Evaluation of the Interface Moisture Conductivity between Control Volumes—Comparison between Linear, Harmonic, and Integral Averaging

Angela Sasic Kalagasidis  Thomas Bednar  Carl-Eric Hagentoft

ABSTRACT

Advanced calculating models have become an essential tool in building physics practice for the prediction of thermal and hygric performance of building envelopes. Successful application of any simulation model is generally affected by the mathematical model on which it is based, the quality of the input data, and, finally, when sensitivity and efficiency of the calculations are to be investigated—the numerical method itself. Simulation of the rapid moisture transfer through a building envelope is a typical process that encounters numerical difficulties. The problem is mostly related to certain building materials, such as bricks, characterized by their low moisture capacity and high hydraulic conductivity in the moisture-saturated region. This paper investigates three numerical techniques for the estimation of the moisture transport coefficients during such processes. Two of them—the harmonic and the linear techniques—are widely used, whereas the integral one is not. It is shown that numerical difficulties can be overcome by choosing a suitable technique.

INTRODUCTION

In numerical terminology the interface conductivity represents the mean conductivity between two grid points. For the finite volume numerical method, this conductivity is allocated at the contact surface of the neighbor volumes. The common practice is to evaluate this value as the harmonic mean of the grid-point conductivities. Since the moisture transfer through porous media is a highly nonlinear process, characterized also by abrupt changes in transport coefficients, this method may obtain the false flux, usually underestimated, if the calculating mesh is not sufficiently refined. As an alternative, arithmetic or integral averaging can be applied to estimate the interface conductivity. Our investigation has been focused on these three different evaluation methods for the interface moisture conductivity. Simulation of the rapid moisture transfer (wetting) through porous media is considered for the case study. Results have shown that, in a qualitative way, arithmetic averaging obtains much better results than the harmonic one, while integral averaging appears to be the most appropriate method.

GOVERNING DIFFERENTIAL EQUATION FOR THE MASS BALANCE IN POROUS MEDIA

The nonisothermal moisture flow thorough porous media, \( g \) (kg/m²s), is to be described by two independent state variables (Claesson 1993). For the sake of modeling, it is assumed that the total moisture flow can be divided into two parts—one resulting from the vapor diffusion \( g_v \) and the other originating from the liquid moisture transport \( g_l \).

\[
g = g_v + g_l
\]

Both vapor and liquid flow are described using the Fickian type of relation, where the flow is linearly proportional to the gradient of the state variable. By choosing water vapor partial pressure \( p \) (Pa) as the state variable for the vapor transport and suction pressure \( P_{suc} \) (Pa) for the liquid transport, the corresponding flows for the one-dimensional case are modeled in the following way:

\[
g_v = -\delta_p \frac{\partial p}{\partial x}
\]

Angela Sasic Kalagasidis is a Ph.D. researcher and Carl-Eric Hagentoft is a professor in the Department of Building Technology, Chalmers University of Technology, Gothenburg, Sweden. Thomas Bednar is an associate professor at the Institute for Building Materials, Building Physics and Fire Protection, University of Technology Vienna, Austria.

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The vapor permeability \( \delta_p \) (kg/msPa) and the liquid water conductivity \( K(s) \) are flow coefficients; both of them depend on the moisture and temperature conditions. For the sake of simplicity, we assume that no air transport is present.

By using \( w \) (kg/m\(^3\)) to denote the total moisture content of the material, a differential form of the mass balance equation reads,

\[
\frac{\partial \psi}{\partial t} = -\frac{\partial g_e}{\partial x} - \frac{\partial g_l}{\partial x}.
\]

\( g_1 = K \cdot \frac{\partial P_{\text{suc}}}{\partial x} \) (3)

The moisture flow coefficient is now equal to one.

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\frac{\partial \psi}{\partial t} = -\frac{\partial g_e}{\partial x} - \frac{\partial g_l}{\partial x}.
\]

\( g_1 = K \cdot \frac{\partial P_{\text{suc}}}{\partial x} \) (4)

**Isothermal Moisture Flow**

As further discussed in Claesson (1993), in the case of the one-dimensional isothermal moisture transport, the total moisture flow can be described using one state variable. It can be, for example, the suction pressure \( P_{\text{suc}} \). Again, the moisture transport equation is of the Fickian type.

\[
g = K_w \cdot \frac{\partial P_{\text{suc}}}{\partial x} \] (5)

where \( K_w \) (s) is the transport coefficient for both vapor and liquid flow. Using the constitutive equations for the moisture transfer (Hagentoft 2002a), the relationship between transport coefficients \( K \) and \( K_w \) can be established.

