

# 3D Simulation of Heat and Moisture Diffusion in Constructions

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**Abstract:** The simulation of heat and moisture transfer represents an essential resource in designing energy efficient buildings. In this paper a time-dependent wall model, consisting of several homogeneous domains, with third-type boundary conditions imposed on the surfaces, is implemented in the COMSOL Multiphysics environment. Temperature and moisture content is calculated inside the construction for different materials and the results are compared with those of commercial heat and moisture transfer programs showing good agreement. The use of COMSOL Multiphysics compared to other commercially available programs is profitable, as it allows also the solution of more complex three-dimensional time-dependent problems. In this paper a model describing the heat and moisture transfer inside a wooden beam-end is addressed.

**Keywords:** Building physics, heat and moisture transfer, beam-end.

## 1. Introduction

The renovation of existing buildings according to high energy efficiency standards will represent a significant contribution concerning the increasing energy demand in our society (EPBD Recast 2010). In particular, solutions with internal insulation for historical buildings have to be developed [1]. However, such solutions require careful planning in order to avoid condensation formation and following degrading of the construction. Wooden elements crossing the insulation such as beam ends can represent critical subjects which require accurate investigation [2]. For this reasons the study of heat and moisture transfer through construction materials is becoming even more relevant in recent times.

Several authors have investigated the mechanisms of heat and moisture transfer through the various materials employed in standard buildings ([3], [4], [5]), numerical solutions have been proposed in order to calculate temperature and moisture content in constructions as function of time and position. Commercial programs specific for hygrothermal simulations are available as well ([6], [7]), however they are restricted to two dimensional problems and do not allow at all or only very limited modeling convective transfer mechanisms. Since convective effects such as in air gaps in the construction may have a relevant influence in many practical cases, a solution in this direction is urgently needed.

COMSOL Multiphysics represents the appropriate tool for the solution of this kind of problems, as it allows also the simulation of 3D geometries and high flexibility concerning the coupling with fluid domains. The capability of COMSOL for hygrothermal simulations has been yet shown by, however till now simplified mathematical models have been used [8].

In this paper a model describing all the transfer mechanisms relevant for the building physics is presented and cross-validated by comparing the results of COMSOL with those calculated with another commercial program.

In order to show the capability of COMSOL Multiphysics by handling transient three dimensional problems, the simulation of a beam-end is given as example.

## 2. Governing Equations and use of COMSOL Multiphysics

Heat and moisture transfer processes in porous materials can be 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. For the one-dimensional case the governing equations system assumes the following form:

$$\frac{\partial u}{\partial \varphi} \frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x} \left( -D_{m,\varphi} \frac{\partial \varphi}{\partial x} - D_{m,T} \frac{\partial T}{\partial x} \right) = 0 \quad (1)$$

$$\frac{\partial h}{\partial T} \frac{\partial T}{\partial t} + \frac{\partial h}{\partial \varphi} \frac{\partial \varphi}{\partial t} + \frac{\partial}{\partial x} \left( -D_{e,T} \frac{\partial T}{\partial x} - D_{e,\varphi} \frac{\partial \varphi}{\partial x} \right) = 0 \quad (2)$$

Temperature  $T$  and relative humidity  $\varphi$  are the dependent variables whereas  $t$  and  $x$  represent time and position.  $u$  is the moisture content and  $h$  the enthalpy.  $D_{m,\varphi}$ ,  $D_{m,T}$ ,  $D_{e,T}$  and  $D_{e,\varphi}$  are material specific diffusion coefficients which assume the following form:

$$D_{m,\varphi} = \frac{p_s D_v}{\mu R_v T} + K_l^* \frac{\partial p_c}{\partial \varphi} \quad (3)$$

$$D_{m,T} = \frac{\varphi D_v}{\mu R_v T} \frac{dp_s}{dT} \quad (4)$$

$$D_{e,T} = \lambda + (h_{lv} + c_{p,v} T) \frac{\varphi D_v}{\mu R_v T} \frac{dp_s}{dT} \quad (5)$$

$$D_{e,\varphi} = (h_{lv} + c_{p,v} T) \frac{p_s D_v}{\mu R_v T} \quad (6)$$

The derivation of the transport coefficients according to the theory of heat and moisture transfer is presented in the following section. The system of equations (1) and (2) can be solved with COMSOL Multiphysics using the PDE mode in the coefficients form. Temperature and relative humidity represent the dependent variables whereas position and time are the independent variables of the problem.

