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TRANSIENT ANALYSIS OF MOISTURE CONDITIONS IN MULTI-LAYER CONSTRUCTIONS

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ABSTRACT

A method to analyze thermal and moisture physical behaviour of building components under transient conditions is introduced. The method is supported by the procedure TRATMO (Transient Analysis of Thermal and Moisture Physical Behaviour of Constructions), which enables the studies of hygrothermal conditions in multi-layer one-dimensional slabs with mixed boundary conditions of first, second and third kind. The numerical algorithm for the solution of the system of two coupled diffusion convection type partial differential equations describing the simultaneous coupled heat and mass transfer in porous media has been formulated using finite difference method with non-equidistant space differentation and the trapezoidal rule for time derivate. To improve the convergence of iteration generating from the non-linear boundary conditions, the so-called quasi-linearization is used. The validity of the procedure is illustrated with an analytical solution for a hygrothermally semi-infinite body and with a field experiment.

1 MODEL EQUATIONS FOR HEAT AND MASS TRANSFER IN POROUS MEDIA

The basic transport equations of any flow system are continuity momentum and energy equations. In multi-phase systems, as which moist porous materials can be considered, the fixed control volume V consists of subvolumes V_i, which are bound by time-dependent surfaces $\partial V_i(t)$. These interfacial surfaces include both interfacial and phase-intrinsic parts. According to the volume averaging theorem, introduced by Slattery [1] and thoroughly discussed by Veverka [2] the transport equation valid for a component of multi-phase system becomes

$$\frac{\partial}{\partial t}\langle \rho_i \Psi_i \rangle = -\nabla\cdot\langle \vec{q}_{eff}\rangle - \nabla\cdot\langle \Psi_i \vec{q}_{M,i}\rangle - \frac{1}{V}\sum_j \int_{\partial V_{ij}} \Psi_i (\vec{q}_{M,i} - \rho_i \vec{w}_{ij})\cdot\vec{n}_{ij}\,dA -$$

$$- \frac{1}{V}\sum_j \int_{\partial V_{ij}} \vec{q}_{eff}\cdot\vec{n}_{ij}\,dA\,, \quad \text{where} \tag{1}$$

Ψ_i is scalar, vector or second-order tensor

$\vec{w}_{ij}$ velocity vector of the interfacial surface ∂V_{ij}.

When Eq. (1) is applied to continuity and energy equations it is obtained

$$\frac{\partial}{\partial t}\langle \rho_i \rangle = -\nabla\cdot\langle \vec{q}_{M,i}\rangle - \frac{1}{V}\sum_j \int_{\partial V_{ij}} \rho_i (\vec{v}_i - \vec{w}_{ij})\cdot\vec{n}_{ij}\,dA \tag{2}$$

$$\frac{\partial}{\partial t}\langle h_i \rho_i \rangle = -\nabla\cdot\langle \vec{q}_i\rangle - \nabla\cdot\langle h_i \vec{q}_{M,i}\rangle - \frac{1}{V}\sum_j \int_{V_{ij}} (\rho_i h_i)(\vec{v}_i - \vec{w}_{ij})\cdot\vec{n}_{ij}\,dA\,. \tag{3}$$

Corresponding equations for multi-phase system are

$$\sum_i \frac{\partial\langle \rho_i \rangle}{\partial t} = -\sum_i \nabla\cdot\langle \vec{q}_{M,i}\rangle + \sum_{\substack{i \\ i\neq j}} \sum_j \langle \dot{q}_{ij}\rangle \tag{4}$$

$$\sum_i \frac{\partial\langle h_i \rho_i \rangle}{\partial t} = -\sum_i \nabla\cdot\langle \vec{q}_i\rangle + \sum_{\substack{i \\ i\neq j}} h_i \sum_j \langle \dot{q}_{ij}\rangle - \sum_i \nabla\cdot(h_i \vec{q}_{M,i})\,. \tag{5}$$

In Eqs (4) and (5)

$\langle \rho_i \rangle$ is locally volume-averaged partial density

$\nabla\cdot\langle \vec{q}_{M,i}\rangle$ divergence of locally volume-averaged mass flow density

$\langle \dot{q}_{ij}\rangle$ locally volume-averaged volumetric rate of phase change ij, $= \frac{1}{V}\int_{\partial V_{ij}} \rho_i (\vec{v}_i - \vec{w}_{ij})\cdot\vec{n}_{ij}\,dA$.