For this particular case, the moisture flow can be described by the gradient of the Kirchhoff’s flow potential, which is defined in Claesson (1993) as

\[
\Psi(P_{\text{suc}}) = \Psi_{\text{ref}} + \int_{P_{\text{suc,ref}}}^{P_{\text{suc}}} K_w dP_{\text{suc}},
\]

(6)

where \( \Psi_{\text{ref}} \) represents the reference value of the suction pressure \( P_{\text{suc,ref}} \). Using \( \Psi \), the moisture flow \( g \) from Equation 5 can be expressed as

\[
g = \frac{\partial \Psi(P_{\text{suc}})}{\partial x} \] (7)

The moisture flow coefficient is now equal to one.

The concept of the Kirchhoff’s flow potential and its application to the nonlinear isothermal moisture transport in porous media is presented in detail in Arfvidsson (1998). One of the advantages of using this concept is that the problem of numerical calculation of the mean transport coefficients between nodes disappears (Cleasson 1993; Arfvidsson 1998). We will refer to this method in our work.

**NUMERICAL SOLUTION OF THE MOISTURE BALANCE EQUATION**

There are a number of different numerical methods that can be used for solving the one-dimensional thermal and moisture transport through building envelopes (Hens 1996; Hagentoft 2002b). For the present investigation, the code based on the finite volumes method and the explicit time discretization scheme is used (Sasic Kalagasidis 2004).

**Discretized Form of the Moisture Balance Equation**

The first step in the control volume technique is to divide the domain into discrete control volumes, as in Figure 1. Although the technique was introduced by Patankar (1980), we keep the same notations here for the volumes as they are given in the original reference: \( P \) stands for the center of the considered volume, while \( W \) and \( E \) denote nodes to the “west” and “east” sides of the considered one. Small letters \( w \) and \( e \) indicate contact surfaces between volumes.

Mass balance over the volume \( P \) is obtained by integrating Equation 4.

\[
\frac{\partial}{\partial t} \int_{W}^{E} g \, dx = \int_{W}^{E} \left( \frac{\partial}{\partial x} \left( \delta_p \frac{\partial P}{\partial x} - K \frac{\partial P_{\text{suc}}}{\partial x} \right) \right) dx
\]

Assuming the uniform moisture content within a volume and the explicit time discretization, a discretized form of Equation 4 reads,

\[
\frac{d w_{P} + d w_{E}}{\Delta t} \left( P_{E} - P_{W} \right) = \left( \delta_{P,s} \frac{P_{E} - P_{P}}{d_{PE}} - K_{s} \frac{P_{\text{suc,E}} - P_{\text{suc,P}}}{d_{PE}} \right) t
\]

\[
+ \left( \delta_{P,w} \frac{P_{W} - P_{P}}{d_{WP}} - K_{w} \frac{P_{\text{suc,W}} - P_{\text{suc,P}}}{d_{WP}} \right) t.
\]

Vapor diffusion coefficients (\( \delta_{P,w} \) and \( \delta_{P,e} \)) and liquid conductivities (\( K_w \) and \( K_e \)) should be calculated as the mean value of transport coefficients between two consecutive nodes, e.g., over distances \( W-P \) and \( P-E \). Since they are allocated to the interfaces between volumes (\( e \) and \( w \), they are known as interface transport coefficients.

**Estimation Methods of the Interface Conductivity**

Interface transport coefficients can be estimated in different ways. In this work, three methods are discussed: the harmonic, the linear, and the integral one. The first two methods are widely used (since they are recommended in the relevant literature, see for example Patankar [1980]), while the

![Figure 1](http://example.com/f1.png)

**Figure 1** Control volume method. Discretization scheme and notations.
1. **Harmonic averaging**

This method assumes equal moisture fluxes over the volume interfaces. For W-P distance, it reads

\[
g_{w,w} = g_{w,P} = g_{w,P}.
\]  

Starting from the above statement, the interface vapor and liquid conductivities at the place \( w \) are calculated as

\[
\frac{d_{wP}}{\delta_{p,w}} = \frac{d_{wP}}{\delta_{p,P}} + \frac{d_{wP}}{K_{w} + \frac{d_{wP}}{K_{P}}}. \tag{11}
\]

For the uniform mesh, interface conductivities calculated in this way represent harmonic averages between nodal values. Since \( d/\delta \) and \( d/K \) represent resistances to vapor diffusion and liquid moisture conduction, this method is also known as the resistance method.

