

Simulation and Verification of Coupled Heat and Moisture Modeling

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Abstract: The modeling of coupled heat and moisture transport is found to be a valuable method in which possible damage-related processes in building materials and components can be predicted.

This paper includes the implementation and comparison of two types of moisture potentials used in the modeling of coupled heat and moisture transport: the natural logarithmic of the suction pressure (LPc) and the relative humidity (Rh). Two finite element models evaluating the coupled thermal and hygric transport have been developed using COMSOL Multiphysics®.

The two developed models were verified with the normative benchmark test of European Provisional Standard prEN 15026. These models appear to be valid predictive tools to investigate the impact of a change in climatic conditions on building materials and components.

Keywords: Heat, moisture, verification, predictive tool

1. Introduction

The driving force of this paper is the Climate for Culture project found within the European Union's 7th framework program. This project attempts to face the challenges of climate change, while acknowledging the need for the preservation of cultural heritage. It is important to consider that a change in climatic conditions can cause not only damage, but can also destroy the basic structure of these sites, as well as their associated interior artefacts. As such, the modeling of coupled heat and moisture transport is found to be a valuable method in which possible damage-related processes in building materials and components can be predicted.

A main issue that has been encountered when modeling coupled heat and moisture transport concerns the choice of the moisture potential from a numerical point of view [3]. The following moisture potentials are numerically not suitable: (1) Moisture content

[kg/m³]. The main problem with this potential is the discontinuity in moisture content at the interface of two materials. (2) Partial vapor pressure [Pa]. While using this potential, a problem can occur if local temperature drops rapidly. Furthermore, the saturation vapor pressure drops simultaneously and the relative humidity could rise above 100% (anomaly). (3) Suction pressure Pc [Pa]. The suction pressure ranges from 1 to ~10⁹ Pa if liquid water transport is included. Especially when liquid water (e.g. rain) is penetrating the material at a boundary that is dry initially, a sudden change from ~10⁹ Pa to 1 Pa is expected. Such a change easily causes numerical instabilities and may produce Pc < 1 Pa (anomaly). (4) Relative humidity Rh [%]. Rh encounters a similar problem as described for Pc. However, if there is no liquid water penetration at the boundaries, the Rh is a suitable moisture potential. The latter will be illustrated in this paper. (5) The natural logarithmic of suction pressure (LPc) [Pa]. This potential seems to be best suitable for extreme conditions as will also be discussed in this paper.

This paper presents the implementation of various moisture potentials namely, the natural logarithmic of the suction pressure (LPc) and the relative humidity (Rh), into the governing equations for coupled heat and moisture modeling. The COMSOL Multiphysics® modeling procedures used for the two case scenarios are discussed; followed by, the verification of the models using a normative benchmark test. Lastly, the numerical simulated results obtained from the two models are compared.

2. Coupled Heat and Moisture Transport

The models are based on one-dimensional conductive heat transfer, q_{cd} , according to Fourier's Law:

$$q = q_{cd} \quad (1)$$

$$q_{cd} = -\lambda \nabla T = - \left(\lambda \frac{\partial T}{\partial x} \right)$$

where T is the temperature [°C, K] and λ is the moisture dependent thermal conductivity [W/mK].

The total moisture transfer, g , includes both one-dimensional vapour, g_v , and liquid flow, g_ℓ . Moisture transport can be characterized by various potentials as is demonstrated in the two developed models, which include natural logarithmic of the suction pressure (LPc) and relative humidity (Rh). The following Equation (2) however describes a general form of the total moisture transfer using partial vapour pressure as the potential:

$$g = g_v + g_\ell$$

$$g_v = -\delta_p \nabla p = - \left(\delta_p \frac{\partial p}{\partial x} \right) \quad (2)$$

$$g_\ell = -D_w \cdot \frac{\xi}{p_{sat}} \nabla p = -D_w \cdot \frac{\xi}{p_{sat}} \left(\frac{\partial p}{\partial x} \right)$$

where p is the partial vapour pressure [Pa]; p_{sat} is the saturation vapour pressure [Pa]; δ_p is the vapour permeability [kg/msPa]; D_w is the liquid transport coefficient [m²/s]; and lastly, ξ is the moisture capacity [kg/m³].