When heat and mass transfer in capillary-porous bodies is discussed, the total mass flux $\Sigma\vec{q}_{M,i}$ includes diffusion, surface diffusion, capillary flow and viscous flows of humid air and liquid water. Model equations for $q_{M,i}$:s are obtained with analyses of momentum equation. It can be shown that diffusion and capillary flows can be related to moisture content and temperature. Consequently, the transient moisture balance equation becomes :

$$\langle\rho_0\rangle \frac{\partial\langle u\rangle}{\partial t} = \sum_{k=1}^{3} \nabla\cdot(\underline{a}_{m,k}^{(u)}\cdot\nabla\langle u\rangle + \underline{a}_{m,k}^{(T)}\cdot\nabla\langle T\rangle + \nabla\cdot(\frac{\underline{K}_{v,14}}{\nu_{14}}\cdot\nabla\langle p_{14}^{(14)}\rangle + \frac{\underline{K}_{v,2}}{\nu_2}\cdot\nabla\langle p_{2,0}^{(2)}\rangle) . \quad (6)$$

Correspondingly, the transient energy balance equations becomes

$$\frac{\partial}{\partial t}(C_{eff}^{'''}\langle T\rangle) = \nabla\cdot(\underline{K}_q\cdot\nabla\langle T\rangle) + \sum_j (l_{ij}\langle\dot{q}_{ij}\rangle - \sum_{i=2,14} \nabla\cdot\langle h_i\vec{q}_{M,i}\rangle . \quad (7)$$

The following transport properties have to be known simulate simultaneous coupled heat and mass transfer in porous bodies

i) moisture and thermal moisture diffusivities, $a_{m,k}^{(u)}$ and $a_{m,k}^{(T)}$
ii) permeabilities for humid air and liquid water flows, $K_{v,14}$ and $K_{v,2}$
iii) thermal capacity and conductivity, $C_{eff}^{'''}$ and K_q .

Methods for the determination of these transport properties are introduced in [3] as well as the derivation of Eqs (6) and (7).

The interface between air and a porous body may be considered as a special case of multi-phase systems. Heat and moisture transfer processes across the boundary layer may be considered as quasi-steady-state, thus the fluxes facing surface equal the fluxes leasing. In building physical applications the following fluxes have to be taken into account

i) thermal radiation fluxes
ii) conduction heat flux
iii) convection heat flux
iv) conduction moisture flux
v) convection water vapour flux
vi) convection liquious water flux (driving rain)
vii) filtration (viscous) flux of water or humid air .

The constitutive equations for the boundary conditions are obtained from Eqs (6) and (7) assuming quasi-steady-state transport processes across boundary layers .

The interface of adjacent layers may be considered in the cases, where there is between the adjacent layers

i) perfect hydraulic contact
ii) no hydraulic contact
iii) non-capacitive layer e.g. the so-called surface resistance
iv) air gap (ventilation of construction) .

When the hydraulic contact is perfect and accumulation of heat and moisture is not allowed at the interface, the following conditions of continuity are valid :

i) temperature distribution and heat flux are continuous
ii) moisture transfer potentials (temperature and water vapour pressure and pressure of capillary condensate) are continuous .

Figure 1 illustrates fluxes and transport potential at different kind of boundary conditions in building physical applications .