### 3. Theory of Heat and Moisture Transfer in Porous Materials

In this section the models that are employed to describe storage and transfer of heat and moisture in the material are described. As suggested by others authors ([3], [4], [9]) a macroscopic approach has been chosen as it allows porous materials to be treated as homogeneous media.

#### 3.1 Moisture Storage

The water content  $u$  inside a porous material can be represented as function of the relative humidity  $\phi$ , whereas its dependence from the temperature can be neglected in most cases (see *Figure 1*).

The relationship between  $u$  and  $\phi$  is described by the water retention curve, which is material-specific and can be obtained in experimental way as shown in [10]. This function has been imported in COMSOL using a linear interpolation method.

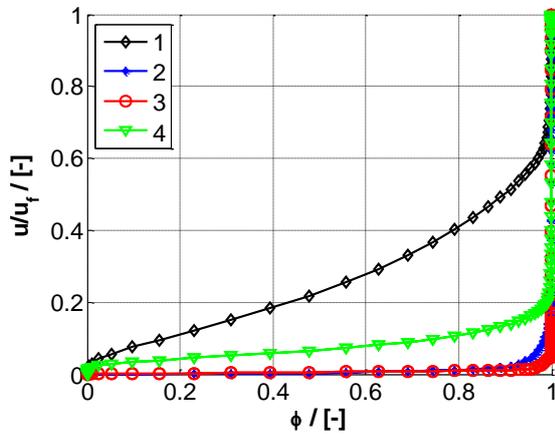


Figure 1 Water retention curve of concrete (1), brick (2), cellulose (3) und spruce(4)

#### 3.2 Enthalpy Storage

The enthalpy storage inside a volume element can be described through the following equation:

$$h = \rho_a c_{p,a} T - w \rho_a c_{p,a} T + w \rho_l c_l T + (w_f - w)(h_{lv} + c_{p,v} T) \rho_v \quad (7)$$

where  $h$ ,  $\rho$ ,  $c$  and  $T$  are the enthalpy, the density, the thermal capacity and the temperature respectively. The indices  $d$ ,  $a$ ,  $v$  and  $l$  represent the dry material (including solid matrix and air inside the pores), the

air replaced by liquid water, the vapor and liquid phase of water respectively. The volume fraction employed by liquid water  $w$  is defined by equation (8):

$$w = \frac{u}{\rho_l} \quad (8)$$

Under the condition of free moisture saturation,  $w$  assumes its maximal value  $w_f$ .

#### 3.3 Moisture Transfer

The mechanisms related to moisture transfer in porous materials are shown in *Figure 2*.

As noticed in [4], the mass transfer due to air pressure or hydraulic pressure differences and the effect of the gravity are negligible within the temperature and pressure ranges relevant for the building physics. Considering that the thermal diffusion can be neglected as well, the remaining transfer mechanisms include the vapor diffusion due to the vapor partial pressure gradient and the liquid flux concerning the capillary suction and the surface diffusion.

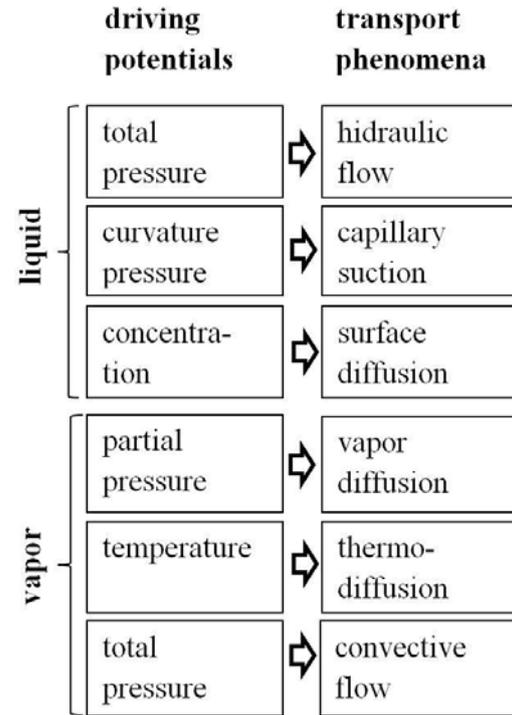


Figure 2 Moisture transfer phenomena in porous materials [10]