As long as the case is one-dimensional, steady-state, without a source term, and where the transport coefficient varies in a stepwise fashion from one control volume to another, this technique has proved to be valid (Patankar 1980). Even in situations with non-zero sources or with continuous variations of the transport property, the technique could perform quite well.

Our experience in numerical modeling of one-dimensional transient heat and moisture transport in porous building materials agrees with the statement above. The common task also includes variable transport properties and source terms and, with a sufficiently fine calculating mesh, realistic solutions could be obtained. However, in cases where (moisture) transport properties vary by several orders of magnitude and gradients are very high (like the wetting of brick), this technique is not effective any more and sometimes not even reliable, which will be illustrated in what follows.

2. **Linear averaging**

Surface conductivities are calculated as linear variations of the neighboring conductivities:

\[
\delta_{p,w} = \frac{d_{wP}}{d_{wP}} \delta_{p,w} + \frac{d_{wP}}{d_{wP}} \delta_{p,P}, \quad K_{w} = \frac{d_{wP}}{d_{wP}} K_{w} + \frac{d_{wP}}{d_{wP}} K_{P}. \tag{12}
\]

For the uniform mesh, interface conductivities calculated in this way represent arithmetic averages between nodal values.

This method is known as being especially efficient in cases where the harmonic averaging method encounters problems. In Galbraith et al. (2001), both harmonic and linear methods are evaluated for the certain number of vapor transport exercises, showing that the linear method produces a less accurate solution for the transient vapor transport in hygroscopic materials and suggesting a compiled calculation method of these two: harmonic averaging for the boundary nodes and linear method for the internal ones.

3. **Integral averaging**

The integral mean value of the vapor transport coefficient over the distance \( W-P \) is defined as

\[
\delta_{p,w} = \frac{1}{(P_{P} - P_{w})} \int_{w}^{P} \delta_{p}(p)p'\,dp'. \tag{13}
\]

\[
K_{w} = \frac{1}{(P_{suc,P} - P_{suc,W})} \int_{w}^{P} K(P_{suc})dP_{suc}.
\]

Comparing these two equations with the definition of the Kirchhoff’s potential given by Equation 6, it is evident that the integral mean value of the transport coefficient represents the mean values of related \( \Psi \) potentials.

It is interesting to note that the measurements of the (total) moisture transport coefficient using the cup method are actually based on the determination of the set of mean values of this coefficient over the ranges of different relative humidities (Arfvidsson 1998; Janz 2000; Galbraith et al. 2003).

**The Problem of the “Moving Boundary”**

At first sight, it is obvious that these three methods exhibit different behaviors and trends. The first two—the harmonic and the linear—depend directly on the mesh refinement (the size of the volume is incorporated in their formulation, Equations 11 and 12), whereas this is not the case for the integral method (Equation 13). This will be illustrated here by comparing the three different numerical solutions for the process of the free moisture uptake, also known as the suction experiment. Numerical methods that are used for these exercises differ only in the estimation method for the surface moisture conductivity.

The numerical problem in simulating the suction experiment is localized at the “wetting front”—the boundary that appears between the already wet partition of the material and the one that should be wetted. Very sharp moisture flow gradients may appear at the wetting front: hydraulic conductivity in the partition saturated with water can be by several orders of magnitude larger than that in the dry region, as shown in Figure 2. The problem is especially pronounced with certain building materials, such as bricks. These materials are characterized by low moisture capacity and high liquid conductivity in the wet region and, as a result of that, the wetting front moves fast through the material when it is exposed to water.

In order to “catch” the moving front, the numerical mesh around it should be very refined. Since the front moves throughout the whole calculation domain, it implies that the mesh should be fine in the whole domain or be possible to be refined at the moment when the wetting starts. Otherwise, the solution can be far from reality.
The "moving" front is a well-known problem in numerical modeling and the related literature treats it by using the so-called auto-adaptive mesh—a mesh that "follows" the front and keeps the refinement only around it (see, for example, Fletcher [1987]). There are not many computational codes for the building physics applications that use the auto-adaptive mesh refining technique, even if it was shown to be very efficient for this type of problem (Roels 2000). The majority of the codes work with the stationary mesh and, in that case, it is not economical to keep the mesh fine all of the time. For example, if we consider a wall that is exposed to normal external climate conditions and where rapid wetting occurs occasionally, during the rain, it is evident that keeping the mesh fine during the periods without wetting (or drying) will significantly slow the simulations. The accuracy of some other processes that take place, such as convective heat and moisture transfer or radiative heat exchange, may not be improved since the good convergence of the solution is already achieved with the less fine mesh. The problem arises even more if several walls are considered at the same time (a common case for the building) during long simulation periods (years).