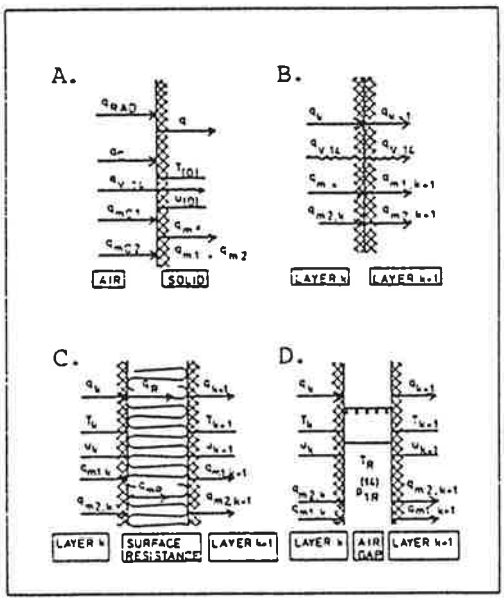

Fig. 1. Fluxes and transport potentials at different kind of boundary conditions in building physical applications

A. Air-solid interface

B. Perfect hygrothermal contact between adjacent layers

C. Surface resistance between adjacent layers

D. Viscous flow in the air gap between layers

2. NUMERICAL SOLUTION OF THE MODEL EQUATIONS

The model equations for the coupled simultaneous heat and moisture transfer in porous bodies are strongly non-linear with non-linear boundary conditions. Therefore, it is reasonable to solve them numerically by computer. In the following a numerical solution algorithm for a system of two coupled non-linear partial differential equations will be introduced. The model equations Eqs (6) and (7) can be written into the following formulae :

$$\frac{\partial (C_{eff}T)}{\partial t} = \frac{\partial}{\partial x_i}\left(a_1^{(T)}\frac{\partial T}{\partial x_i} + a_2^{(T)}\frac{\partial u}{\partial x_i}\right) + a_3^{(T)}\frac{\partial T}{\partial x_i} + a_4^{(T)}\frac{\partial u}{\partial x_i} \tag{8}$$

$$\frac{\partial (\rho_0 u)}{\partial t} = \frac{\partial}{\partial x_i}\left(a_1^{(u)}\frac{\partial T}{\partial x_i} + a_2^{(u)}\frac{\partial u}{\partial x_i}\right) + a_3^{(u)}\frac{\partial T}{\partial x_i} + a_4^{(u)}\frac{\partial u}{\partial x_i}, \tag{9}$$

where coefficients a_i^j are functions of variables T and u.

Some other coupled transport phenomena obey Eqs (8) and (9), too. This means that the following numerical algorithm and the corresponding computer code have applications wider than in the hygrothermal analyses of building constructions.

When central differentation is used, the second and first derivates will have the following approximations:

$$\frac{\partial}{\partial x}\left(a_i^{(j)}\frac{\partial f}{\partial x}\right) \approx \sum_{k=L-1}^{L+1} \bar{a}_k f_k \tag{10}$$

$$a_i^{(j)}\frac{\partial f}{\partial x} \approx \overline{a_i^{(j)}}(L) \sum_{k=L-1}^{L+1} b_k f_k . \tag{11}$$

The first derivate at L = 1 achieves the formula

$$\left(\frac{\partial f}{\partial x}\right)_{L=1} = \sum_{k=1}^{3} c_k f_k . \tag{12}$$

Table 1 gives the formulaes for $\bar{a}_k$, b_k and c_k.

When differentation formualue (10) and (11) are applied to Eqs (8) and (9), they are transformed to two ordinary differential equations :

$$\frac{d}{dt}(C_{eff}^{'''}T)_L \approx \sum_{k=L-1}^{L+1} \{[\bar{a}_k^{TT} + \overline{a_3^{(T)}}\, b_k]T_k + [\bar{a}_k^{TU} + \overline{a_4^{(T)}}\, b_k]U_k\} \equiv F_1(T_k, U_k) \tag{13}$$

$$\frac{d}{dt}(\ {}_0u)_L \approx \sum_{k=L-1}^{L+1} \{[\bar{a}_k^{UT} + \overline{a_3^{(T)}}\, b_k]\, T_k + [\bar{a}_k^{UU} + \overline{a_4^{(u)}}\, b_k]\, U_k\} \equiv F_2(T_k, U_k). \tag{14}$$