The diffusive vapor flux takes the following form according to [9]:

$$j_v = - \frac{D_v}{\mu R_v T} \frac{\partial p_v}{\partial x} \quad (9)$$

where  $p_v$  represents the partial pressure of vapor,  $D_v$  the diffusivity of vapor in air,  $\mu$  the vapor diffusion resistance factor and  $T$  the absolute temperature. Equation (10) gives the relation between the partial pressure of vapor  $p_v$ , the relative humidity  $\phi$  and the saturation pressure  $p_s$ , which is a function of the temperature:

$$p_v = \phi p_s(T) \quad (10)$$

From (9) and (10) it follows:

$$j_v = -\frac{\phi D_v}{\mu R_v T} \frac{dp_s}{dT} \frac{\partial T}{\partial x} - \frac{p_s D_v}{\mu R_v T} \frac{\partial \phi}{\partial x} \quad (11)$$

According to [4] the liquid flux  $j_l$  due to the capillary suction gradient can be described by (12):

$$j_l = -K_l \frac{\partial p_c}{\partial x} \quad (12)$$

where  $p_c$  represents the capillary pressure and  $K_l$  the liquid conductivity which is a material specific moisture dependent parameter.

This parameter is obtained in experimental way ([10], [7]). Equation (12) can be written in the following form, showing explicit the gradient of  $\phi$ .

$$j_l = -K_l \frac{\partial p_c}{\partial \phi} \frac{\partial \phi}{\partial x} = K_l^* \frac{\partial \phi}{\partial x} \quad (13)$$

The transport coefficient  $K_l^*$  is:

$$K_l^* = -K_l \frac{\partial p_c}{\partial \phi} \quad (14)$$

and is shown in Figure 3 taking concrete as an example.

The liquid flux represents a significant contribution to the whole moisture transfer for higher moisture contents.

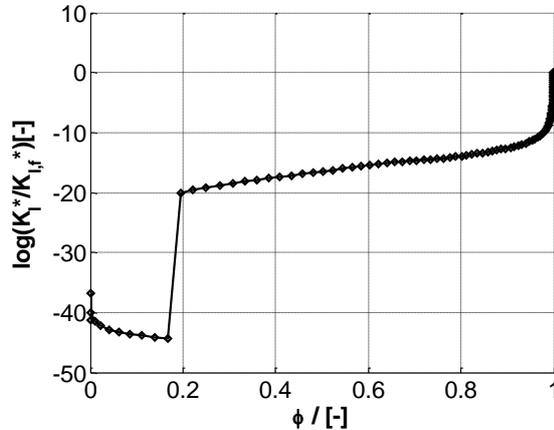


Figure 3 Liquid transfer coefficient  $K_l^*$  (concrete)

### 3.4 Energy Transfer

The energy transfer through a porous material can be described according to [4] by:

$$q = -\lambda \frac{\partial T}{\partial x} + (h_{lv} + c_{p,v}T)j_v \quad (15)$$

Where  $q$  represents the total energy flux and  $\lambda$  the real thermal conductivity of the material. The enthalpy flux due to mass transfer is represented by the term  $(h_{lv} + c_{p,v}T)j_v$ , where  $j_v$  represent the vapor flux. The contribute of the liquid flux can be neglected as observed in [4].

The real thermal conductivity of the moist material is a function of the water content, whereas its dependence on the temperature can be neglected for standard building physics problems.

## 4. Results

### 4.1 One-Dimensional Wall Model

For the cross-validation of the Comsol model with [7], a one dimensional case representing a double layer wall with cellulose insulation on the warm side and brick on the cold side is implemented.

The boundary conditions imposed on the surfaces are described by equations (16) and (17).

$$-D_{m,\phi} \frac{\partial \phi_k}{\partial x} - D_{m,T} \frac{\partial T_k}{\partial x} = \beta_k (p_{v,k} - p_{v,\infty,k}) \quad (16)$$

$$-D_{e,\phi} \frac{\partial \phi_k}{\partial x} - D_{e,T} \frac{\partial T_k}{\partial x} = \alpha_k (T_k - T_{\infty,k}) \quad (17)$$

With  $k = 1, 2$  representing left and right boundary. and:

		$k=1$	$k=2$
$T_{\infty,k}$	[°C]	$T_{\infty,1}(t)$	20
$\phi_{\infty,k}$	[-]	0.8	0.5
$\alpha_k$	[w/(m² K)]	25	10
$\beta_k$	[s/m]	2e-7	3e-8

$T_{\infty,1}(t)$  is a cosine curve with annual period. The main material properties are reported in the following table.

