SIMULATION OF MOISTURE TRANSPORT TO ASSESS DURABILITY ASPECTS OF COMPOSITE WALLS

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ABSTRACT
Simulation of dynamic moisture transport processes in building structures under varying conditions re quires the solution of the partial differential equations of coupled moisture and beat transport.
Our research focuses on the moisture transport equation as this is generally the harder one to solve. We will report on two related research projects that are motivated by durability-aspects of construction walls, being dependent on specific transport phenomena occurring during operation (first case) and construction (second case).
The first case deals with moisture migration as a result of both moisture and temperature gradients in concrete walls with a polymer finish.
The second case deals with the construction of masonry walls during which the rapid migration of moisture which occurs from the fresh mortar into the bricks has a great effect on the resulting bond strength of the masonry wall.

INTRODUCTION

In order to predict the durability of composite external building walls affected by water transport during operation as well as during their construction, adequate simulations will help to assess these transport phenomena with a sufficient degree of accuracy. We will show how the simulations were performed in two specific cases, each requiring a different approach and each requiring the definition of a particular problem specific formulation in terms of the computational model. The two cases were both motivated by durability assessments which we will introduce first.
The first case deals with the durability of the surface coating of concrete walls used to protect against chemical substances in the environment and thus preserve the quality of the construction. It was found that in many cases the coating deteriorated rapidly without a known cause. The hypothesis was that the observed failure of a coating could possibly be ascribed to water migration due to moisture and temperature gradients. The stagnated fluid behind the coating could then cause stress fractures of the coating at freezing temperatures.
The other case deals with one of the durability aspects of masonry walls. The bond between the brick and the mortar is essential to ensure the structural stability and water tightness of masonry walls. The early rate of water flow from "wet" mortar into brick greatly influences this bond as the particle migration on the interface determines the rate of drying and hardening of the mortar (Groot, 1993).

A brief introduction of the general moisture and heat transport equations will first be given. Neglecting gravity forces, the moisture transport equation (Philip and De Vries, 1957) is described by:

$$\partial\psi/\partial t=\nabla(D_\psi\nabla\psi)+\nabla(D_T\nabla T) \qquad (1)$$

wherein ψ is the moisture content, T is the temperature, D_ψ and D_T denote the diffusivities due to moisture and temperature gradients.
In general, D_ψ and D_T depend on the moisture content ψ and the temperature T.
The temperature results from the well known Fourier equation (2). Note that an added convective transport term due to the moisture migration (including latent heat effects of evaporation and condensation of the liquid in the pores of the material) as well as a moisture gradient forcing term have been suppressed as the influence of both effects can usually be neglected in the cases that are considered here:

$$\rho c\partial T/\partial t=\Lambda_T\nabla T) \qquad (2)$$

Λ_T is the heat conductivity, weakly dependent on T and (usually) strongly dependent on ψ. Equations (1) and (2) can be solved to give ψ (D_ψ, D_T, x, t) where the dependence on the diffusion coefficients and the independent space and time co-ordinates is expressed explicitly.
In both cases the above equations were solved numerically with the f.e.m. toolbox BFEP (Augenbroe,

1986) which was used to calculate the temperature straightforwardly (2) and then solve the highly non-linear equation (1) for one dimensional flow. These computations require accurate estimations of the prevalent coefficients (mainly D_ψ) . Special attention has to be given to the description of boundary and interface conditions.

MOISTURE MIGRATION IN CONCRETE WALLS WITH POLYMER FINISH.

The first case to be considered is the moisture transport in a concrete wall with a polymer finish at both sides. The transport due to a constant temperature gradient with initially a uniform distributed moisture content will be studied in detail in order to check the hypothesis that a temperature gradient alone could cause the stagnation of sufficient fluid behind the coating to cause the damaging effects. For that to happen it must be shown that the migration under the regime of a temperature gradient can be the dominant factor over the moisture gradient driven transport that will try to regain a uniform moisture distribution.

By virtue of the assumptions made above, the temperature field remains steady and we will just have to solve equation (1) assuming that we have accurate information about D_ψ and D_T, which is of course essential to prove the hypothesis.

