ON THE CONSERVATION OF MASS AND ENERGY IN HYGROTHERMAL NUMERICAL SIMULATION WITH COMSOL MULTIPHYSICS

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ABSTRACT

In this paper, two different forms of the non-linear PDE-system for heat and mass transfer in porous materials and their implementation with COMSOL Multiphysics are considered.

The φ -based form presents the relative humidity as system variable and leads in general to nonconservative solutions. The u-based form uses the water content as variable and is conservative.

This study aims to select the most appropriated form for the implementation of the heat and mass transfer problem in COMSOL Multiphysics, comparing the quality of the numerical solutions and the solver performances.

As first test-example, the simulation of a onedimensional porous layer with a moisture flux imposed on one of the boundaries is presented.As second example, the moisture redistribution inside a partially saturated layer is simulated.

INTRODUCTION

COMSOL Multiphysics can be used for solving transient heat and moisture transfer problems inside construction materials (Schijndel, 2008), (Bianchi Janetti, 2012). This FEM software allows 3D-modeling and the coupling with convection inside air gaps in the construction. Moreover, the possibility of an easy integration with Matlab/Simulink is given. These features can represent an advantage compared to other available programs specific for hygrothermal simulation ("WUFi Software," 2011) ("Delphin Software," 2011).

However, the numerical error of the model implemented in COMSOL has to be investigated. In particular the error concerning the conservation of global mass and energy over the domain has to be quantified.

Heat and moisture transfer processes in porous construction materials are described by a system of two partial differential equations derived by imposing the equilibrium balance of mass and energy within an infinitesimal element of volume (Nicolai, 2008). This system is non-linear since the material properties depend on the temperature and moisture distribution. It is known that conservation of mass and energy over the domain depends on the formulation of the PDE-system (Celia, 1990). In order to obtain a conservative formulation, the dependent variables have to be properly chosen.

In order to select the best form for the system, both the described variants will be evaluated considering the influence of the numerical errors on the results.

The determination of the numerical precision of the model implemented in COMSOL Multiphysics for heat and moisture transfer represents an important step in the evaluation of the usability of this program for the solution of problems such as moisture transfer inside constructions.

TEST PROBLEM 1

We consider a porous layer with a constant water flux *j* imposed on the left boundary (Figure 1). The thickness of the layer is one centimeter (L=1 cm).

The right boundary is closed to both, mass and energy transfer.

The initial temperature and moisture distributions inside the layer are uniform.

This problem is implemented in COMSOL Multiphysics using both the φ -based and the u-based form.



Figure 1 Schematic representation of the 1D test problem (here with $j=5.5E^{7}[Kg/(m^{2}s)]$)

φ-based form

We write the system of partial differential equations governing the transport inside the layer as follows (eqs. (1) and (2)):

$$\frac{du}{d\varphi}\frac{\partial\varphi}{\partial t} = \frac{\partial}{\partial x} \left(D_{m,\varphi} \frac{\partial\varphi}{\partial x} + D_{m,T} \frac{\partial T}{\partial x} \right) \tag{1}$$

$$C\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(D_{e,T} \frac{\partial T}{\partial x} + D_{e,\varphi} \frac{\partial \varphi}{\partial x} \right)$$
(2)

The boundary conditions are given by eqs. (3) to (6):

$$-D_{m,\varphi}\frac{\partial\varphi(0,t)}{\partial x} - D_{m,T}\frac{\partial T(0,t)}{\partial x} = j$$
⁽³⁾

$$-D_{e,T}\frac{\partial T(0,t)}{\partial x} - D_{e,\varphi}\frac{\partial \varphi(0,t)}{\partial x} = 0$$
⁽⁴⁾

$$-D_{m,\varphi}\frac{\partial\varphi(L,t)}{\partial x} - D_{m,T}\frac{\partial T(L,t)}{\partial x} = 0$$
⁽⁵⁾

$$-D_{e,T}\frac{\partial T(L,t)}{\partial x} - D_{e,\varphi}\frac{\partial \varphi(L,t)}{\partial x} = 0$$
⁽⁶⁾

Notice that the energy fluxes on the boundaries are given by equations (4) and (6) and are equal to zero, thus we aspect the process to be almost isothermal, since the temperature can change only due to moisture gradients.