Table 1		Material properties	
		Brick	Cellulose
$\rho$	[kg/m³]	1979.11	55.21
$c$	[J/(kg K)]	833.76	2544.42
$\lambda$	[w/(m K)]	0.996	0.04
$\mu$	[-]	45.1	2.06
$u_f$	[kg/m³]	240.6	700

The results of Comsol are compared with those obtained with [7] showing good agreement. In Figure 4 and Figure 5 the profiles of relative humidity (water activity) and temperature, respectively, are shown at different time steps.

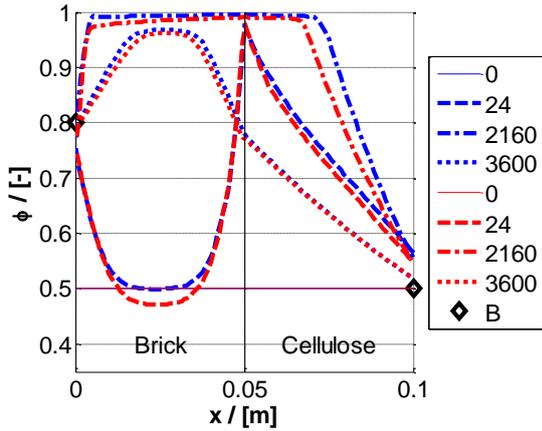


Figure 4 Profiles of relative humidity in the wall at different time steps (hours). Blue line: Comsol; red line: [7]; B: Boundary

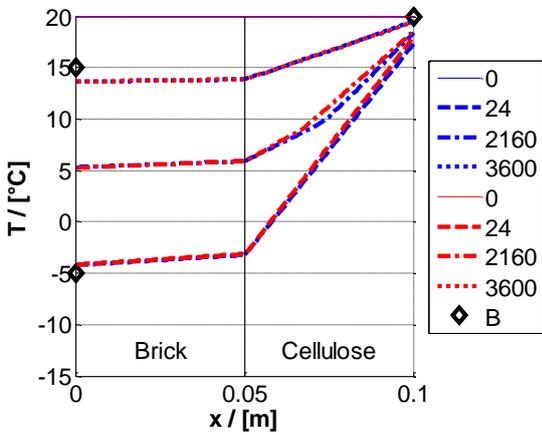


Figure 5 Profiles of temperature in the wall at different time steps (hours). Blue line: Comsol; red line: [7]; B: Boundary

In the considered case, the liquid flux  $j_l$  influence significantly the moisture distribution as can be observed comparing Figure 4 with Figure 6.

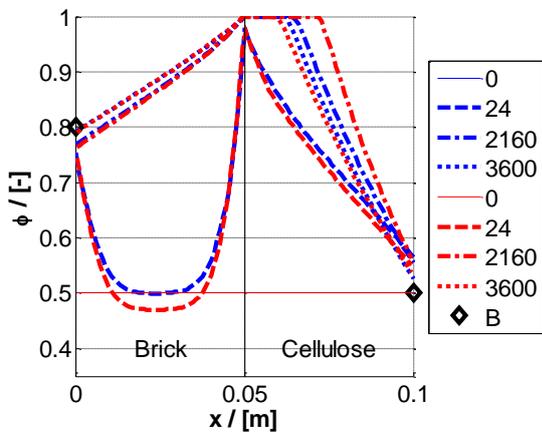


Figure 6 Profiles of relative humidity in the wall at different time steps (hours). Blue line: Comsol; red line: [7]; B: Boundary. Model without liquid transfer.

## 4.2 Beam-end Model

The three-dimensional wall model presented in this section don't refer to a real construction but is to be considered as a generic example. The materials employed in the simulation are concrete, PU foam (internal insulation) and spruce (beam). The main material properties are reported in Table 1. The three domains are shown in Figure 7. Two symmetry planes are used, as shown in Figure 8.