Furthermore, PDEs for energy and moisture balance are used to express dynamic heat and moisture transport mechanisms. These balance equations can be expressed by:

$$c_p \rho \frac{\partial T}{\partial t} = -\nabla(-\lambda \nabla T) \quad (3)$$

$$\frac{\partial w}{\partial t} = -\nabla \left(\underbrace{(-\delta_p - D_w \cdot \frac{\xi}{p_{sat}})}_{g_v + g_\ell} \nabla p \right) \quad (4)$$

where c_p is the specific heat capacity [J/kgK]; ρ is the density [kg/m³]; t is time [s]; and lastly, w is moisture content [kg/m³].

The transformation of Equations (3) and (4) using LPc and Rh as moisture potentials is described respectively in Sections 3 and 4.

3. LPc model

The heat and moisture transport can be described by the following PDEs using LPc as potential for moisture transfer [1].

$$\begin{aligned} C_T \frac{\partial T}{\partial t} &= \nabla \cdot (K_{11} \nabla T + K_{12} \nabla LPc) \\ C_{LPc} \frac{\partial LPc}{\partial t} &= \nabla \cdot (K_{21} \nabla T + K_{22} \nabla LPc) \end{aligned} \quad (5)$$

With:

$$LPc = {}^{10} \log(Pc)$$

$$C_T = \rho \cdot c$$

$$K_{11} = \lambda$$

$$K_{12} = -l_v \cdot \delta_p \cdot \phi \cdot \frac{\partial Pc}{\partial LPc} \cdot P_{sat} \cdot \frac{M_w}{\rho_a RT},$$

$$C_{LPc} = \frac{\partial w}{\partial Pc} \cdot \frac{\partial Pc}{\partial LPc} \quad (6)$$

$$K_{22} = -K \cdot \frac{\partial Pc}{\partial LPc} - \delta_p \cdot \phi \cdot \frac{\partial Pc}{\partial LPc} \cdot P_{sat} \cdot \frac{M_w}{\rho_a RT}$$

$$K_{21} = \delta_p \cdot \phi \cdot \frac{\partial P_{sat}}{\partial T},$$

where t is time [s]; T is temperature [°C, K]; P_c is capillary pressure [Pa]; ρ is material density [kg/m³]; c is specific heat capacity [J/kgK]; λ is thermal conductivity [W/mK]; l_v is specific latent heat of evaporation [J/kg]; δ_p vapour permeability [s]; ϕ is relative humidity [-]; P_{sat} is saturation pressure [Pa]; $M_w = 0.018$ [kg/mol]; $R = 8.314$ [J/molK]; ρ_a is air density [kg/m³]; w is moisture content [kg/m³]; and K is liquid water permeability [s].

4. Rh Model

In the Rh model, the heat transport is described by the energy balance PDE presented in Equation (3).

The moisture transport is formulated to include relative humidity, ϕ , as the moisture potential. Accordingly, the total moisture transfer shown in Equation (2) is expressed in the following [2]:

$$g_v = -\delta_p \cdot p_{sat} \nabla \phi = -\delta_p \cdot p_{sat} \left(\frac{\partial \phi}{\partial x} \right) \quad (7)$$

$$g_\ell = -D_w \cdot \xi \nabla \phi = -D_w \cdot \xi \left(\frac{\partial \phi}{\partial x} \right)$$

