Adaptive integration of element matrices in finite element moisture transfer simulations

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Published in:
Proceedings of the XVI International Conference on Computational Methods in Water Resources

Publication date:
2006

Document Version
Publisher's PDF, also known as Version of record

'ADAPTIVE INTEGRATION' OF ELEMENT MATRICES IN FINITE-ELEMENT MOISTURE TRANSFER SIMULATIONS

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ABSTRACT

The article introduces adaptive integration, an optimisation measure for numerical simulations of moisture transfer in porous materials. It is shown that application of adaptive integration drastically reduces the computational expense of moisture transfer simulations, by easing the errors on the numerical integration of the element permeability matrices at the sharp moisture fronts characteristic of moisture transport in porous materials. Extension to multi-dimensional simulations, coupled models and other discretisation methods concludes the article.

1. INTRODUCTION

Porous building materials, such as ceramic bricks, cementitious and lime-based materials, comprise a broad range of pore radii, varying from 10^{-9} to 10^{-2} m. As a result, moisture transfer in such materials highly depends on the pore pressure or moisture content. At low moisture contents, a few monolayers of adsorbed water strongly adhere to the pore walls, and yield a practically immobile water film. For such low moisture contents the moisture transfer process is governed by molecular vapour diffusion, Knudsen diffusion and bulk flow of the gas phase. As the moisture content increases, wetting fluid starts to fill the smaller pores, creating dispersed water-filled regions by capillary condensation. Liquid water transfer in those water-filled regions is far more efficient, leading to an increase of the moisture permeability. As the moisture content further increases, the water-filled regions expand and, at the critical moisture content, ultimately coalesce to form a continuous liquid water phase.

As a consequence of these microscopic phenomena, the macroscopic continuum description of moisture transport results in strongly non-linear transfer equations. Moisture permeability shows a notable increase due to capillary condensation, and a jump at the critical moisture content; moisture storage equally depends on the capillary pressure. These non-linearities are illustrated for ceramic brick in Figure 1. While exemplified for a common building material, similar observations can be made for soils.

Due to the sharp rise in moisture content and permeability over a limited capillary pressure range (Figure 1), the wetting and drying of porous building materials or soils generally produces sharp moving moisture fronts. These render numerical simulations computationally expensive: a fine spatial discretisation throughout is required to accurately capture these moving fronts. Such fine discretisation throughout is inefficient though, since the small elements are only required at the actual moisture front, while less active regions can be modelled with relatively larger elements.

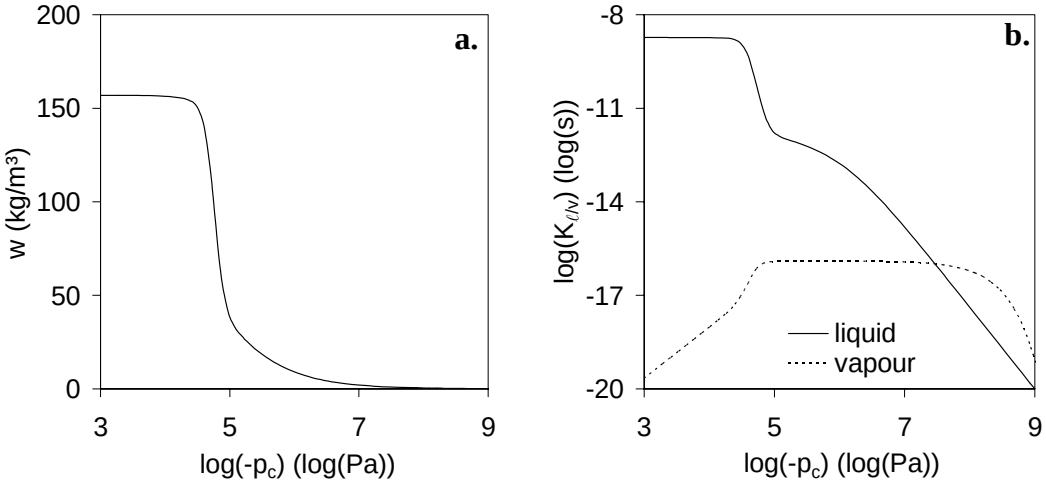

FIGURE 1. Moisture retention curve (a) and permeability (b) of ceramic brick.

This article will show that the requirements on the spatial discretisation for finite-element simulation of moisture absorption into a porous material are primarily determined by the integration error on the element permeability matrices. It will subsequently introduce adaptive integration as optimisation measure targeting this error, thus easing the requirements on the needed discretisation for such simulation.