Table 2

		Material properties		
		Concrete	PU	Spruce
$\rho$	$[\text{kg}/\text{m}^3]$	2320.2	35	528.29
$c$	$[\text{J}/(\text{kg K})]$	850	1320	2000
$\lambda$	$[\text{W}/(\text{m K})]$	2.1	0.028	0.13
$\mu$	$[-]$	110	5	236.2
$u_f$	$[\text{kg}/\text{m}^3]$	143	950	695.4

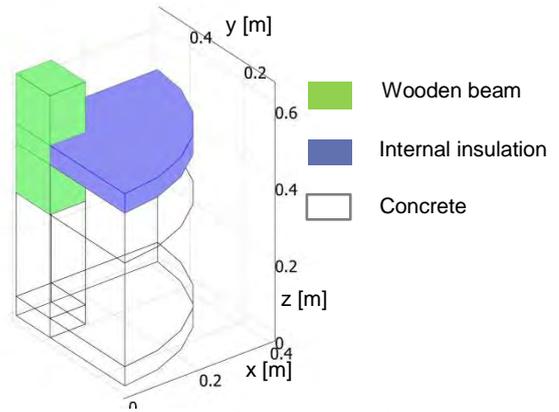


Figure 7 Domains of the beam-end model

Third kind boundary conditions are imposed on the internal and external surfaces according to equations (16) and (17).

The following initial conditions are employed:

$$T(0, x, y, z) = 20^\circ\text{C}$$

$$\varphi(0, x, y, z) = 0.5$$

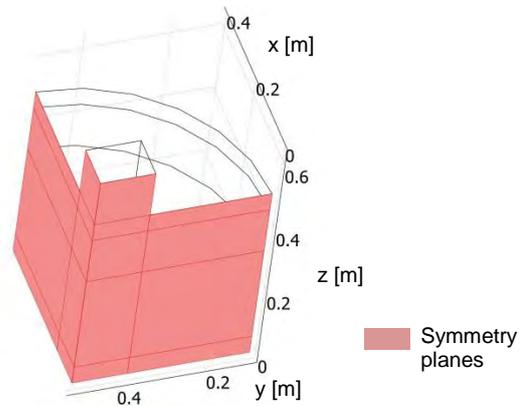
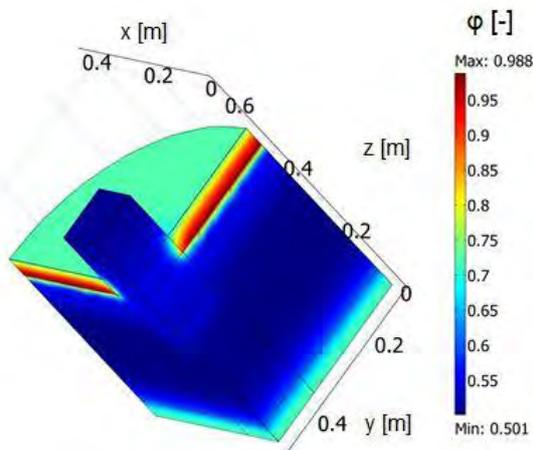


Figure 8 Symmetry planes

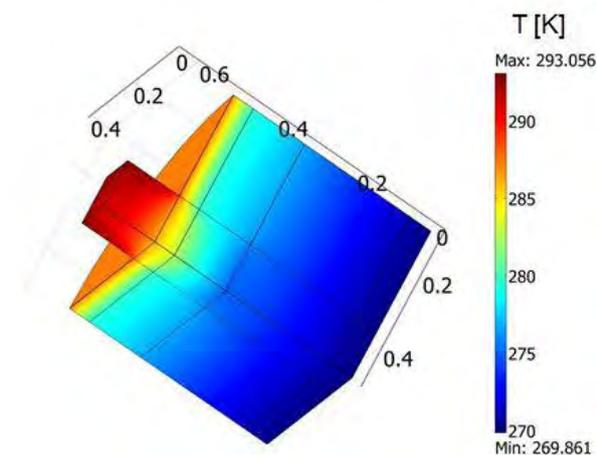
The moisture and temperature distribution over the wall after two years are shown in *Figure 9* and *Figure 10*.

In order to design the insulation properly with regard to appropriate thickness and material (e.g. capillary active), it is essential to predict the development of the moisture content inside the wooden beam and to identify the most critical position. Too high moisture content over prolonged periods of time would allow bacteria increasing and consequent wood damaging.

