldsymbol{\phi}$, **J** are defined by:

$$\boldsymbol{\phi} = [\mathbf{T}, \mathbf{U}]^T; \ [\mathbf{J}_q, \mathbf{J}_m]^T. \quad (19)$$

Typical matrix elements are [10, 12]

$$K_{rs} = \sum \int_{\Omega^e} K\left(\frac{\partial N_r}{\partial X}\frac{\partial N_s}{\partial X}+\frac{\partial N_r}{\partial Y}\frac{\partial N_s}{\partial Y}\right)d\Omega \quad (20)$$

$$C_{rs} = \sum \int_{\Omega^e} CN_rN_s d\Omega \quad (21)$$

and

$$(J_r)_q = \sum \int_{\mu_e} (J_q^*+J_m^*K_\varepsilon/K_m)N_r d\Gamma \quad (22)$$

$$(J_r)_m = \sum \int_{\mu_e} (J_m^*+J_q^*K_\delta/K_q)N_r d\Gamma \quad (23)$$

where $(r, s = 1, M)$.

The preceding summations are taken over the contributions of each element and the boundary conditions are applied only on the appropriate surfaces.

The system of equations (17) is linear in **K** and **C** but non-linear in **J** as the fluxes are functions of the external node potentials. Values at three consecutive time steps are then used to march in time, which results in the following recurrence scheme:

$$\boldsymbol{\phi}^{n+1} = -[\mathbf{K}^n/3+\mathbf{C}^n/(2\Delta\theta)]^{-1} \times [\mathbf{K}^n\boldsymbol{\phi}^n/3+\mathbf{K}^n\boldsymbol{\phi}^{n-1}/3-\mathbf{C}^n\boldsymbol{\phi}^{n-1}/(2\Delta\theta)+\mathbf{J}^n] \quad (24)$$

where the superscript n refers to the time level and $\Delta\theta$ is the time step.

It can be seen that central values of the matrices **K**, **C** and **J** are used in equation (24) which circumvents the necessity for iterating on the non-linear vector **J**. The scheme requires two starting values of $\boldsymbol{\phi}$ for initiation, but this presents no difficulty as known stationary values can be easily assumed.

At this point, however, it must be noted that the unconditionally stable, three level scheme first proposed by Lees [14], is utilised in a slightly modified form. The equivalent fluxes **J** are not averaged over the three time levels, and in certain circumstances, this can lead to oscillations in the numerical solution. However, these instabilities can usually be eliminated by means of some artifice [15]. Extensive numerical experiments by the authors have shown that dramatic improvements in stability can be achieved by redefining $\boldsymbol{\phi}^{n-1}$ at every new time step, as:

$$\boldsymbol{\phi}^{n-1} = (\boldsymbol{\phi}^n+\boldsymbol{\phi}^{n-1}+\boldsymbol{\phi}^{n-2})/3 \quad (25)$$

and continuing with the solution as before.

SOME ILLUSTRATIVE EXAMPLES

In the program, two-dimensional isoparametric elements describe the various regions and these are also capable of incorporating curvilinear sides. The integrations in equations (20)–(22) were carried out numerically as shown in [16]. Since the **K** and **C** matrices are time independent, a Gaussian elimination technique was first used to obtain a partial inverse, which was then utilised to back substitute the variable vector occurring at each stage of the calculation.

Example 1. *Drying of a brick*

Temperature and moisture transfer distributions were determined in a brick subjected to a drying process of relatively high intensity. The geometry considered and the mesh used are represented in Fig. 1(a). By utilising the symmetry of the problem only a quarter of the entire domain need be analysed.