The initial conditions are:

$$\varphi(x,0) = 0.01 \tag{7}$$

$$T(x,0) = 283.15K \tag{8}$$

The dependent variants of the system written in this form (φ -based) are the temperature T(x,t) and relative humidity $\varphi(x,t)$.

The coefficients $D_{m,\varphi}$, $D_{m,T}$, $D_{e,\varphi}$ and $D_{e,T}$ are functions of material specific parameters, describing heat and moisture diffusion through the layer.

The moisture storage inside the porous medium is described through the derivative of the water content u with respect to φ in the left hand side of equation (1), whereas the energy storage is taken into account due to the coefficient C (left hand side of equation (2)). This coefficient represents the equivalent heat capacity of the moist material.

In general, all the transfer and the storage parameters are strongly depending on temperature and moisture distributions $(T(x,t) \text{ and } \varphi(x,t))$. This makes the problem (1)-(8) non-linear and only solvable using a numerical method.

It has been demonstrated that numerical schemes applied to PDE presenting non-linear storage terms can lead to non-conservative solutions (Celia et al., 1990).

In order to verify this for the set of equations (1)-(8), we consider just the dependence of the water content (*u*) on the relative humidity (φ), while all the others coefficients are assumed to be constant (see Table 1).

Even if this assumption is not realistic from the physical point of view, it is justified for two reasons:

First, we are primarily interested in investigating the effect of the storage-terms non-linearity, thus the transfer-terms non-linearity can be neglected. Moreover, the dependence of the coefficient C on the dependent variables is not as relevant as that of the moisture retention on the relative humidity.

Second, due to this simplification, the model is much simpler allowing an easier overview and reproduction.

According to (Holm, 2002), the relation between the water content u and the relative humidity φ can be

approximately described with the following close form expression:

$$u(\varphi) = \frac{u_f}{1 + \left(\frac{-\rho_w R_v T_{ref} ln(\varphi)}{k_1}\right)^{k_2}}$$
(9)

Here, u_f is the water content at saturation, ρ_w is the density of water, R_v is the individual gas constant for water vapour, T_{ref} is the reference absolute temperature and k_1 and k_2 represent two material specific fitting parameters.

Figure 2 shows *u* and its derivative with respect to φ . The plot has been obtained using the data in Table 1 and in Table 2.

Since the derivative $du/d\varphi$ assumes very high values for both, relative humidity φ approaching zero and one, we aspect numerical difficulties when the material is dry and close to the water saturation.



Figure 2 Moisture retention curve $u(\varphi)$ and its derivative

Table 1 Material parameters

Parameter	Unit	Value
$D_{m,\varphi}$	[kg/(m s)]	2.715493e-9
$D_{m,T}$	[kg/(m s K)]	9.107562e-11
$D_{e,\varphi}$	[W/m]	6.639e-3
$D_{e,T}$	[W/(m K)]	1.6
С	$[W/(m^3 K)]$	1.430417e6
k1	[Pa]	2.997117e6
k2	[-]	0.51671
<i>u</i> _f	$[Kg/m^3]$	180

Table 2 Constants

Constant	Unit	Value
$ ho_w$	$[Kg/m^3]$	1000
R_{v}	[J/(Kg K)]	462
T _{ref}	[K]	283.15

u-based form

Writing the system in the u-based form, we obtain the set of equations (10) to (15).