Furthermore, the left-hand side of the PDE describing the moisture balance in Equation (4) is simplified in order to be a function of relative humidity. The simplification is accomplished by expanding the partial derivative of moisture content and introducing general definitions for moisture capacity and relative humidity:

$$\frac{\partial w}{\partial t} = \frac{\partial w}{\partial p} \cdot \frac{\partial p}{\partial t} = \frac{\partial w}{\partial p} \cdot \frac{\partial \varphi}{\partial p} \cdot \frac{\partial p}{\partial t}$$

$$\frac{\partial w}{\partial \varphi} = \xi \quad (8)$$

$$\varphi = \frac{p}{p_{\text{sat}}} \rightarrow \frac{\partial \varphi}{\partial p} = \frac{1}{p_{\text{sat}}}$$

These above relationships are subsequently introduced to yield the final form of the moisture balance equation for this model:

$$\xi \frac{\partial \varphi}{\partial t} = -\nabla \cdot ((-\delta_p \cdot p_{\text{sat}} - D_w \cdot \xi) \nabla \varphi) \quad (9)$$

As observed in Equation (9), the moisture balance is now expressed solely as a function of relative humidity.

Lastly, the boundary value problem is formulated with the inclusion of two Neumann boundary conditions, namely the convective thermal and hygric fluxes:

$$q_c = \alpha_c \cdot (T_s - T_a)$$

$$g_\varphi = \beta_\varphi \cdot (\varphi_s - \varphi_a) \quad (10)$$

where α_c is the convective heat transfer coefficient [W/m²K]; β_φ is the moisture transfer coefficient [kg/m²s]; subscript s denotes the surface boundary condition; and lastly, subscript a denotes the surrounding air boundary condition.

5. Use of COMSOL Multiphysics

The finite element method was used to evaluate coupled one-dimensional thermal and hygric transport by means of COMSOL. The Coefficient Form PDE Interface (c) multiphysics modeling tool was used to describe the combined transport mechanisms for both LPc and Rh models.

5.1 Modeling equations

The energy and moisture balance equations described for both models were simulated in COMSOL using the multiphysics modeling tool entitled Coefficient Form PDE Interface (c). This tool contains the feature of a scalar coefficient form equation that is described by a balance equation and boundary conditions. The simplified PDE problem neglecting convective heat transfer inside the material is described by the following:

$$d_a \frac{\partial u}{\partial t} = -\nabla \cdot (-c \nabla u) \quad \text{in } \Omega$$

$$n \cdot (c \nabla u) = g - h^T \mu \quad \text{on } \partial \Omega \quad (11)$$

$$u = r \quad \text{on } \partial \Omega$$

where u is a dependent variable on the computational domain Ω ; d_a is a damping/mass coefficient; c is a diffusion coefficient; g is a boundary source term; h is a boundary coefficient; μ is a Lagrange multiplier; n is an outward unit normal vector on the domain boundary $\partial \Omega$; and lastly, r is a known vector.

The dependent variable, u , can be expanded into a vector including two dependent variables describing both heat and moisture transports [2]:

$$u = \begin{bmatrix} T \\ LPc \end{bmatrix} \quad \text{or} \quad u = \begin{bmatrix} T \\ \varphi \end{bmatrix} \quad (12)$$

Furthermore, the damping and diffusion coefficients are accordingly expanded into vector form. For example, the following matrices describe the coefficients used in the Rh model:

$$d_a \cdot \frac{\partial u}{\partial t} = \begin{bmatrix} d_{a,T} & 0 \\ 0 & d_{a,\varphi} \end{bmatrix} \cdot \begin{bmatrix} \frac{\partial T}{\partial t} \\ \frac{\partial \varphi}{\partial t} \end{bmatrix} \quad (13)$$

With:

$$d_{a,T} = \rho c_p$$

$$d_{a,\varphi} = \xi$$

$$-\nabla \cdot (-c \cdot \nabla u) = \nabla \cdot \begin{bmatrix} c_T & 0 \\ 0 & c_\varphi \end{bmatrix} \cdot \begin{bmatrix} \nabla T \\ \nabla \varphi \end{bmatrix}$$