The concrete wall is discretizised in 1D space using linear finite elements, leading to the solution of the discretised moisture content $\underline{\psi}(t)$, containing the values in the nodes of the discretised domain. The known transient temperature field likewise can be discretised and will be represented by $\underline{T}(t)$. Applying the standard finite element technique a discretised form of equation (1) can be derived:

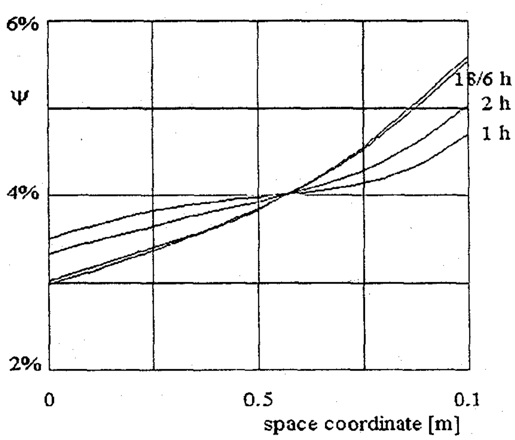

Fig.1. Moisture contents in concrete

$$M\frac{\partial \underline{\psi}}{\partial t} = S(D_\psi)\underline{\psi} + U(D_T)\underline{T} = 0 \qquad (3)$$

Wherein M is the Mass matrix and S and U express the discrete form of the exchange due to the two driving forces. S and U are assembled over all elements, i.e.

$$S = \sum_{elements} S^e \quad ; \quad U = \sum_{elements} U^e$$

BFEP offers the opportunity to the user to define his own element, which is an option that must be used in this case in order to build S and U according to the known dependency on D_ψ (ψ,T) and D_T (ψ,T). For the linear element with two nodes the following element matrix calculations were defined in user supplied subroutines:

$$S^e = a/h * \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} ;$$

$$a = (D_\psi(\psi_1, T_1) + D_\psi(\psi_2, T_2))/2$$

$$U^e = b/h * \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} ;$$

$$b = (D_T(\psi_1, T_1) + D_T(\psi_2, T_2))/2$$

Apart from these problem specific extensions the simulations were done in a straightforward manner. With proper begin and boundary conditions the discrete set of ordinary differential equations (3) are solved using a Runge-Kutta numerical time integrator (Augenbroe, 1986) with a recalculation of S and U at each time step.

Calculation results are shown in figure 1. They are based on the dependencies of D_ψ and D_T depicted in figure 2, which are taken from (Kusters, 1989) based on the original work in (Kiessl,1977).

In this example a steady state temperature distribution is assumed going from 10 °C (right side) to 0 °C (left side). After 18 hours apparently an equilibrium between the moisture transport due to the temperature gradient and the moisture transport caused by the moisture content gradient was established. Other examples with different wall thickness and a range of temperature fields showing similar results led to the conclusion that the hypothesis was correct and that special care must be taken with respect to the temperature gradient that is allowed in walls with this type of coating.