Transport equations:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(D_{m,u} \frac{\partial u}{\partial x} + D_{m,T} \frac{\partial T}{\partial x} \right) \tag{10}$$

$$C\frac{\partial T}{\partial t} = \frac{\partial}{\partial x} \left(D_{e,T} \frac{\partial T}{\partial x} + D_{e,u} \frac{\partial u}{\partial x} \right)$$
(11)

Boundary conditions:

$$-D_{m,u}\frac{\partial u(0,t)}{\partial x} - D_{m,T}\frac{\partial T(0,t)}{\partial x} = j$$
(12)

$$-D_{e,T}\frac{\partial T(0,t)}{\partial x} - D_{e,u}\frac{\partial u(0,t)}{\partial x} = 0$$
(13)

$$-D_{m,u}\frac{\partial u(L,t)}{\partial x} - D_{m,T}\frac{\partial T(L,t)}{\partial x} = 0$$
(14)

$$-D_{e,T}\frac{\partial T(L,t)}{\partial x} - D_{e,u}\frac{\partial u(L,t)}{\partial x} = 0$$
(15)

The initial water content u(x,0), is calculated using equation (9) with eq. (7). The initial temperature is given by eq. (8).

It can be observed that the system (10)-(15) is equivalent to (1)-(8) from the analytical point of view, since the coefficients $D_{m,u}$ and $D_{e,u}$ are obtained from $D_{m,\varphi}$ and $D_{e,\varphi}$ using the equations (16) and (17) where $\varphi(u)$ is the inverse function of (9).

$$D_{m,u} = D_{m,\varphi} \frac{d\varphi}{du} \tag{16}$$

$$D_{e,u} = D_{e,\varphi} \frac{d\varphi}{du} \tag{17}$$

We observe that the coefficient of the time derivative in the first member side of equation (10) is constant (equal to one). This guarantees the mass conservation of the solution calculated with COMSOL Multiphysics, as shown in the results of this study.

IMPLEMENTATION IN COMSOL MULTIPHYSICS

For the solution of the set of equations (1)-(8) and (10)-(15) the COMSOL version 3.4 is employed ("COMSOL Multiphysics Software," 2011).

This program, based on the finite element method (Galerkin), allows the solution of various nonlinear PDE Systems of equations having the following generic form valid in the domain:

$$e_{a}\frac{\partial^{2}\boldsymbol{u}}{\partial t^{2}} + d_{a}\frac{\partial\boldsymbol{u}}{\partial t} +$$

$$+\nabla \cdot (-c\nabla \boldsymbol{u} - \alpha \boldsymbol{u} + \gamma) + \beta \cdot \nabla \boldsymbol{u} + a\boldsymbol{u} = f$$
(18)

With Neumann boundary conditions given by the following equation:

$$\vec{n} \cdot (-c\nabla \boldsymbol{u} - \alpha \boldsymbol{u} + \gamma) + q \boldsymbol{u} = g \tag{19}$$

Equations (18) and (19) can be easily adapted to the φ -based form described by equations (1) to (6) putting:

$$u = \{\varphi, T\}$$

$$e_{a} = \alpha = \beta = a = f = q_{1} = q_{2} = g_{1} = \{0, 0\}$$

$$d_{a} = \{du/d\varphi, C\}$$

$$c = \{D_{m,\varphi}, D_{e,T}\}$$

$$\gamma = \{-D_{m,T'} dT/dx, -D_{e,\varphi'} d\varphi/dx\}$$

$$g_{2} = \{j, 0\}$$

The subscripts 1 and 2 refer to the left and the right hand side boundary, respectively. With the u-based form is possible to proceed in analogous way.

Notice that COMSOL would accept also other forms for the same problem. For example, it is possible to include the time derivative of the water content $u(\varphi)$ in the coefficient *f*, modifying the previous defined coefficients as follows:

$$f = \{ \partial u(\boldsymbol{\varphi}) / \partial t, 0 \}$$
$$d_a = \{ 0, C \}$$

The performance evaluation of such alternative mixed forms in Comsol may be part of future work.

The equations (18) and (19) can be set in the graphical user interface of COMSOL directly in their analytical form, whereas the software performs the numerical discretisation and linearization of the system.

The user has to specify the shape function for the simulation (Physics \rightarrow Subdomain settings \rightarrow Element): in this study, linear and quadratic Lagrange-elements are investigated.

The simulations are performed with the following solver parameters (standard settings, with exception of relative and absolute tolerance):

Linear system solver: Direct UMFPACK; relative tolerance: 1e-5; absolute tolerance: 1e-5.