The problem that appears in the numerical domain is actually the consequence of the modeling. Equation 8 indicates that flows over the volume boundaries should be the result of the integration. In the discretized form (Equation 9), this demand is not obvious anymore, thereby leaving us the possibility of choosing a suitable method for the estimation of the discretized transport properties. In the majority of the applications, it is the harmonic method, since it secures the flow balance over the surface. Furthermore, this method usually does not encounter any problems when being applied to processes where transport coefficients have the linear form or are moderately nonlinear (such as the heat conduction or water vapor diffusion).

**NUMERICAL EXAMPLE: SIMULATION OF THE SUCTION EXPERIMENT**

A 0.2 m thick material sample is immersed in water for the free moisture uptake. Material data are fictitious: the moisture uptake coefficient, $A$, is constant and equals $10 \text{ kg/m}^2\text{h}^{0.5}$ and the water retention curve is defined by the following relation:

$$w(P_{\text{suc}}) = 300 \cdot (1 + 10^{-6} \cdot P_{\text{suc}})^{-1}$$  \hspace{1cm} (14)

The total moisture conductivity $K_w$ is modeled as

$$K_w(P_{\text{suc}}, n) = \frac{\partial w(P_{\text{suc}})}{\partial P_{\text{suc}}}, \quad \frac{n + 1}{\frac{\partial w(P_{\text{suc}})}{\partial P_{\text{suc}}}} \left( \frac{A}{300} \right)^2 \left( \frac{w(P_{\text{suc}})}{300} \right)^n \left( n + 1 - \left( \frac{w(P_{\text{suc}})}{300} \right)^n \right),$$  \hspace{1cm} (15)

where $n$ is a free parameter (Bednar 2000). An analytical solution for this case is available: the total amount of water taken by the material specimen during the time is

$$A \sqrt{t}.$$  \hspace{1cm} (16)
For the one-dimensional problem, the sample is wetted from one side, while the other side is sealed against the water vapor exchange with the surroundings. Initial conditions for the sample are: 20°C and 0% relative humidity. Heat and vapor transfer coefficients at the boundaries are: 10 W/m²K and 0 s/m. The isothermal moisture uptake is considered.

**Case 1.** The variable \( n \) is equal to 13. The water retention curve, \( w(P_{\text{swc}}) \), the hydraulic conductivity, \( K_w(P_{\text{swc}},n) \), and the integrated hydraulic conductivity, \( PSI(P_{\text{swc}},n) \), are given in Figure 3. This fictitious material has thermal and moisture properties close to a common brick.

The moisture content of the sample increases with time. It is expressed as the saturation degree: the present moisture content is compared to the maximum value of 300 kg/m³.

After ten hours, saturation is 53% (the analytical solution). Figure 4 shows results obtained by the linear and integral averaging and for the different mesh refinements: with 5 nodes—20 and 100. Only the uniform mesh is concerned. By refining the mesh, both methods give solutions that converge to the analytical one. The integral method provides a solution that is close to the analytical one, already with the very coarse mesh (five nodes), while the linear method significantly overestimates the correct solution.

The solution with the harmonic method gives 0% saturation degree after ten hours, despite the mesh refinement. However, this is not surprising; the conductivity \( K_w \), given by Equation 5, is zero for the absolutely dry sample, which gives rise to the infinite moisture transport resistance on the dry side (Equation 11). In this theoretical case, the value “close to zero” is on the order of \( 10^{-50} \). The method is further tested and the wetting is finally “initiated” by the nonuniform mesh with the cell size of \( 10^{-15} \) m close to the boundary.

The actual moisture uptake coefficients during simulations are given in Figure 5; they additionally clarify the results.

**Figure 3** Water retention curve \( w(P_{\text{swc}}) \), total hydraulic conductivity \( K_w(P_{\text{swc}}) \), and integrated hydraulic conductivity \( PSI(P_{\text{swc}}) \) for the test materials.

**Figure 4** Saturation degree of the sample for Case 1. Study of the different averaging techniques and different mesh refinements.