With: (14)

$$c_T = \lambda$$

$$c_\varphi = \delta_p \cdot p_{\text{sat}} + D_w \cdot \xi$$

Introducing the above coefficient matrices into the simplified PDE yields the following formulation:

$$\begin{bmatrix} \rho c_p & 0 \\ 0 & \xi \end{bmatrix} \begin{bmatrix} \frac{\partial T}{\partial t} \\ \frac{\partial \varphi}{\partial t} \end{bmatrix} + \begin{bmatrix} \lambda & 0 \\ 0 & \delta_p \cdot p_{\text{sat}} + D_w \cdot \xi \end{bmatrix} \begin{bmatrix} \nabla^2 T \\ \nabla^2 \varphi \end{bmatrix} \quad (15)$$

The methodology presented above is also applied to the LPc model. This formulation also holds for two- or three-dimensional cases, as well as non-isotropic materials. The directional properties can be described accordingly in the relevant coefficients.

6. Model Verification

The verification of the LPc and Rh models was completed by means of the normative benchmark test of European Provisional Standard prEN15026 [4]. This benchmark test is based on an analytical solution for one-dimensional coupled thermal and hygric transport in a homogeneous semi-infinite domain. Figure 1 shows the 20 m domain that is used for verification.

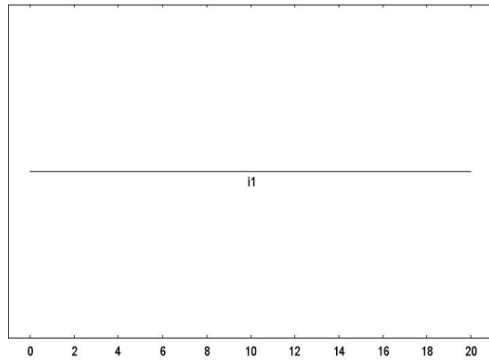


Figure 1. Overview of the domain used in the verification.

The exterior boundary of the domain is defined at 0 m, and as such the interior boundary is located at 20 m. As per the benchmark, the domain is in equilibrium with constant surrounding conditions of $T=20^{\circ}\text{C}$ and $Rh=50\%$. The domain is thereafter exposed to a step change to $T=30^{\circ}\text{C}$ and $Rh=95\%$ at the exterior boundary. The boundary conditions are introduced using Neumann boundary conditions, similar to those presented in Equation (10).

Boundary resistances and moisture sources (rain) are to be neglected according to the benchmark. Nonetheless, it is necessary to include heat and moisture transfer coefficients in the models to solve the PDE boundary value problem. The transfer coefficients were selected to ensure that constant boundary conditions are maintained during the numerical simulations. For example, low surface transfer coefficients were applied at the interior boundary in order to eliminate any influence

that the internal boundary conditions may have on the domain. Accordingly, the changes in the temperature and moisture distributions taking place from the exterior to the interior can be captured adequately in the numerical simulation profiles.

Temperature and moisture profiles after 7, 30 and 365 days are to be calculated by the model. These profile results are required to fall within $\pm 2.5\%$ of the analytical solution.

The hygrothermal material properties and general data used in the verification are specified by the prEN15026 benchmark test.

6.1 LPc model verification

MatLab is used for the implementation of the material functions. These functions are used to convert measurable material properties such as K , ϕ , δ_p and λ . These material properties are dependent on the moisture content into PDE coefficients and also dependent on the LPc and T. This is schematically shown in Figure 2.

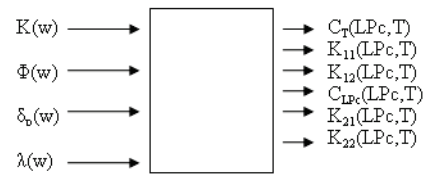


Figure 2. The conversion from measurable material properties into PDE coefficients.

The results of the conversion from material property into PDE coefficients are presented in Figure 3.