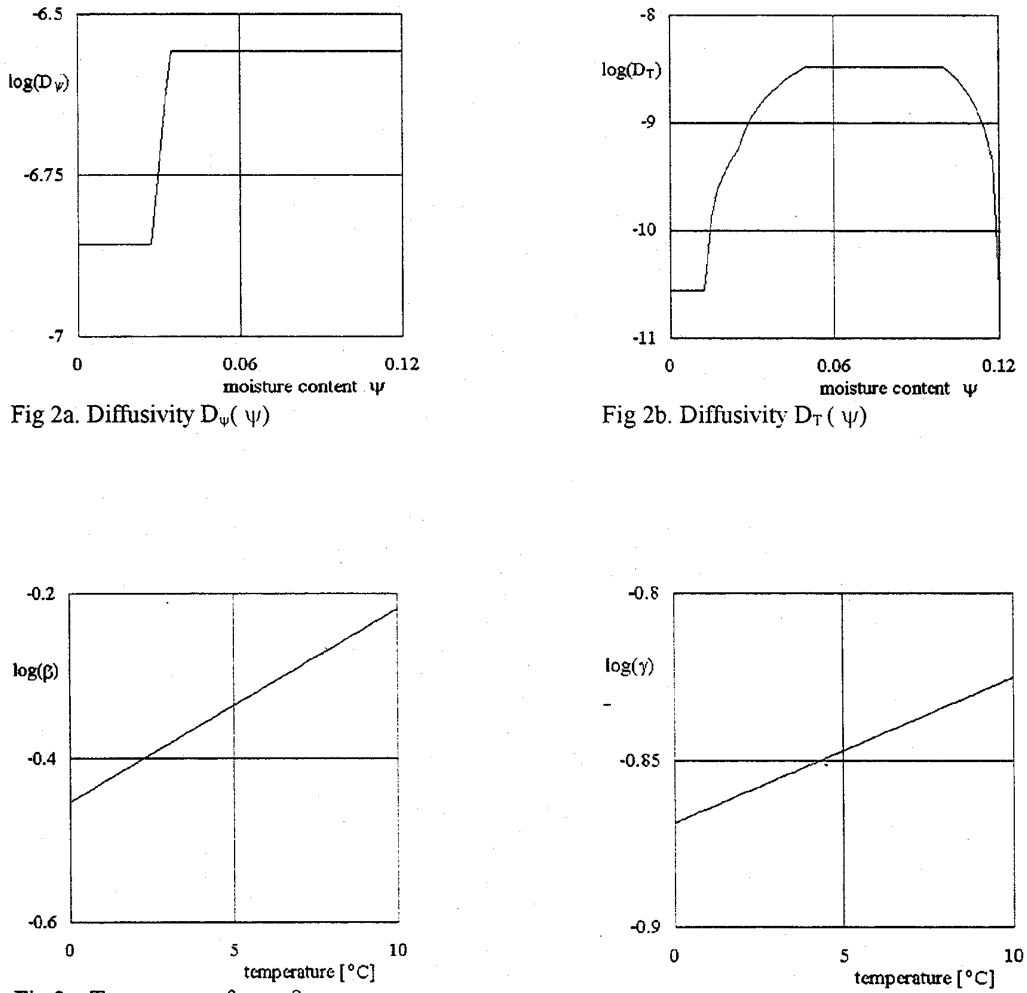

Fig 2a. Diffusivity $D_\psi(\psi)$

Fig 2b. Diffusivity $D_T(\psi)$

Fig 2c. Temperature factor β

Fig 2d. Temperature factor γ

Fig.2. Diffusivities in concrete, $D_\psi(\psi,T)=\beta D_\psi(\psi)$; $D_T(\psi,T)=\gamma D_T(\psi)$

MASONRY WALL UNDER CONSTRUCTION

The second application of moisture simulation deals with a phenomenon that relates to the construction of masonry walls during which rapid migration of moisture transport from fresh "wet" mortar into the brick occurs. In this example the simulations were restricted to the isothermal case, as the overriding factor in the transport process is the way in which the suction pressure in the brick leads to the extraction of water particles from the mortar. This is a process that starts with a high transfer rate at the initial time of contact, and then gradually slows down as extraction gets more difficult and the edge zones of the brick become saturated with water. The complexity of the problem lies in the unknown diffusivities of both materials (they are expected to be strongly dependent on moisture content) as well as in the intricate physical process that takes place at the interface and needs to be expressed as an internal boundary condition.

The process is governed by:

$$\partial\psi/\partial t = \nabla (D_\psi \nabla \psi) \qquad (4a)$$

or in its discretised form:

$$M\frac{\partial \underline{\psi}}{\partial t} = S(D_\psi)\underline{\psi} \qquad (4b)$$

Special care has to be taken in formulating the conditions at the interface where the two materials are put in contact. Whereas the moisture potential P_ψ (defined as suction pressure devided by the water density) is continuous over this boundary, the moisture content is not. At the interface a continuous moisture potential P_m is assumed which results from the pressure balance of the vapour in the adjoing pores in the two materials.

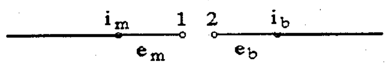

Fig 3.