Time stepping: BDF (Backward Differentiation Formula), maximum BDF order: 5; minimum BDF order: 1

RESULTS OF THE TEST PROBLEM 1

The distributions of relative humidity, water content and temperature inside the porous layer at different time steps are reported in Figure 3, Figure 4 and Figure 5, respectively.

These results have been calculated with five equal linear elements ($\Delta x = 2mm$).

The ϕ -based form and the u-based form show a good agreement for temperature and relative humidity.

For the water content distribution, the difference becomes relevant just if u approaches to the saturation (φ approaching to unity).



Figure 3 Relative humidity distribution at different time steps. Five equal mesh elements.



Figure 4 Water content distribution at different time steps. Five equal mesh elements.



Figure 5 Temperature distribution at different time steps; five equal mesh elements

Considering the water content calculated on the left boundary, we notice that the φ -based form solution overestimates the exact value, whereas the u-based form solution underestimates it. Both the solutions converge to the same value by refining the mesh (see Figure 6). In order to show this more clearly, it is convenient to write the deviation between the two models as follows:

$$\Delta u(0,t) = u_{\varphi}(0,t) - u_{u}(0,t)$$
⁽²⁰⁾

In eq. (20), $u_{\varphi}(0,t)$ and $u_u(0,t)$ represent the solutions calculated at the position x=0 with the φ -based and the u-based form, respectively.

The values of Δu after one hundred hours (t=100 h) are reported in Figure 7 as function of the mesh element number M. Linear and quadratic shape functions have been employed.

The deviation between the two models can be reduced by refining the mesh. However, it remains significant also using fine meshes (M = 20 $\rightarrow \Delta u > 40 \text{ Kg/m}^3$, for linear elements).



Figure 6 water content distribution after 100h for a fine (100 elements) and a coarse mesh (5 elements)

This can be explained, considering that the derivative of the moisture retention curve assumes extremely high values when u approaches the saturation (see Figure 2) leading to a high numerical approximation error in both the φ -based and u-based models. We can conclude that, for a precise prediction of the water content on the left surface an extremely fine mesh is required, independently of the employed PDE-form.

Mass conservation

In this subsection, the aim is to investigate the conservation of total mass and energy for both the implemented PDE forms, giving a measure of the solution quality.

For the cases presented in this study, the energy results are necessary conservative since the effective heat capacity is supposed to be constant.

In general, it can be shown that, if the coefficients of the time derivatives are constants (in COMSOL: the damping/mass coefficient d_a), the solution results conservative. Therefore, here, the u-based form results conservative for both energy and mass whereas the φ -based form only for the energy.

Notice that the water content distribution calculated with the φ -based form over a coarse mesh overestimates the fine mesh solution (lower part of Figure 6). Assuming that the fine mesh solution approaches, with good approximation, the exact solution, we can deduce that the φ -based form does not conserve the mass, since the total mass in the domain is overestimated.

In order to quantify the deviation from the conservative solution, we introduce a mass balance ratio *MB*, as suggested by (Celia et al., 1990):

$$MB(t) = \frac{\int_0^L u(x,t) \, dx - j \cdot t}{\int_0^L u(x,0) \, dx}$$
(21)

The numerator represents the total moisture in the domain at a given time t minus the total flux into the domain up to that time. The denominator represents the total initial moisture content. Thus, for a perfectly conservative solution, the parameter MB has to be equal to one.



Figure 7 $\Delta u(0,t^*)$ as a function of the number of mesh elements $M(t^*=100h)$

The upper part of Figure 8 shows the evolution of the mass balance ratio calculated with the ϕ -based form for different mesh refinements using Lagrange linear elements.

Significant deviations from the conservative solution can be observed at the end of the simulation when the

left side of the layer becomes saturated. Smaller deviations are also present in the first part of the simulation (for the dry material).

This behaviour can be explained, considering again the form of the moisture retention curve (see Figure 2).

A mesh refinement improves the solution quality obtained with linear Lagrange elements (Figure 8, bottom). It is also obvious that the finer the mesh, the less is the improvement with a further refinement. (in the considered case, more than twenty elements do not lead to any significant furter improvement of the mass conservation).