2. FINITE-ELEMENT MODELLING OF MOISTURE TRANSFER

2.1 Transfer equation

The isothermal transfer of moisture in porous materials can concisely be described with:

$$c_m \frac{\partial p_c}{\partial t} - \nabla^T k_m \nabla p_c = 0 \tag{1}$$

where p_c is the capillary pressure, t the time, c_m the moisture capacity and k_m the moisture permeability. Due to the pore sizes involved in building materials, the effect of gravity on moisture transfer is commonly considered insignificant in building physics. Capillary pressure p_c is normally applied in building physics as moisture transfer potential and can easily be related to the matric head ψ, proper to the domain of soil physics: $p_c = \psi \cdot \rho_l \cdot g$, where ρ_l is the density of water and g the gravitational acceleration.

2.2 Spatial and temporal discretisation

A finite-element based spatial discretisation is preferred for the presented model, since the possibility to integrate a continuous variation of the independent variables over the calculation domain is considered numerically superior. Finite differences or control volumes on the other hand, assume the capillary pressures piecewise constant. An implicit finite-difference temporal discretisation is favoured for its superiority in stability, efficiency and realism. The spatial and temporal discretisation convert equation (1) to a system of non-linear algebraic equations:

$$\left(\mathbf{C}^{t+\Delta t} + \Delta t \mathbf{K}^{t+\Delta t}\right)\mathbf{P}_c^{t+\Delta t} = \mathbf{F}^{t+\Delta t}\Delta t + \mathbf{C}^{t+\Delta t}\,\mathbf{P}_c^{t} \tag{2}$$

where $\mathbf{C}$ is the capacity matrix, $\mathbf{K}$ the permeability matrix, $\mathbf{P_c}$ the capillary pressure vector, $\mathbf{F}$ the external load vector and Δt the time step. More detailed information on the numerical implementation can be found in (Janssen et al., 2005).

The capacity and permeability matrices are composed from their element matrices:

$$C_{ij}^{e} = \int_{\Omega^e} c_m N_i N_j d\Omega \tag{3}$$

$$K_{ij}^{e} = \int_{\Omega^e} k_m \nabla^{\mathbf{T}} N_i \nabla N_j d\Omega \tag{4}$$

where $N_{i/j}$ are the finite element shape functions. Commonly, numerical integration is applied to resolve the integrals in (3-4).

2.3 Simulation example

In free water uptake experiments, the under side of a beam-shaped sample is put in contact with water and the moisture accumulation in the sample is recorded. The accumulation should theoretically progress proportionally with $t^{0.5}$, and the proportionality is defined the 'capillary absorption coefficient' A_{cap} of the material. The initial and boundary conditions for a free water uptake simulation of a 9 cm high ceramic brick sample are:

$$t < 0\,\mathrm{s}: \quad x \in [0; 0.09]\,\mathrm{m} \qquad p_c = -10^8\ \mathrm{Pa} \tag{5}$$

$$t \geq 0\,\mathrm{s}: \quad x = 0\,\mathrm{m} \qquad p_c = 0\ \mathrm{Pa} \tag{6}$$

$$x = 0.09\,\mathrm{m} \qquad \text{impermeable}$$

The simulation is continued for 4500 s, with alphanumeric output every 100 s. The resulting moisture content profiles and moisture accumulation are illustrated in Figure 2.

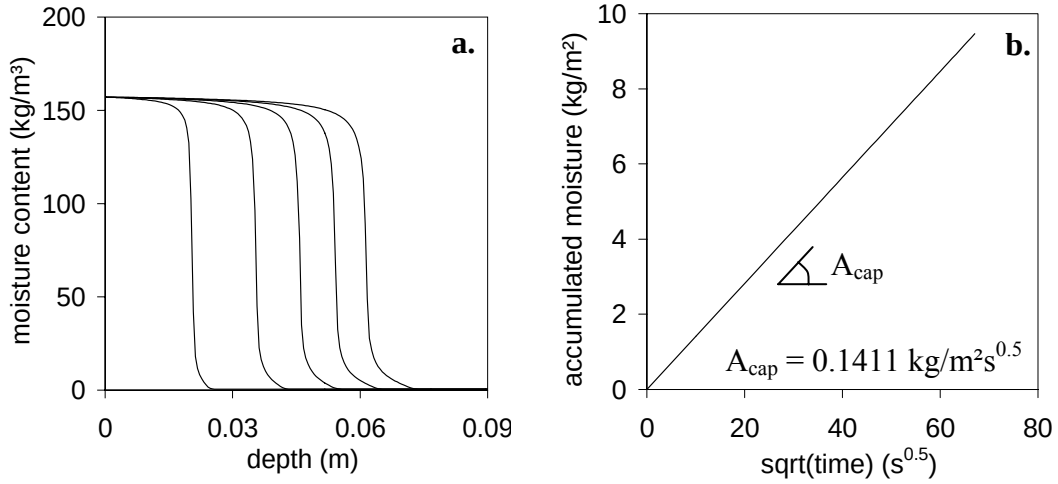

FIGURE 2. Moisture content profiles at 500, 1500, 2500, 3500, 4500 s (a) and moisture accumulation (b) during free water uptake in 9 cm ceramic brick.