Figure 3 shows the two materials and their discretisation in linear two-node elements. The figure also shows an example of the type of mesh refinement that is applied in the vicinity of the inner boundary. Note that two nodes (i_m and i_b) are introduced at the interface representing the moisture contents in either material. Furthermore two fictitious nodes (1 and 2), connected to resp. i_m and i_b are introduced in order to express the inner boundary conditions which can be expressed as:

$$\alpha\ (\psi_1 - \psi(i_m)) = \alpha\,(\psi(i_b) - \psi_2) \qquad (5a)$$

$$P_\psi(\psi_1) = P_\psi(\psi_2) = P_{\psi m} \qquad (5b)$$

In discretised form, the two materials are 'detached' with both boundaries connected to two artificial surface elements (e_m and e_b). The boundary conditions are expressed in the values of ψ_1 and ψ_2 that need to be determined at each time. The moisture transmittance α in the elements e_m and e_b is chosen arbitrarily large (but equal).
The prescribed moisture contents in 1 and 2 are determined at each time step such that over the boundary a continuous moisture flux occurs and the suction forces are consistent with the moisture potentials at either side.

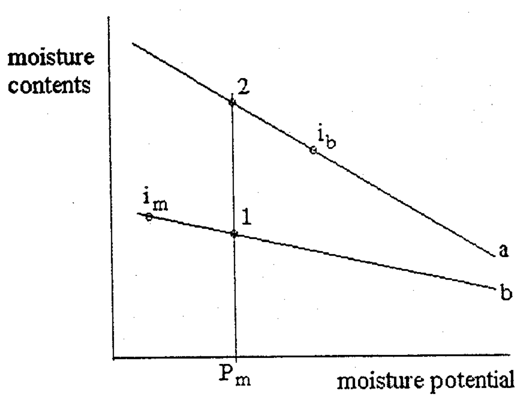

Fig 4.

Figure 4 illustrates the procedure schematically. It shows the relation between the moisture content and the moisture potential for both mortar (curve b) and a specific brick (curve a). Satisfying equation (5) whilst demanding a continuous moisture potential across the interface requires the determination of P_m as the root of

$$\psi(i_m) - \psi_m(P_m) - (\psi_b(P_m) - \psi(i_b)) = 0$$

With this approach the simulation comes down to solving the non-linear equation (4) in each material separately and calculating ψ_1 and ψ_2 at each time step, based on the latest values of the state ψ at either side of the boundary. It should be well recognised that this calculation for each time step requires the solution of a non-linear algebraic equation, which is being done iteratively in the BFEP program.
In order to perform actual simulations it is required that one has good knowledge of the diffusivities in both materials (as a function of ψ) and of the dependence between the moisture potential P and ψ. The research started off with the experimental determination of the diffusivity in the brick material $D_{\psi b}(\psi)$ and the moisture potential $P_{\psi b}(\psi)$. Results of those studies, i.e. solving the inverse problem, were reported earlier (Pel,1993; Tumbuan,1993). In these studies experiments were done with a neutron radiosity technique allowing accurate measurement of $\psi(x,t)$ and ensuing parameter estimation based on the repeated solution of equation (4) and a parameter search algorithm.
In our case we are faced with a special problem as these data for the fresh mortar were not available. This required tackling the inverse problem before any accurate simulations could be performed on the direct problem (4). The inverse problem of equation (4) deals with estimating $D_{\psi m}$ and $P_{\psi m}$ of a mortar from known experimental values of the moisture contents ψ in brick and mortar after contact, at different x and t.

APPROACH TO INVERSE PROBLEM

The 'direct' problem (4) enables us to solve ψ ($D_{\psi m}$, $P_{\psi m}$, $D_{\psi b}$, $P_{\psi b}$; x,t) for given or estimated functions $D_{\psi m}$, $P_{\psi m}$ and $D_{\psi b}$, $P_{\psi b}$ denoting the diffusivities and moisture potentials in mortar and brick. The inverse problem deals with estimating these functions of ψ using as criterion that the 'difference' between experiment and model outcome shall be minimised. This is accomplished by requiring the mean square difference between the model output ψ^m and the outcome of an experimental process ψ^P to be as small as possible, i.e. to minimise:

$$\int_{t=0}^{t_{end}} \sum_{i=1}^{N} (\psi^p(x_i,t) - \psi^m(x_i,t))^2 dt \qquad (6)$$

where the integration extends over the duration of the experiment (0 to t_{end}) and N is the number of discrete measuring locations. In order to deal with this problem as a parameter estimation problem the unknown functions must be parametrised, i.e. assuming a certain type of function with discrete parameters.