Since the system is non-linear with non-linear boundary conditions, general conditions for the stability of the numerical algorithm can not be established. Therefore, it is preferable to use such approximations for time derivate, for example the Crank-Nicholson method, which convergence without stability criteria. In the Crank-Nicholson method the trapezoidal rule is applied :

$$(C'''_{eff}T)_L^{s+1} = (C'''_{eff}T)_L^{s} + \frac{\Delta t}{2}[F_1^{s+1}(\underline{x}_i) + F_1^{s}(\underline{x}_i)] \tag{15}$$

$$(\rho_0 u)_L^{s+1} = (\rho_0 u)_L^{s} + \frac{\Delta t}{2}[F_2^{s+1}(\underline{x}_i) + F_2^{s}(\underline{x}_i)]. \tag{16}$$

When the formualue of the functions $F_1(x_i)$ and $F_2(x_i)$ are substituted to equations (13) and (14) two matrixes [A] and [B] are obtained, which are double tridiagonal type matrixes and which equal equations (17) [the ordinary differential equations (15) and (16) are transformed to the linear system of equations

$$[A]^{s+1}(x_1^{s+1}, x_2^{x+1}, \ldots)^T = [B]^{s}(x_1^{s}, x_2^{s}, \ldots)^T + (z_1^{s+1}, z_2^{s+1}, \ldots)^T, \tag{17}$$

where x_{2k-1} and x_{2k} equal temperature and moisture content in the grid point k, respectively.

The matrix equation (17) is solved using NAG-library programs F01BRF, F04AXF [4]. Elements a_{1j}, a_{2j}, a_{i-1} in matrix A and elements z_1, z_2 and z_i in column matrix z are evaluated from the boundary conditions equations of the temperature and moisture distribution. When temperature T and moisture content u are chosen to be transport potentials, the value of the water vapour flow in the boundary condition equations has to be solved by iteration. The convergence of iteration may be improved by quasi-linearizing. If function $F(x_i) = 0$ is dependent on variables x_i, so

$$dF(x_i) = \sum_i \frac{\partial F(x_i)}{\partial x_i} dx_i \quad \text{or}$$

$$F(x_i)^{(p)} \approx F(x_i)^{(p-1)} + \sum_i \left\{\frac{\partial F(x_i)}{\partial x_i}\right\}^{(p-1)} [x_i^{(p)} - x_i^{(p-1)}]. \tag{18}$$

The values of vapour pressure and its partial derivates needed in quasi-linearization are evaluated from the water vapour pressure table with bicubic spline interpolation routines (IBCICU and DBCEVU, respectively [5]) .

TABLE 1. Formulaes for the approximations of first and second derivates .

$$\bar{a}_{L-1} = \frac{\overline{a_i^{(j)}(L-\tfrac{1}{2})}}{0{,}5\Delta x_B(L)\,[\Delta x_B(L) + \Delta x_F(L)]}$$

$$\bar{a}_{L} = -\frac{\overline{a_i^{(j)}(L+\tfrac{1}{2})}\,\Delta x_B(L) + \overline{a_i^{(j)}(L-\tfrac{1}{2})}\,\Delta x_F(L)}{0{,}5\Delta x_B(L)\,\Delta x_F(L)\,[\Delta x_B(L) + \Delta x_F(L)]}$$

$$\bar{a}_{L+1} = \frac{\overline{a_i^{(j)}(L+\tfrac{1}{2})}}{0{,}5\Delta x_F(L)\,[\Delta x_B(L) + \Delta x_F(L)]}$$

$$b_{L-1} = -\frac{\Delta x_F(L)}{2\,\Delta x_B(L)\,\Delta x_F(L)}$$

$$b_{L} = \frac{\Delta x_F(L) - \Delta x_B(L)}{2\,\Delta x_B(L)\,\Delta x_F(L)}$$

$$b_{L+1} = \frac{\Delta x_B(L)}{2\,\Delta x_B(L)\,\Delta x_F(L)}$$

$$c_1 = \frac{\Delta x_F(L+1) + 2\,\Delta x_B(L+1)}{\Delta x_B(L+1)\,[\Delta x_F(L+1) + \Delta x_B(L+1)]}$$

$$c_2 = \frac{\Delta x_F(L+1) + \Delta x_B(L+1)}{\Delta x_F(L+1)\,\Delta x_B(L+1)}$$

$$c_3 = \frac{\Delta x_B(L+1)}{\Delta x_F(L+1)\,[\Delta x_F(L+1) + \Delta x_B(L+1)]}$$