3. ADAPTIVE INTEGRATION OF ELEMENT MATRICES

Due to a history of predominantly linear problems, with constant material properties, commonly low-order schemes are favoured for the numerical integration of the element capacity and permeability matrices (Zienkiewicz and Taylor, 1994). The introduced model makes use of third and fifth order accurate Gauss-Legendre cubature formulae for its linear and quadratic elements respectively, translating to two and three gauss points for one-dimensional elements.

It will be shown below that the combination of sharp moving moisture fronts and low-order numerical integration adversely affects the required discretisations, increasing the computational cost of numerical simulations of moisture absorption into a porous material.

3.1 Numerical integration and required discretisation

3.1.1 Influence on discretisation

The influence of applying low-order numerical integration schemes on the required discretisation is illustrated with the simulation of free water uptake by 9 cm ceramic brick, by comparison of 'acceptable minimal' discretisations determined for a low-order (3 gauss points per quadratic element) and high-order (10 gauss points per quadratic element) numerical integration scheme. The acceptable minimal discretisation is defined as the minimal number of nodes required to approximate a fine-discretisation reference solution within certain deviations.

The global capillary absorption coefficient $A_{cap,global}$ is defined as the slope of the accumulated moisture versus $t^{0.5}$ relation for the complete simulation, while the momentary $A_{cap,moment}$ is the quotient of the current amount of accumulated moisture and current $t^{0.5}$. Both definitions are illustrated in Figure 3(a). The 'acceptability' of a discretisation is decided from the deviation between $A_{cap,global}$ from the reference and minimal discretisation, and deviations between $A_{cap,global}$ and $A_{cap,moment}$ for the minimal discretisation:

$$\frac{A_{cap,global}^{minimal} - A_{cap,global}^{reference}}{A_{cap,global}^{reference}} \leq 1\% \tag{7}$$

$$\frac{A_{cap,moment}^{minimal} - A_{cap,global}^{minimal}}{A_{cap,global}^{minimal}} \leq 1\% \quad \forall t \in [100\,s,\ 200\,s,\ 300\,s,\ ...,\ 4500\,s] \tag{8}$$

both should remain less than 1 %. The first criterion (7) hence concerns the global deviation between the reference and the minimal discretisation, the second (8) is connected to the deviations from the straight line for the minimal discretisation. It is opted here to focus on the global transfer process only, but other criteria could involve the preservation of the moisture content profiles: such analysis would yield similar qualitative conclusions.

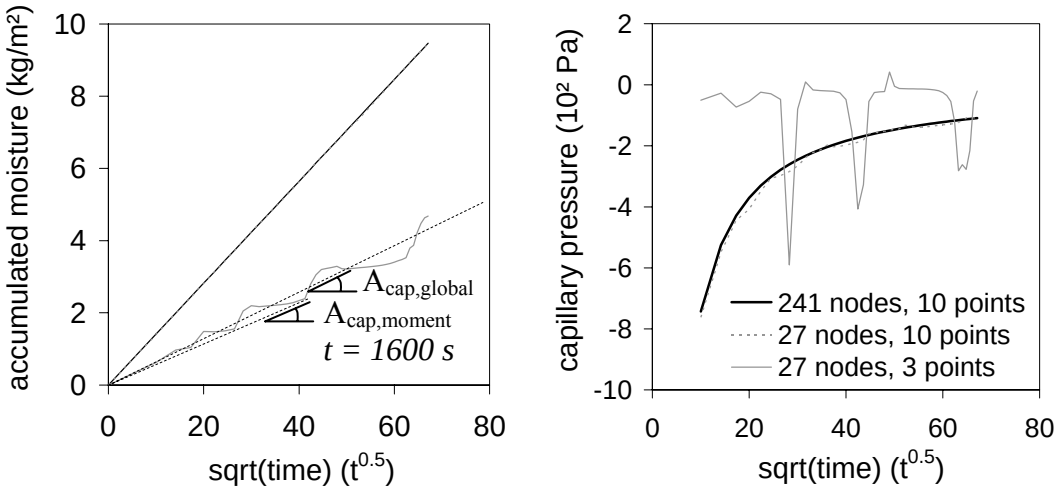

FIGURE 3. moisture accumulation (a) and capillary pressure at 2 10^{-4} m (b) during free water uptake by 9 cm ceramic brick.