The actual parameter estimation is then performed using a random search technique which calls a BFEP simulation run for the solution of equation (4) at each iterative step. The search technique used is insensitive to random measurement errors and it can easily handle a large number of constraints that the parameter values have to obey. In many cases these constraints are necessary to ensure that they determine a physically possible function whereas other constraints must ensure the well-posedness of the direct problem at each evaluation step of the search algorithm.

RESULTS

Figure 5 gives the results of the estimation of $D_{\psi m}$ and $P_{\psi m}$, based on neutron radiography measurements applied to cross sections of brick and mortar in an experimental set up (Groot,1989). This set-up used an initial moisture content in a fired clay brick of 1.3 % of the volume.

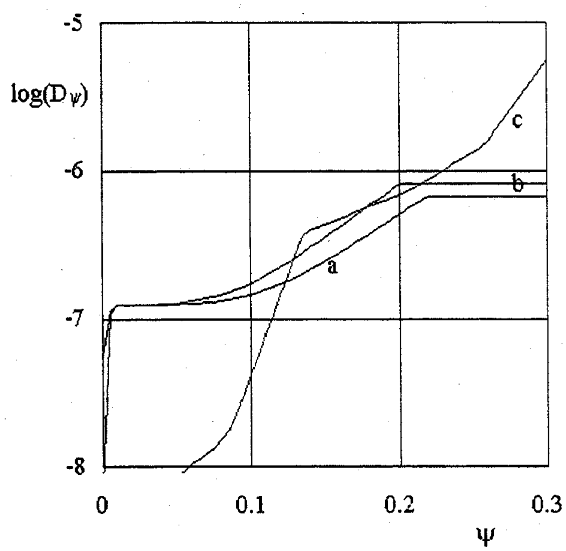

Fig. 5a. Estimated diffusivities in mortar.
a. mortar close to interface
b. mortar elsewhere.
c. known value in brick

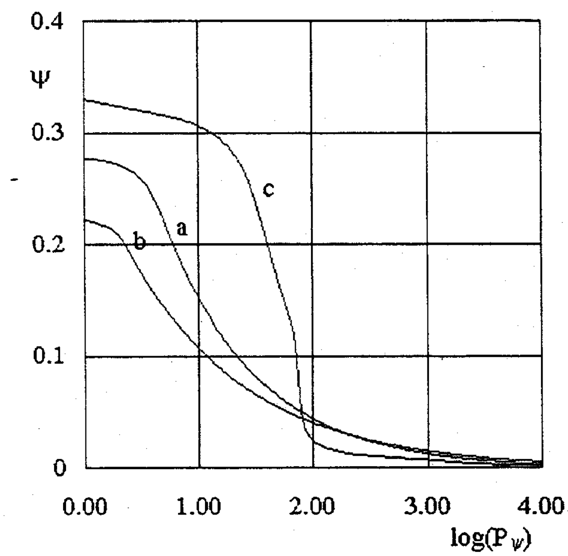

Fig. 5b. Estimated moisture potential in mortar.
a. mortar close to interface
b. mortar elsewhere.
c. known value in brick