In the calculations the following values of physical properties were used:

$$\rho = 1200\,\text{kg/m}^3; \quad c_q = 879\,\text{J/kg}\cdot\text{K};$$
$$k_q = 0.44\,\text{W/m}\cdot\text{K}; \quad \delta = 0.56\,°\text{M}\cdot\text{K}^{-1};$$
$$c_m = 1.8\times10^{-3}\,\text{kg}_{\text{moisture}}/\text{k}_{q\text{dry body}}\,°\text{M};$$
$$\lambda = 2.5\times10^6\,\text{J/kg}; \quad \varepsilon = 0.3;$$
$$k_m = 6.04\times10^{-8}\,\text{kg}_{\text{moisture}}/\text{m}\cdot\text{s}\,°\text{M}.$$

Convective boundary conditions have been considered, with higher values of transfer coefficients at the external surface:

$$\alpha_q = 35\,\text{W/m}^2\cdot\text{K};$$
$$\alpha_m = 8.64\times10^{-6}\,\text{kg}_{\text{moisture}}/\text{m}^2\cdot\text{s}\cdot°\text{M}$$

lower values at the internal surface:

$$\alpha_q = 17.5\,\text{W/m}^2\cdot\text{K};$$
$$\alpha_m = 4.32\times10^{-6}\,\text{kg}_{\text{moisture}}/\text{m}^2\cdot\text{s}\cdot°\text{M}$$

and the same values of equilibrium potentials:

$$t_a = 60°\text{C}; \quad u_a = 11°\text{M}.$$

Constant stationary initial conditions have been assumed throughout the domain:

$$t_i = 10°\text{C}; \quad u_i = 111°\text{M}.$$

Potential distributions at different levels of time are shown in Fig. 1(b) and Fig. 1(c). As can be seen, large moisture potential gradients occur at the corners indicating a possible failure zone due to the different shrinkages induced. Therefore, in this particular case, recourse to a less intense drying process would be recommended.

The order of accuracy reached with the numerical calculations was evaluated by considering a section where essentially a one-dimensional distribution of

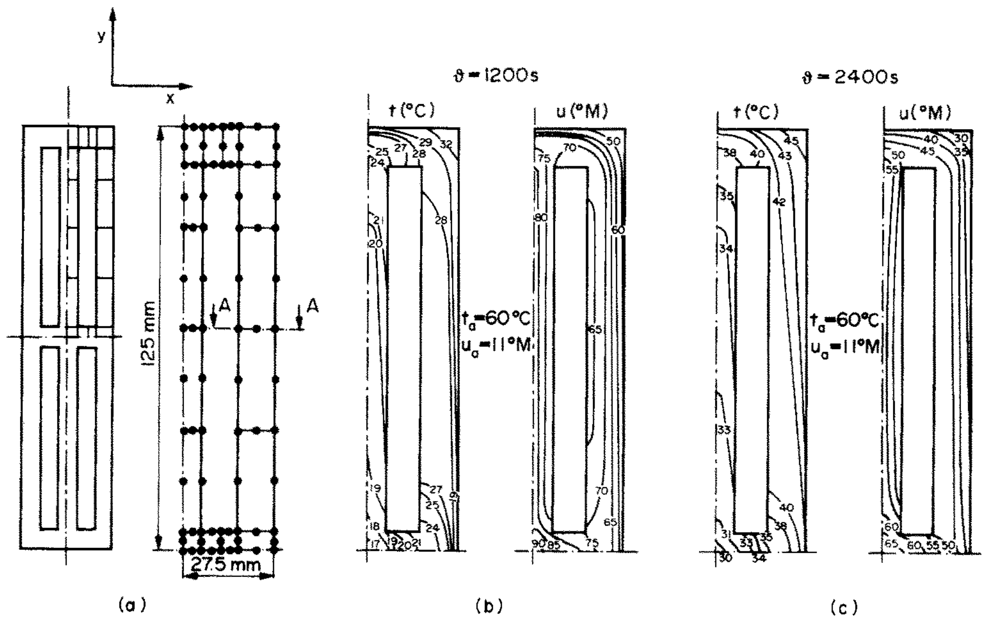


FIG. 1. Drying of a brick. (a) Mesh used. (b) Potential distributions at $\vartheta = 1200$ s. (c) Potential distributions at $\vartheta = 2400$ s.

potentials exist and assuming, for comparison purposes, the same convection coefficients on both sides of the "slab". Reference to the centre of section AA (Fig. 1a) and to the following values of convection coefficients:

$$\alpha_q = 35\,\mathrm{W/m^2 \cdot K}; \quad \alpha_m = 8.64 \times 10^{-6}\,\mathrm{kg/m^2 \cdot s \cdot {}^\circ M}$$

yields the results presented in Fig. 2. A not unsatisfactory agreement is seen to exist between the analytical solution given in ([8], p. 52) and the finite element solution obtained using the mesh of Fig. 1(a).