The reference solution applies 241 nodes – first internode distance Δx_1: 10^{-5} m, internode distance growth factor ζ: 1.05, maximal internode distance Δx_{max}: 5 10^{-4} m – and 10 gauss integration points per quadratic element. Minimal discretisations are determined for the low-order and high-order numerical integration scheme. For the low-order scheme, the acceptability limits are reached for 153 nodes (Δx_1: 3 10^{-5} m, ζ: 1.03, Δx_{max}: 5 10^{-3} m), while the high-order scheme requires only 27 nodes (Δx_1: 2 10^{-4} m, ζ: 1.20, Δx_{max}: 1 10^{-2} m). These differences indicate that the spatial discretisation for finite-element simulation of moisture absorption into a porous material is mainly determined by the integration error on the element capacity and permeability matrices and that the use of low-order numerical integration thus has an adverse effect on the required discretisation.

3.1.2 Cause of inaccuracy

From all element matrices, the variability of the moisture permeability with capillary pressure is most pronounced, and particularly so at sharp moisture fronts characteristic for moisture absorption into a porous material (see Figures 1-2). The inaccurate low-order numerical integration of element matrices must thus result primarily from an imperfect estimate of the integral of the element moisture permeability (3). The numerical integration of moisture permeability over a one-dimensional quadratic element is illustrated in Figure 4. Capillary pressure is assumed to vary linearly – acceptable for a sharp moisture front – from -3 10^4 to -3 10^5 Pa. Such capillary pressures correspond with the primary drops in moisture content and in permeability (Figure 1), and are not uncommon in ceramic brick free water uptake simulations.

Whereas the capillary pressure only varies over one order of magnitude, the permeability variation exceeds three orders of magnitude. The exact permeability integral over the element is 8.0 10^{-11} s. The low-order numerical integration scheme leads to 1.3 10^{-11} s, while the high-order scheme results in 7.7 10-11 s, which is respectively 16 and 96 % of the correct value.

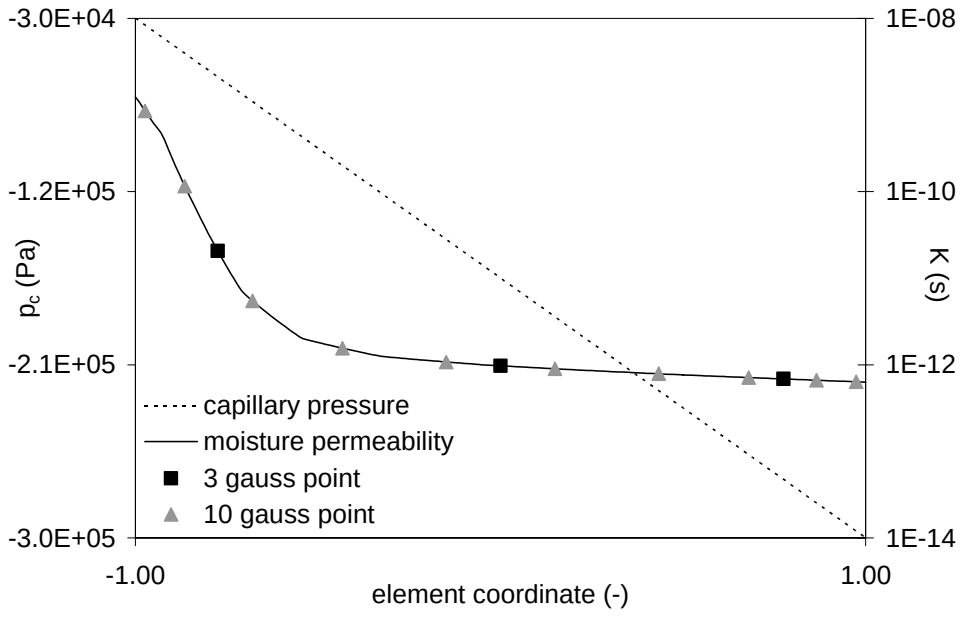

FIGURE 4. 3- and 10-point numerical integration of the moisture permeability over a one-dimensional quadratic element.