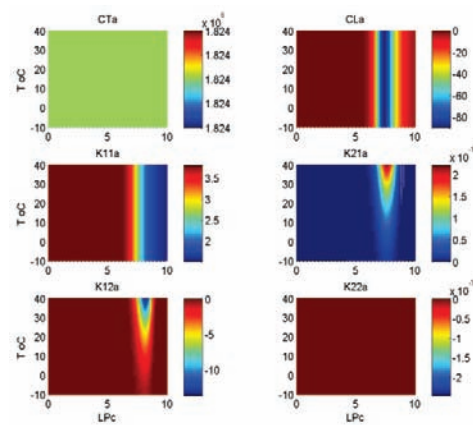


Figure 3. PDE coefficients CT, CLPc, Kij as functions of LPc and T calculated

At each point in the material the vapour pressure can be calculated using similar corresponding functions.

The governing PDE Equations (5) are implemented using the coefficients from Figure 3. Table 1 provides the specific boundary values, which are defined as Neumann type boundary conditions.

Table 1: Boundary conditions

No	Boundary condition
2 – 4	{0;0}
1	{ $100*(30*\text{flc2hs}(t,10)-T)$; $2e-8*(4037.5*\text{flc2hs}(t,10)-P_v(\text{LpC},T))$ }

In the boundary No. 1 condition, which corresponds to the interior boundary, the command flc2hs is implemented to create a Heaviside function. The vapour pressure p_v at the surface can be expressed as a function of LPc and T similar to the coefficients of Figure 2.

The numerical simulation included a calculation period of 1 year and time steps of 1 hour. A mesh containing 1639 triangular elements with at the exterior boundary a maximum element size of 0.001 and an element growth rate of 1.2 was observed to be quite sufficient.

The heat and moisture profile results pertaining to the LPc model were plotted for 7, 30, and 365 days against the required permissible error range specified by the benchmark. The numerical simulation results were found to meet the requirements stated by the benchmark as is depicted below in Figure 4 and Figure 5.

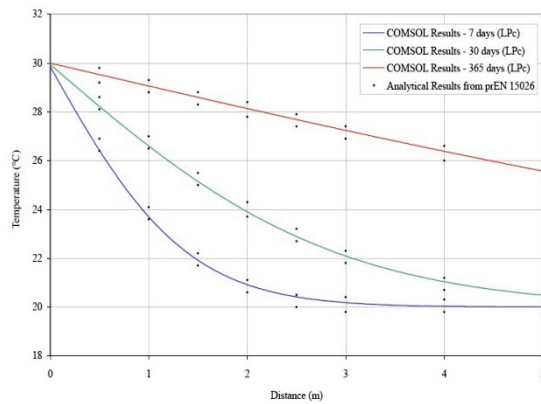


Figure 4. The numerically simulated temperature distribution calculated using the LPc model.

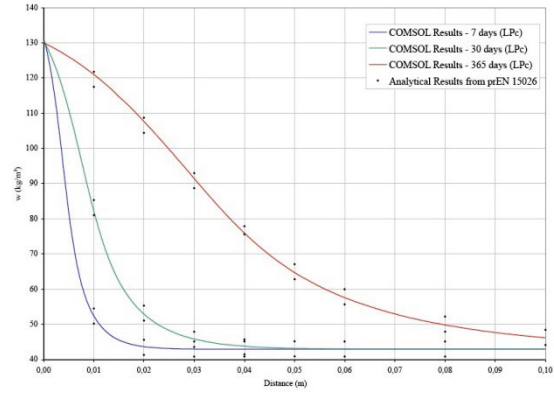


Figure 5. The numerically simulated moisture distribution calculated using the LPc model.

The LPc model is shown to be a valid predictive tool to investigate the impact of variable thermal and hygric conditions on building materials according to the verification results.

6.2 Rh model verification

In the Rh model, the initial and boundary conditions specified by the benchmark are introduced into COMSOL using global definitions. The heat and moisture transfer coefficients shown in Table 2 were selected to ensure constant boundary conditions in the calculations.

Table 2: Heat and moisture transfer coefficients used for the verification of the Rh model.