**Figure 5** Calculated moisture uptake coefficients for Case 1. Study of the different averaging techniques and different mesh refinements.
from Figure 4. In the case of the linear method, the value for $A$ is overestimated, but it steadily converges to the value of 10 kg/m²h⁰.⁵⁻¹, both with the time and the mesh refinement. For the integral method, the calculated moisture uptake coefficient is underestimated in the beginning (the solution with five nodes), but it converges much faster, both with time and the mesh refinement.

**Case 2.** The variable $n$ is equal to 1. The moisture retention curve remains the same as in the first case, but the hydraulic conductivity and its integrated value, the PSI, are changed, as shown in Figure 3. The hydraulic conductivity in the dry region is on the order of $10^{-20}$ s. This value still causes a high moisture resistance, but not numerically high, as in the previous example.

The saturation degree of the sample becomes 53% again, after ten hours. Solutions are obtained with all three methods (Figure 6). The linear and the integral method give results similar to those from the previous case. For the harmonic method, the wetting is initiated only with a mesh of 100 nodes but is still underestimated—the saturation is 14% after ten hours. By performing the further mesh refinement, the solution with the harmonic method approaches the analytical one.

The calculated values for the moisture uptake coefficients for this case are given in Figure 7. For the linear method, the moisture uptake coefficient does not converge so steadily with the mesh refinement as in Case 1 (compare the values for 20 and 100 nodes). The result obtained by the integral method exhibit the same tendency as before. The solution for the harmonic method is not presented here, since it underestimates significantly the correct solution.

**CONCLUSION**

This work has shown that it is possible to produce an accurate solution for the problem of the “moving boundary” using a stationary mesh by choosing the proper method for the estimation of the interface conductivity. Furthermore, an addi-
tional demand to keep the coarse mesh is also fulfilled. For this purpose, two theoretical suction experiments are simulated. In both cases, the analytical solution is available.

In Case 1, the moisture transport properties of the material are modeled to represent the ones of the common brick: the material is nonhygroscopic, but highly capillary active. It is shown that the harmonic method drastically underestimates the moisture flow over the wetting boundary and, as a consequence of that, the solution, which is far from reality, is produced. The linear and integral methods are able to produce an accurate solution for the case treated. However, if the mesh is not sufficiently refined, the linear method overestimates the flow, and the solution based on this method can significantly differ from the accurate one. The integral method gives a realistic solution with a coarse mesh. Even with moderate mesh refinement, the solution obtained with the integral method converges rapidly to the analytical one.

In Case 2, only the hydraulic conductivity of the sample is changed so that the material is capillary active also in the unsaturated region. By this, the moisture flow gradient over the wetting front is decreased and an “easier” numerical problem is generated. Solutions obtained by each of the three methods, for the estimation of the interface moisture conductivity, are similar to the ones from Case 1. However, the difficulties and discrepancies are not as pronounced.

The integral method appears to be the most accurate one for the estimation of the interface moisture conductivity. It is very insensitive to the mesh refinement and, thus, inspires confidence in the solution. The application of this method for the nonisothermal moisture transport problems is to be further investigated. Finally, it is important to mention that this method is extremely sensitive to the quality of the input data. The integration for generating the Kirchhoff’s potentials, described by Equation 13, should be performed with the special caution.

**NOMENCLATURE**

\( A \) = moisture uptake coefficient, \( \text{kg/m}^2\text{h}^{0.5} \)  
\( g \) = moisture flow, \( \text{kg/m}^2\text{s} \)  
\( K \) = liquid water conductivity, \( \text{s} \)  
\( K_w \) = total hydraulic conductivity, \( \text{s} \)  
\( p \) = water vapor partial pressure, \( \text{Pa} \)  
\( P_{\text{sc}} \) = suction pressure, \( \text{Pa} \)  
\( t \) = time, \( \text{s or h} \)  
\( w \) = moisture content, \( \text{kg/m}^3 \)  
\( x \) = space coordinate, \( \text{m} \)  
\( \delta_p \) = vapor diffusivity, \( \text{kg/m}^2\text{sPa} \)  
\( \Psi \) = integrated total hydraulic conductivity, \( \text{kg/m}^3\text{s} \)

**Subscripts**

\( e \) = at the east contact surface (to the right of the P node)  
\( E \) = at the east node (to the right)  
\( l \) = liquid water  
\( P \) = at the middle node  
\( \text{ref} \) = reference value  
\( w \) = at the west contact surface (to the left)  
\( W \) = at the west node (to the left)

**REFERENCES**