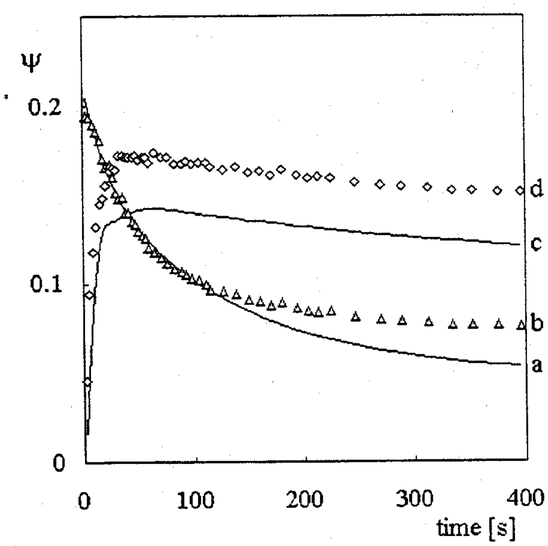

Fig.6a. Moisture contents as function of time.
Initial moisture content in brick 1.3 %.
a : calculated moisture values
b : measured moisture values
c : calculated brick values
d : measured brick values
Calculated values after convergence of the parameter estimation process.

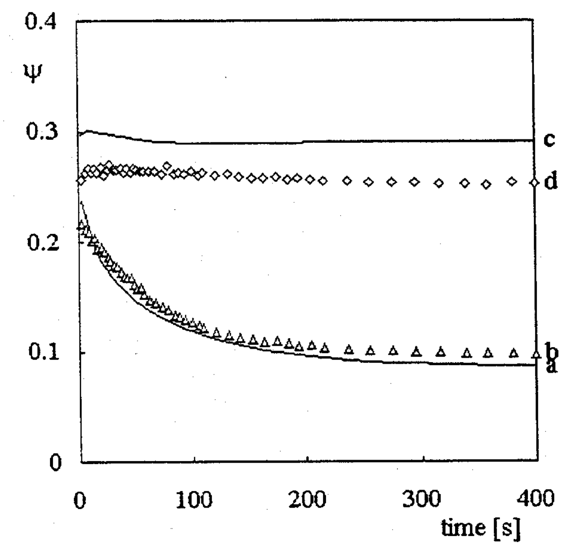

Fig.6b. Moisture contents as function of time.
Initial moisture content in brick 15 %.
a : predicted mortar values
b : measured mortar values
c : predicted brick values
d : measured brick values

In the mortar it is assumed that different pore structures in the region close to the interface exists compared to elsewhere. For both regions a different function $D_{\psi m}$ and $P_{\psi m}$ has thus to be assumed and entered in the estimation process. This adds to the complexity of the inverse problem in that the number of parameters increases. Solving the inverse problem proved to be computationally demanding; an extreme case solution of the inverse problem involved:

- 33 parameters to be estimated, obeying 95 constraint expressions
- 1200 evaluations (each requiring solution of equation 4) before convergence was reached
- 200.000 time steps to numerically solve equation 4 for the time interval using BFEP (the extremely fast process and steep gradients in the boundary region as well as the sensitivity of the calculation of P_m at the interface mandates very small time steps)
- a rebuild of $S(\psi)$ at each time step and the iterative solution of the interface conditions at each time step

This leads to a number of $24*10^7$ time step calculations done in an estimation run. On a 486 50mhz PC this takes about 80 hours. A direct run, e.g. to predict the moisture transport in a certain condition with the use of known (prior estimated) $D_{\psi m}$ and $P_{\psi m}$ will normally only take 4 minutes.

The obtained values of $D_{\psi m}$ and $P_{\psi m}$ were subsequently used to predict the moisture contents in a mortar/brick combination with an initial moisture content of 15 % in the brick. Figure 6 shows the results and compares them with the measurements. The difference between predicted and measured moisture contents in the brick are due to uncertainties in diffusivity and moisture potential of the brick. In view of the validity of the estimated parameters shown by figure 5, the model is now being used to do a study on the optimal moisture conditions during masonry work, for different types of mortar and bricks.

CONCLUSIONS

Two cases where moisture transport has a major importance on the durability of building components have been successfully studied by using simulation and experiments. In case of moisture transport driven by a temperature gradient a hypothesis concerning the damaging of the coating was effectively proven.

The solution of the non-linear direct problem proved to be a straightforward affair with the chosen build-

ing simulation toolbox. Using it at the heart of a parameter estimation technique also led to rather reliable results for the inverse problem.
Further experiments are in progress to extend our knowledge about material properties and refine the functions with which to describe them. New experiments will enable continued validation of the approach.

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