Name	Expression	Description
α_e	1.00E4 [W/m ² K]	Exterior heat transfer coefficient
α_i	1.11E-10 [W/m ² K]	Interior heat transfer coefficient (adiabatic)
β_e	1.00E2 [kg/m ² s]	Exterior moisture transfer coefficient
β_i	7.78E-5 [kg/m ² s]	Interior moisture transfer coefficient (adiabatic)

The material properties are tabulated and inputted into the Rh model by means of material interpolation functions defined in COMSOL.

The numerical simulation included a calculation period of 365 days and time steps of 3600 s. A mesh containing 1000 elements distributed with a geometric sequence and an element ratio of 10 was found to adequately

capture the rapidly decreasing moisture profile at the exterior boundary.

The heat and moisture profile results pertaining to the Rh model were plotted for 7, 30, and 365 days against the required permissible error range specified by the benchmark. In accordance with Figure 6 and Figure 7, the numerical simulation results meet the requirements stated by the benchmark.

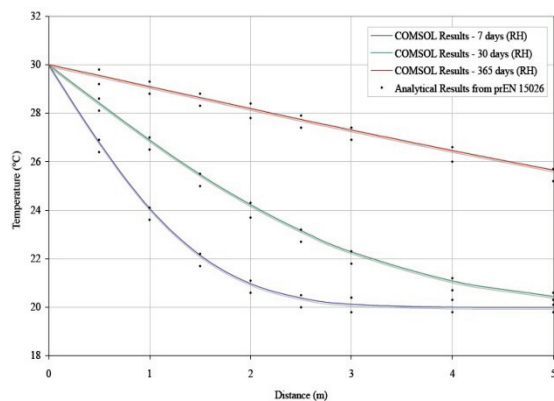


Figure 6. The numerically simulated temperature distribution calculated using the Rh model.

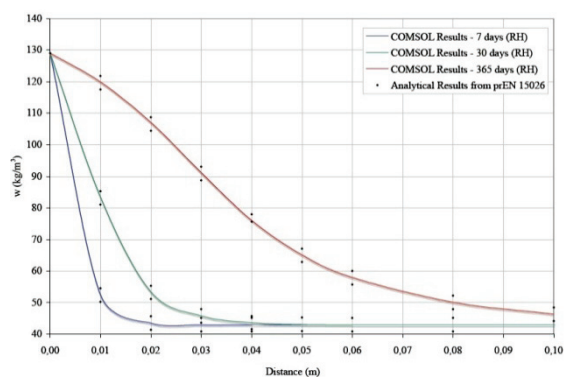


Figure 7. The numerically simulated moisture distribution calculated using the Rh model.

As such, this model appears to be a valid predictive tool to investigate the impact of variable thermal and hygric conditions on building materials.

7. Model Comparison

Although both models produce similar results, they differ in moisture potentials and space dimensions. A small comparison of the models using COMSOL 4.2.0.228: The LPc model consists of 290 elements, 1742 degrees of freedom and a solution time of 19 s. The Rh

model consists of 1000 elements, 4002 degrees of freedom solved and a solution time of 11 s.

8. Conclusions

Two types of moisture potentials used in the modeling of coupled heat and moisture transport: the natural logarithmic of the suction pressure (LPc) and the relative humidity (Rh) developed models were verified with the normative benchmark test of European Provisional Standard prEN 15026. These models appear to be valid predictive tools to investigate the impact of a change in climatic conditions on building materials and components.

The Rh based model has the advantage that the measured material properties can be directly implemented as functions in COMSOL. The disadvantage is that this model is numerical not suitable for liquid water fluctuations at the boundaries.

The LPc model is the best suitable for extreme conditions at the boundaries including liquid water fluctuations. The main disadvantage is the PDE coefficients are calculated from the measured material properties as using MatLab as a pre-processor. If an error occurs in this pre-processing phase, it could be challenging to notice possible errors from the PDE coefficient.

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