The solution calculated with quadratic Lagrange elements is almost conservative, independently from the number of mesh elements. However, in some cases quadratic elements lead to oscillations in the solution. This has been investigated on the basis of a second test problem (see test problem 2).



Figure 8 Mass balance ratio as a function of time for different numbers of grid elements calculated with the φ -based form (top). Mass balance ratio vs. number of grid elements (M) after 100h (bottom)

Notice that the u-based form solution on a coarse mesh in part overestimates and in part underestimates the fine solution (lower part of Figure 6). However, the mass balance ratio results to be exactly equal to one for every mesh refinenment. This prooves that this solution is conservative.

Solver performance

In COMSOL the time step is variable and determined by the internal software algorithm. The φ -based form leads to fewer time steps if compared with the ubased form, and thus, to a lower solution time. This can represent a drawback of the u-based form, especially for large models.

No significant difference concerning the number of Jacobian matrices which have to be evaluated has been observed between the two variants for the considered cases.

In Table 3 and in Table 4 the solver performance statistics for both the φ -based and the u-based forms are reported for linear Lagrange elements (processor: intelTM CoreTM i7 CPU M, 620 @ 2.67GHz, one core, RAM: 4.00GB).

Table 3 Solver performance φ-based form linear Lagrange elements

М	Time steps	Number of Jacobians	Solution time [s]
3	97	21	0.91
5	113	26	1.037
10	126	22	1.089
20	128	19	1.111
100	154	17	1.3

Table 4 Solver performance u-based form linear Lagrange elements

М	Time steps	Number of Jacobians	Solution time [s]
3	853	15	4.134
5	955	16	4.893
10	1012	17	5.191
20	1043	18	5.566
100	1058	30	5.851

Similar results are obtained also using quadratic Lagrange elements (Table 5 and Table 6).

Table 5 Solver performance φ-based form quadratic Lagrange elements

М	Time steps	Number of Jacobians	Solution time [s]
3	102	22	0.967
5	129	19	1.207
10	135	17	1.23
20	148	16	1.268
100	172	17	1.511

Table 6 Solver performance u-based form quadratic Lagrange elements

М	Time steps	Number of Jacobians	Solution time [s]
3	949	17	4.678
5	997	16	4.869
10	1021	18	5.052
20	1058	28	5.527
100	1030	35	5.6

TEST PROBLEM 2

Since the φ -based form leads to a lower number of time steps and to faster solutions, it is in general advantageous to use it instead of the u-based form.

Despite the non-conservative solution, the errors concerning the conservation of mass and energy remain in an acceptable range in many tested cases. Higher errors can occur in case of steep gradients or at saturation conditions.

In this section, the φ -based form is tested, employing a second 1D-problem presenting these critical conditions.

We consider a layer (5 cm) closed on the boundaries to both the energy and the mass transfer. The initial temperature inside the layer is uniform (20 °C), whereas the initial relative humidity is a step-function (100% on the left and 20% on the right side of the layer).

In this case, realistic transfer and storage parameters, depending on both temperature and moisture content are employed. The diffusion coefficients are defined as follows according to (Janetti, 2012):

$$D_{m,\varphi} = \frac{p_s D_v}{\mu R_v T} - K_l \quad \frac{\partial p_c}{\partial \varphi} \tag{22}$$

$$D_{m,T} = \frac{\varphi D_v}{\mu R_v T} \frac{dp_s}{dT}$$
(23)

$$D_{e,T} = \lambda + \left(h_{lv} + c_{p,v}T\right) \frac{\varphi D_v}{\mu R_v T} \frac{dp_s}{dT}$$
(24)

$$D_{e,\varphi} = \left(h_{lv} + c_{p,v}T\right) \frac{p_s D_v}{\mu R_v T}$$
(25)

(26)

RESULTS FOR TEST PROBLEM 2

In Figure 9, Figure 10 and Figure 11 the results calculated with COMSOL are compared with those of the simulation program ("Delphin Software," 2011).

The software Delphin, developed specifically for modeling heat and moisture transfer in constructions, is based on the Finite Volume Method and is conservative. The performances of this software

 $C = \rho c$

concerning numerical accuracy and computational effort have been investigated by (Nicolai, 2008).