Since the underestimation of element permeability integrals by low-order numerical integration is limited to sharp moisture fronts, and furthermore depends on the capillary pressures involved, its occurrence is erratic. The affected elements can however only ensure continuity of flow by a raised gradient in capillary pressure, perturbing the simulation. The accumulated moisture, and the capillary pressure at $2\ 10^{-4}$ m (the first node above the sorption surface) into the brick are shown in Figure 3 for the 27 node simulations with low-order and high-order numerical integration. It is easily observed that the free water uptake simulation with 27 nodes and low-order integration is significantly affected by the inaccurate permeability integration. The jerky behaviour of the capillary pressure at $2\ 10^{-4}$ m indicates the erratic underestimation of element moisture permeability integrals and their effect on the simulation is obvious from Figure 3(a). It can furthermore be observed that the limit of acceptability is also reached for the 27 nodes, high-order integration simulation.

3.2 Adaptive integration

A general application of high-order numerical integration requires less computational expense than the low-order scheme: every iteration, only 13 elements with 10 integration points are to be evaluated and just 27 equations are to be solved. The low-order scheme on the other hand necessitates evaluating 76 elements with 3 integration points and solution of 153 equations. The accuracy – and computational expense – of the high-order scheme is though only required at the sharp moisture fronts: general application is inefficient.

Adaptive integration can thus save computation time where possible and provide accuracy where required: high-order numerical integration is used for elements with large permeability variations, low-order for all other elements. A sensitivity analysis reveals that the high-order scheme should be applied for all elements with a permeability variation of one order of magnitude or larger. Application of adaptive integration in the 27-nodes simulation demonstrates that a similar accuracy is obtained, while 80 % of all element integrations can still be executed with a low-order scheme. This measure diminishes the average number of integration points for one single iteration to 57.2 instead of 130 for 10-point and 228 for 3-point numerical integration. Adaptive integration for free water uptake by ceramic brick thus requires 4 times less integrations points and 5 times less nodes than the low-order minimum discretisation. Adaptive integration thus considerably reduces the computational expense for finite-element simulations of moisture absorption into a porous material.

3.3 Conclusion

While adaptive integration has been introduced for one-dimensional free water uptake, its extension to multi-dimensional simulations is straightforward, and even more rewarding. The reduction of integration points and nodes is possible in all dimensions, and will hence result in significant reductions of the global computational cost. Multi-dimensional equivalents of the high-order integration scheme are on hand in literature (Liu and Vinokur, 1999; Cools, 2003).

Its merit is moreover not limited to simulations of moisture absorption into a porous material. Simulations of building components (or soils) under atmospheric excitation can similarly benefit from the technique, since it efficiently takes care of the occasional sharp moving moisture fronts arising from drying under sunshine or from absorption of precipitation. Simulation of phenomena coupled to moisture transfer – heat-moisture-deformation models for example – can likewise gain from the application of adaptive integration for the numerical integrations of element matrices.

Mesh-adaptive methods (Roels et al., 1999) outperform the adaptive integration presented here, but require the solution of an additional diffusion equation, and prove difficult to control in multi-dimensional simulations. Adaptive integration on the other hand, solely requires two separate numerical integration schemes and can easily be extended to multidimensional simulations.

4. CONCLUSIONS

In this article it was demonstrated that the common preference for low-order numerical integration adversely affects the required discretisation for simulation of moisture absorption into a porous material. It was shown that a fine discretisation throughout was needed to accurately capture the sharp moving moisture fronts. Such fine discretisation throughout is inefficient though, as the small elements are only required at the actual moisture front, while less active regions can be modelled with relatively larger elements.

The reason for this adverse influence was pinpointed in the inaccurate numerical integration of the element permeability matrices, a consequence of the strong non-linear relationship between capillary pressure and moisture permeability. Consequently adaptive integration was introduced, targeting these integration errors and hence easing the requirements on the needed discretisation. For the free water uptake in ceramic brick, it was shown that the computational cost could be significantly reduced by application of adaptive integration: 4 times less integration points and 5 times less nodes were needed, while the accuracy remained untouched.

While seemingly specific to finite-element based simulation models for moisture transfer in porous materials, the other spatial discretisation methods – finite differences and control volumes – can equally benefit from adaptive integration. Kalagasidis et al. (2004) evaluated different averaging schemes for the inter-node permeabilities in a control-volume discretisation, and observed that integral averaging performed best. For all-purpose applicability the integral averaging also has to employ numerical integration schemes, which hence calls for the application of adaptive integration.

ACKNOWLEDGEMENTS

The results presented in this article have been obtained within the frame of the SBO IWT 03175 project ‘Structural damage due to dynamic excitations: a multi-disciplinary approach’, funded by ‘IWT Vlaanderen’, the Institute for the Promotion of Innovation by Science and Technology in Flanders. This financial support is gratefully acknowledged.

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