3 COMPUTER CODE TRATMO

In order to simulate coupled heat and mass transfer in porous materials the computer code TRATMO (Transient Analysis Code for Thermal and Moisture Physical Behaviour of Constructions) has been formulated [6]. The numerical algorithm for the general system of two non-linear partial differential equations introduced above is utilized. Consequently most blocks of TRATMO are applicable in TRATMO-modifications, which are valid for the simulations of coupled transport phenomena described by Eqs (8) and (9). The applications of the present version of TRATMO are in the field of building technology e.g. the subprograms including transport properties and calculations of boundary conditions are formulated for building physical applications. TRATMO is written in FORTRAN-4 language for CDC CYBER-173. A short description of the outlines of TRATMO will be given.

Input data

The following input data are given in subprogram INPUPR :

i) number of layers and material code of layers
ii) number and mesh intervals of space steps
iii) initial temperature and moisture content distributions
iv) surface resistances for heat and mass transfer at boundary layers and interfacial surfaces of adjacent layers

v) reading instructions of environmental conditions (natural or artificial environment)
vi) execution parameters and options
vii) output options .

Environment conditions

The environment conditions for transient simulations are evaluated by ENVIRO-subprogram. The boundary conditions inside and outside the construction are described by temperature, vapour pressure or humidity ratio of humid air, solar radiation and wind velocity, from which the outside heat transfer coefficient is estimated. The environment conditions can be read from a special weather file including the quantities listed above and the time step, which may, due to Crank-Nicholson method, vary from step to step. In the weather file the environment data are time averaged values for each time step. The environment file is made by a separate program from an hourly weather file, which is commonly used in computer codes for the energy analyses of buildings. When necessary, environment data can be described by internal functions in ENVIRO-subprogram. For the execution of TRATMO the modified ENVIRO-subprogram can be compiled and added in loading without compiling the whole program.

Material and transport properties

Library subprograms MATER and VAPOR include material and transport properties of various materials. Each material has its own number code identifizing the material in input.

Subprogram MATER includes the following material and transport properties :

i) density (function of u)
ii) thermal conductivity and volumetric thermal capacity (functions of T and u)
iii) moisture diffusivities (functions of T and u)
iv) thermal moisture diffusivities (functions of T and u) or
v) temperature gradient coefficient (function of u) .

Subprogram VAPOR includes the vapour pressure table of absorbed moisture (sorptio isotherms) for each material. Vapour pressure is a function of moisture content and temperature for hygroscopic materials but only of temperature for non-hygroscopic materials. The partial derivates needed due to quasi-linearization of the boundary conditions are calculated using bicubic spline interpolation (IMSL-library program IBCICU and DBCEVU [5]) .

Output options

Two independent output files can be formed. One is for the printer and the other for the CALCOMP-drum plotter. The CALCOMP - Figures illustrate a function using time as abscissa, while from the printer output file the moisture distribution curves using time as a parameter can be drawn.

The following items can be stored into the files

i) environment conditions
ii) temperatures and moisture contents at grid points
iii) heat and moisture fluxes at surfaces
iv) water vapour pressures at surfaces and
v) cumulative heat and moisture fluxes at inner and outer surfaces of the construction .