The chosen constants and material parameters used for this example are reported in the following table:

Parameter	Dimension	Value
λ	W/(m K)	1.774
ρ	kg/m ³	2452.91
С	J/(kg K)	702.156
μ	-	53.798
K_l	S	1e-15
u_f	kg/m ³	54.052
$C_{p,v}$	J/(kg K)	2050
h_{lv}	kJ/kg	2445
D_v	m ² /s	2.662e-5
R_{v}	J/(kg K)	462

Table 7Parameters for the test problem 2

The solutions show a good agreement on the right side of the layer, whereas on the left side (saturated side) the COMSOL solution presents oscillations (Figure 10). Thus, even if the error concerning the mass conservation remains always under 3% (Figure 12), the solution quality is not adequate in case of saturation.

Notice that this simulation is performed with linear elements. Using quadratic elements, even larger oscillations occur and the calculation crashes.

The model can be improved modifying the solver parameter (linear solver, time stepping), anyway this leads to longer calculation time. Further optimization work should be performed in this direction.

Further tests have shown that with lower relative humidity on the left hand side (99%), the quality of the solution is satisfactory and the mass conservation error becomes negligible. Thus, the use of COMSOL is already profitable for calculations in this moisture range.



Figure 9 distribution of relative humidity in the layer; comparison between COMSOL (C) and Delphin (D)



Figure 10 distribution of water content in the layer; comparison between COMSOL (C) and Delphin (D)



Figure 11 Temperature distribution in the layer; comparison between COMSOL (C) and Delphin (D)



Figure 12 Development of mass balance ratio for the Test problem 2

CONCLUSION

The use of COMSOL Multiphysics as solver for modeling heat and moisture transfer problems is profitable. The mathematical model can be easily modified and adapted by the user, allowing high flexibility. Moreover, coupling with other programs and multidimensional simulation are possible. However the quality of the numerical solution has to be evaluated, with respect to different possible forms of the PDE system.

In this paper we consider the numerical performance of the ϕ -based form and of the u-based form.

The u-based form leads always to a conservative solution but in general presents higher numerical effort.

The quality of the φ -based form solution is in general acceptable, with exception of calculations at saturation conditions. In this case, oscillations occur.

The influence of solver type and setting and time stepping parameters will be investigated in future works. Moreover, the results may be extended to 2D and 3D cases.

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NOMENCLATURE

C	$[J/(m^{3} K)]$	Equivalent heat capacity
с	[J/(kg K)]	Heat capacity
$D_{m,\varphi}$	[kg/(m s)]	
$D_{m,T}$	[kg/(m s K)]	Transport
$D_{e,arphi}$	[W/m]	Coefficients
$D_{e,T}$	[W/(m K)]	
D	$[m^2/s]$	Diffusivity
h	[J/kg]	Enthalpy
j	$[kg/(m^2 s)]$	Mass flux
K	[s]	Conductivity
k1	[Pa]	Water retention
k2	[-]	function parameters
L	[m]	Layer thickness
M	[-]	Number of mesh elements
$M\!B$	[-]	Mass balance ratio
р	[Pa]	Pressure
R	[J/(kg K)]	Gas constant
t	[s]	Time
T	[K]	Temperature
θ	[°C]	Temperature
u	$[kg/m^3]$	Volumetric water content
X	[m]	Position
λ	[W/(m K)]	Thermal conductivity
μ	[-]	Vapour diffusion resistance
ρ	$[kg/m^3]$	Density
φ	[%]	Relative humidity

Subscripts

c capillary	
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- f Free saturation
- I Liquid
- lv Liquid-vapour
- p Constant pressure
- ref Reference
- u u-based form
- v Vapor
- w Liquid water
- φ ϕ -based form

COMSOL coefficients

- *c Diffusion coefficient*
- a Absorption coefficient
- f Source term
- *e_a* Mass coefficient
- d_a Damping/Mass coefficient
- α Conservative flux convection coefficient
- β Convection coefficient
- *γ Conservative flux source term*
- q Boundary condition coefficient
- g Boundary condition coefficient

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