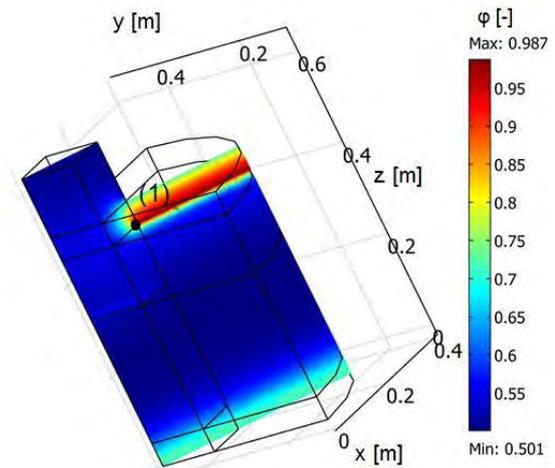
As expected, the point presenting highest humidity inside the wood is situated at the intersection of the beam edge with the interface plane between insulation and masonry (see *Figure 11*). The relative humidity development over two years is shown in *Figure 12*.



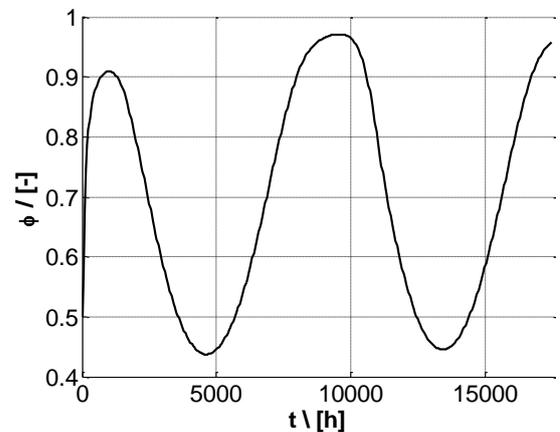
*Figure 9* Relative humidity distribution in the construction after two years



*Figure 10* Temperature distribution in the construction after two years



*Figure 11* Highest moisture content position in the wooden phase (Point 1)



*Figure 12* Relative humidity progress at point (1) over two years

## 5. Convection

Convection in cracks in the beam or in voids between the beam and the internal insulation has to be prevented or at least limited to non-critical values. The influence of convection through air gaps between beam and wall can be simulated assuming one-dimensional convective flux along the gap's axis. The driving equations describing this one-dimensional problem have to be coupled with the three-dimensional heat and moisture transfer in the construction. This coupling can be implemented in the COMSOL environment using the *weak form* on the boundary of the solid domain limiting the air gap and will concern future development.

## 6. Outlook

In this study it is shown that COMSOL Multiphysics is well suited for solving three-dimensional problems in the building physics such as to predict moisture condensation inside wooden beams.

The 1D and 2D models are cross-validated against commercially available programs. Validation of the 3D model against measured data will be part of future work in the framework of the EU-project 3ENCULT [11]

Further developments will concern the coupling with building models in order to allow for whole building simulations.

## 7. Nomenclature

$c$	$[J/(kg\ K)]$	Heat capacity
$D$	$[m^2/s]$	Diffusivity
$Dm, \varphi$	$[kg/(m\ s)]$	Transport coefficients
$Dm, T$	$[kg/(m\ s\ K)]$	
$De, \varphi$	$[w/m]$	
$De, T$	$[w/(m\ K)]$	
$h$	$[J/m^3]$	Enthalpy
$j$	$[kg/(m^2\ s)]$	Mass flux
$p$	$[Pa]$	Pressure
$q$	$[w/(m^2)]$	Heat flux
$R$	$[J/(kg\ K)]$	Gas constant
$t$	$[s]$	Time
$T$	$[K]$	Temperature
$u$	$[kg/m^3]$	Water content
$x, y, z$	$[m]$	Position
$\alpha$	$[w/(m^2\ K)]$	Heat transfer coefficient
$\beta$	$[s/m]$	Mass transfer coefficient
$\lambda$	$[w/(m\ K)]$	Heat conductivity
$\mu$	$[-]$	Vapor diffusion resistance
$\rho$	$[kg/m^3]$	Density
$\varphi$	$[-]$	Relative humidity

### Subscripts

$a$	Air
$c$	Capillary
$d$	Dry
$f$	Free saturation
$p$	Constant pressure
$l$	Liquid
$s$	Saturated
$v$	Vapor
$\infty$	Out of boundary layer

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