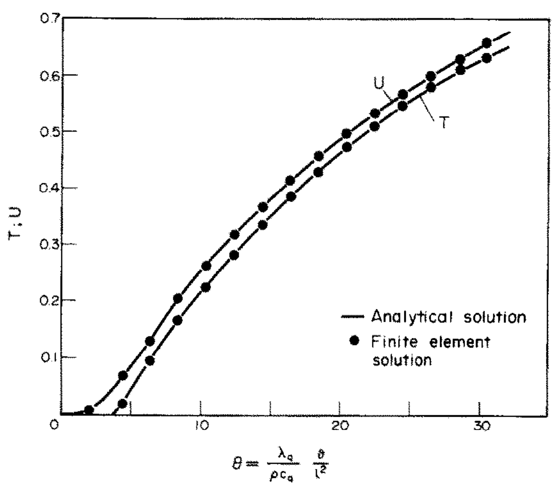


FIG. 2. Comparison of analytical and finite element solutions for the central point of slab AA in Fig. 1(a).

Example 2. *Drying of a ceramic electric insulator*

The complicated geometry considered in this example is modelled by the finite element mesh shown in Fig. 3(a). The axial symmetry is dealt with, as suggested in ([16], p. 302), by assuming $x \equiv r$ utilizing "equivalent" values of physical properties: $(\rho c)^* \equiv r\rho c$, $(k)^* \equiv rk$ and taking into account the circular development of the domain in the evaluation of external surface areas.

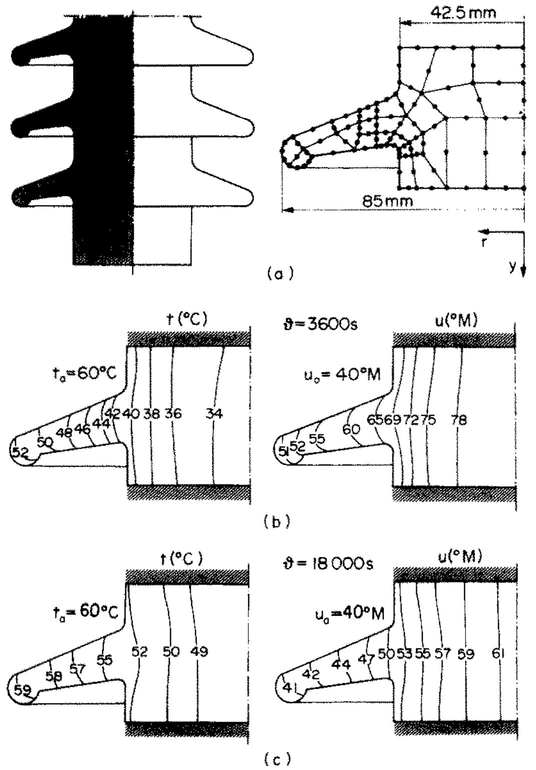


FIG. 3. Drying of an axi-symmetric electric insulator made of ceramic material. (a) Mesh used. (b) Potential distributions at $\vartheta = 3600$s. (c) Potential distributions at $\vartheta = 18\,000$s.

Values of physical parameters and of boundary and initial conditions have been assumed as follows:

$$\rho = 2000\,\mathrm{kg/m^3}; \quad c_q = 607\,\mathrm{J/kg \cdot K};$$

$$k_q = 0.34\,\mathrm{W/m\cdot K};\quad \delta = 0.56\,^\circ\mathrm{M\cdot K^{-1}};$$
$$c_m = 1.8\times10^{-3}\,\mathrm{kg_{moisture}/kg_{dry\ body}\cdot{}^\circ M};$$
$$\lambda = 2.5\times10^{6}\,\mathrm{J/kg};\quad \varepsilon = 0.3;$$
$$k_m = 2.4\times10^{-7}\,\mathrm{kg_{moisture}/m\cdot s\cdot{}^\circ M};\quad \alpha_q = 20\,\mathrm{W/m\cdot{}^\circ K};$$
$$\alpha_m = 5.0\times10^{-6}\,\mathrm{kg_{moisture}/m^2\cdot s\cdot M};\quad t_a = 60^\circ\mathrm{C};$$
$$u_a = 40^\circ\mathrm{M};\quad t_i = 25^\circ\mathrm{C};\quad u_i = 80^\circ\mathrm{M}.$$

The analysis on drying cycles for ceramic electric insulators is a problem of great practical importance and as can be inferred from Figs. 3(b) and 3(c), such an objective can be achieved by means of a finite element analysis.

Example 3. *Heat and moisture transfer in a foundation basement*

It is known that excessive mass transfer in cold stone walls can seriously damage their thermal insulation. Thus, vapour barriers are usually utilized to reduce such moisture migration. However, it is possible for the barrier to be wrongly positioned and in such circumstances the moisture content in the thermal insulation can rise dangerously.

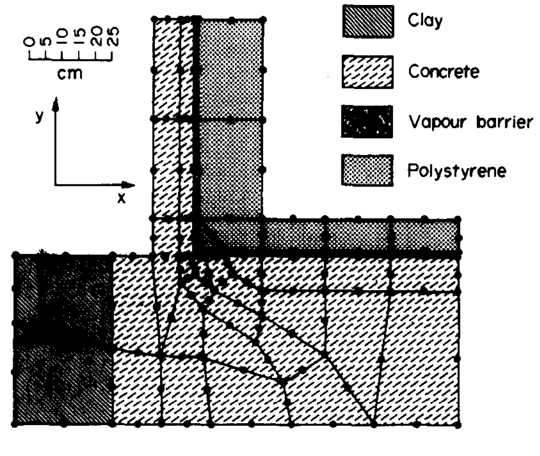
A steady state finite element analysis with the mesh shown in Fig. 4(a) was used to demonstrate the applicability of the method in such cases. Boundary conditions of the first kind and non-conductive external surfaces are referred to, as indicated in the figures. The physical property values utilized were as follows:

concrete: $k_q = 0.32\,\mathrm{W/m\cdot K}$;
$k_m = 1.4\times10^{-8}\,\mathrm{kg_{moisture}/m\cdot s\cdot{}^\circ M}$

soil (clay): $k_q = 1.143\,\mathrm{W/m\cdot K}$;
$k_m = 1.1\times10^{-7}\,\mathrm{kg_{moisture}/m\cdot s\cdot{}^\circ M}$

polystyrene: $k_q = 0.03\,\mathrm{W/m\cdot K}$;
$k_m = 1.05\times10^{-9}\,\mathrm{kg_{moisture}/m\cdot s\cdot{}^\circ M}$

vapour barrier: $k_q = 1\,\mathrm{W/m\cdot K}$;
$k_m = 2.8\times10^{-12}\,\mathrm{kg_{moisture}/m\cdot s\cdot{}^\circ M}$.