4. VERIFICATIONS OF TRATMO

4.1 Accuracy of TRATMO compared with an analytical solution for a semi-infinite body

When considering the diffusion and capillary flows of gaseous and liquious moisture, the linearized balance equations become (for simplicity symbols of local averaging are left out) :

$$C'''_{eff} \frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + l_{12}\varepsilon_{12} \frac{\partial u}{\partial t} \quad \text{and} \tag{19}$$

$$\frac{\partial u}{\partial t} = a_m^{(u)} \left(\frac{\partial^2 u}{\partial x^2} + \delta_T^{(u)} \frac{\partial^2 T}{\partial x^2}\right) , \tag{20}$$

for which the solution is [7].

$$\bar{T}(x,s) = \sum_{n=1}^{4} C_n \, e^{-\mu_n \sqrt{\frac{s}{a}} x} \tag{21}$$

$$\bar{u}(x,s) = \frac{1}{\varepsilon_{12} Ko} \sum_{n=1}^{4} C_n \, (1-\mu_n^2) \, e^{-\mu_n \sqrt{\frac{s}{a}} x} . \tag{22}$$

The roots of the characteristic equation are

$$\mu_{1,2}^2 = \frac{1}{2} \left[(1+Fe+1/Lu) \pm \sqrt{(1+Fe+1/Lu)^2 - 4/Lu} \right] \tag{23}$$

Fe is Feodorovs modulus $= \varepsilon_{12} Ko \, \delta_T^{(u)} = \frac{\varepsilon_{12} l_{12} \rho_0}{C'''_{eff}} \frac{a_m^{(T)}}{a_m^{(u)}}$, where

ε_{12} and l_{12} are the so-called phase change criteria and heat of phase change, respectively, and

Lu is Luikovs modulus $= a_m^{(u)}/a = a_m^{(u)}/(\lambda/C'''_{eff})$.

The solution in time domain for the case of step change of surface temperature ΔT_p and moisture content Δu_p is [6]

$$[\, T(x,t) , \, u(x,t) \,]^T = \{G\} \, (\Delta T_p , \, \Delta u_p)^T . \tag{24}$$

The elements of transfer matrix {G} are of form

$q_{ij} = a_{ij} \operatorname{erfc} \frac{\mu_j x}{2\sqrt{at}}$, where a_{ij}:s are elements of matrix {A}

$$\{A\} = \frac{1}{\mu_2^2 - \mu_1^2} \begin{bmatrix} \mu_2^2 - 1 & \varepsilon_{12}\,Ko \\ \mu_1^2 - 1 & -\varepsilon_{12}\,Ko \end{bmatrix} .$$

Figure 2 illustrates the results from an analytical and TRAT computations [6]. The following input data were used $\lambda = 0.14$ W/mK, $\rho_0 = 550$ kg/m^3, $C'''_{eff} = 0.7$ MJ/m^{3}K, $a_m^{(u)} = 1.4 \cdot 10$ m^2/s and $a_m^{(T)} = 7.0 \cdot 10^{-11}$ m^2/s K. The space steps in TRATMO computation were Δx_i = 2,3,4,10,15,15,50,100,300 mm. Slight oscillation and deviation when using the time step Δt = 1 ks, and no oscillation and smaller deviation when using the time steps Δt = 0,1 ks, may be seen between the numerically and analytically calculated results. By decreasing the time, or increasing the space step oscillation is decreased. Correspondingly deviation is increased when space step is increased. Although the comparison is not rigorous in any way, it shows, however, that it would be preferable to use floating space or time steps in order to optimize the accuracy of solution with respect to the computation costs. This is possible but not done in the present version of TRATMO.