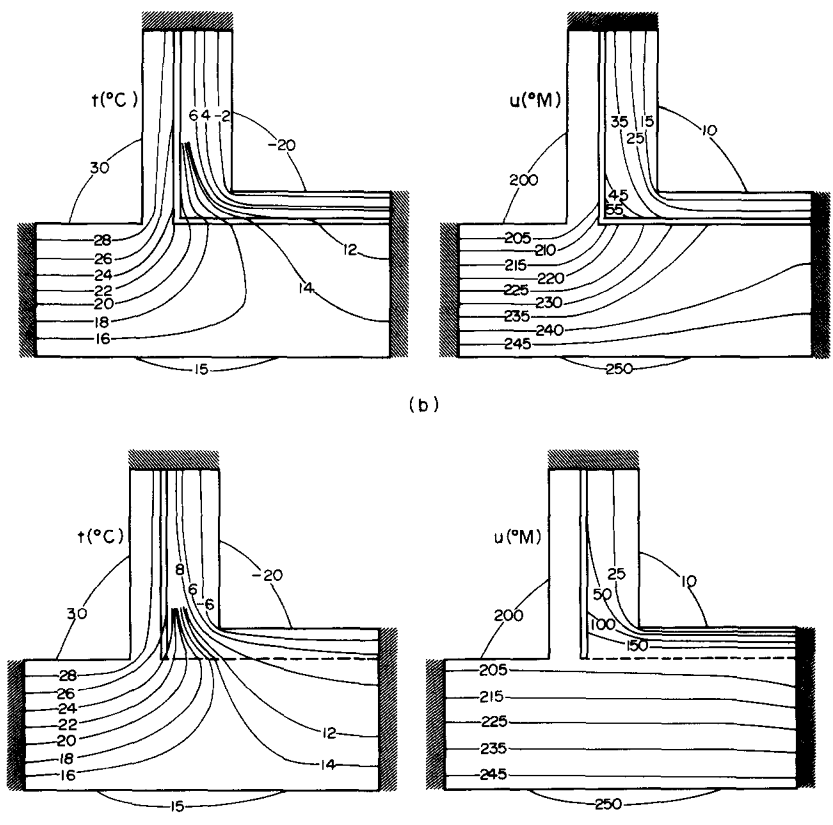


FIG. 4. Heat and moisture transfer in the foundation basement of a cold store. (a) Mesh used. (b) Steady state potential distributions with a complete vapour barrier. (c) Steady state potential distributions with the vapour barrier removed from the floor.

Any moisture transfer was assumed to occur only in vapour from ($\varepsilon = 1$) and the same value of the thermogradient coefficient: $\delta = 0.5°M \cdot K^{-1}$ was used for all materials.*

The potential distributions with two different arrangements of the vapour barrier are given in Figs. 4(b) and 4(c). As can be inferred from the results, the vapour barriers must be extended to the floors in order to be effective.

CONCLUSIONS

The approach to the solution of heat- and mass-transfer problems in porous bodies proposed in this paper has wide applications and has been shown to give accurate results.

The versatility of the finite element method in dealing with complicated geometries and physical property variations makes possible the solution of practical problems in the fields of drying theory, building thermophysics and, in more general, heat and mass transfer in porous materials.

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*In such a case vapour diffusion has no influence on the thermal field, but temperature distributions still affect moisture potential distributions (see, for details, [5] and [3] p. 247).

RESOLUTION NUMERIQUE DES PROBLEMES BIDIMENSIONNELS DE TRANSFERT DE CHALEUR ET DE MASSE

Résumé—On utilise la méthode des éléments finis pour résoudre les problèmes de transfert de chaleur et de masse dans les milieux poreux. La formulation est donnée sous forme générale et n'est pas limitée à un type particulier d'élément. L'article démontre que la souplesse de la technique permet une méthode de résolution du système d'équations de Luikov utile dans ses applications pratiques nouvelles.

EINE NUMERISCHE LÖSUNG ZWEIDIMENSIONALER PROBLEME DES WÄRME- UND STOFFÜBERGANGS

Zusammenfassung—Zur Lösung zweidimensionaler Wärme- und Stoffübergangsprobleme in porösen Stoffen wird die Methode der finiten Elemente angewandt. Die Formulierung wird in allgemeinen Ausdrücken gegeben und ist nicht auf spezielle Elementtypen beschränkt. In der Arbeit wird gezeigt, daß die Vielseitigkeit dieser Methode zu günstigen Lösungsverfahren für neue, praktische Anwendungsfälle des Luikov-Gleichungssystems führt.

ЧИСЛЕННОЕ РЕШЕНИЕ ДВУМЕРНЫХ ЗАДАЧ ТЕПЛО- И МАССООБМЕНА

Аннотация — Для решения двумерных задач переноса тепла и массы в пористых средах используется метод конечных элементов. Дается общая формулировка, не ограниченная определенным типом элемента. Показано, что гибкость метода позволяет эффективно применить систему уравнений Лыкова к решению новых практических задач.