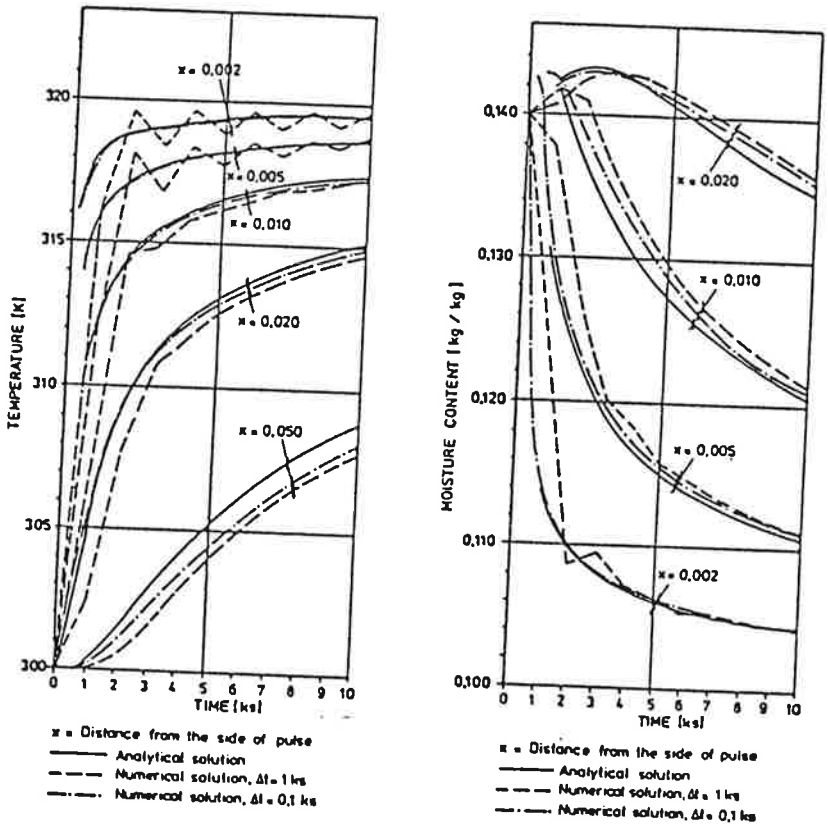

Fig. 2. Temperature and moisture content in semi-infinite body caused by step change of surface temperature and moisture content.

4.2 Accuracy of TRATMO compared with a field experiment

A field experiment under natural climate conditions has been carried out in order to verify the validity of TRATMO. The wall construction from outside to inside was :

i)	wood board	22 mm
ii)	ventilated air gap	22 mm
iii)	expanded polystyrene	50 mm
iv)	light mineral wool	100 mm
v)	plastic sheet as water vapour barrier	
vi)	woodchipboard with latex paint 12 mm .	

The purpose of this experiment was not find out if expanded polystyrene can be used as wind cover without risks of moisture failures.

In order to determine experimentally the hygrothermal conditions in the construction, samples of polystyrene, mineral wool and the woodchips located on the surface between polystyrene and mineral wool have been taken. Figure 3 gives the computed and from time to time measured moisture contents in the test wall.

A rather good agreement between calculations and measurements can be found. The results themselves show that there are neither net accumulation of moisture into polystyrene (thermal resistance will be preserved) in long run nor surface condensation at the interfacial surface of mineral wool and expanded polystyrene.

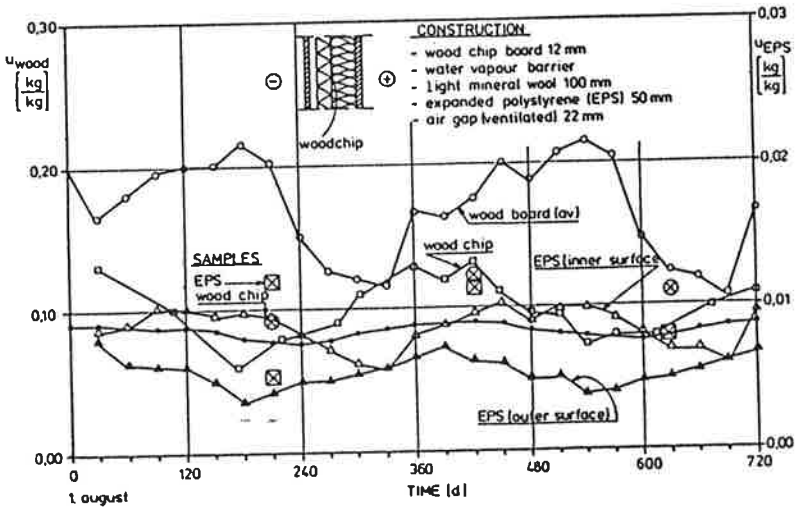

Fig. 3. Moisture conditions in a timber wall with wind cover of expanded polystyrene .

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