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IMPLEMENTATION OF FULLY COUPLED HEAT AND MASS TRANSPORT MODEL TO DETERMINE TEMPERTATURE AND MOISTURE STATE AT ELEVATED TEMPERATURES.

R. PECENKO[*], T. HOZJAN[*] AND S. SVENSSON[†]

[*] University of Ljubljana
Faculty of Civil and Geodetic Engineering
Department of Mechanics
Jamova 2, 1000 Ljubljana, Slovenia
e-mail: robert.pecenko@fgg.uni-lj.si

[†] Technical University of Denmark
Dept. Civil Engineering
Brovej 118, 2800 kgs. Lyngby, Denmark
email: nss@byg.dtu.dk

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Abstract. The aim of this study is to present precise numerical formulation to determine temperature and moisture state of timber in the situation prior pyrolysis. The strong formulations needed for an accurate description of the physics are presented and discussed as well as their coupling terms. From these the weak formulation is deducted. Based on the weak formulation two case studies are conducted. The results of this case is presented.

1 INTRODUCTION

In an open porous hygroscopic material such as wood, heat and moisture transport is a complex system of coupled processes. Inside timber, different phases of water can be observed, i.e., free water, bound water and gas phase of water (water vapour and air). Conservation equations for each phase with the exchange of mass between the different phases have to be considered. Different transfer phenomenon's can be applied for each phase. The bound water transfer model is assumed to follow Fick's law [1]. More complex is the transfer of gaseous mixture. Transfer of water vapour and air has to be combined by a convective and diffusive model of transport. For the convective part Darcy's law is usually applied and for the diffusive part Fick's law is used [2]. The free water constitutive relation is usually assumed to follow the generalized Darcy's law [3]. All three processes are connected with each other through the exchange of mass between the different phases, i.e., the conversion of vapour to free water and vice versa (condensation and evaporation), the conversion of vapour to bound water and vice versa (sorption) and the conversion of free water to bound water and vice versa. Thermal interaction on mass transfer is seen as temperature dependent diffusion coefficients where Fick's law is applied and temperature dependent mass velocity where Darcy's law is used as well as the Soret effect. The equations describing the conservation of mass must also be supplemented with an equation describing the conservation of enthalpy [2]. This equation takes three phenomena into account. Firstly, the usual conduction of heat thru solid, described by Fourier's law. Secondly, the changes in enthalpy resulting from change of phase, i.e. sorption, evaporation and condensation. And finally, the convective transfer of heat, i.e. the effect that heat is carried in the mass flux. These equations with corresponding initial and boundary conditions are generally non-linear and can rarely be if at all solved analytically. Therefore, numerical methods have to be employed.

2 CONSERVATION EQUATIONS

The coupled system of differential equations for heat and mass transport is derived from the following basic laws for mass and energy conservation.

- Free water conservation

$$\frac{\partial\left(\varepsilon_{FW}\rho_{FW}\right)}{\partial t}=-\nabla J_{FW}-\dot{E}_{FW} \tag{1}$$

- Bound water conservation

$$\frac{\partial c_b}{\partial t}=-\nabla J_b+\dot{c} \tag{2}$$

- Water vapour conservation

$$\frac{\partial\left(\varepsilon_G\tilde{\rho}_V\right)}{\partial t}=-\nabla J_V+\dot{E}_{FW}-\dot{c} \tag{3}$$

- Dry air conservation

$$\frac{\partial\left(\varepsilon_G\tilde{\rho}_A\right)}{\partial t}=-\nabla J_A \tag{4}$$

In eqs. (1) – (4), J_i and ε_i denotes the mass flux and the volume fraction of the phase *i*. Indices *FW*, *b*, *G*, *V* and *A* stands for free water, bound water, gaseous mixture, water vapour and air. ρ_i is phase density defined per unit volume of gaseous mixture, c_b the concentration of bound water, $\dot{E}_{FW}$ is the amount of vaporized free water and $\dot{c}$ is the sorption rate which within time interval *dt* represent the amount of water vapour absorbed to bound water or vice versa.

- Energy conservation equation

$$\left(\rho C\right)\frac{\partial T}{\partial t}=-\nabla\left(-k\nabla T\right)-\Delta h_{sorp}\dot{c}-\lambda_E\dot{E}_{FW}-\left(\rho Cv\right)\nabla T\ . \tag{5}$$

In the eq. (5) ρC denotes specific heat of timber, k is the coefficient of thermal conductivity of timber, Δh_{sorp} is heat of sorption, λ_E is latent heat of evaporation and ρCv represents the energy transport by fluid convection.

3 CONSTITUTIVE RELATIONS

3.1 Bound water

The model for temperature dependent bound water diffusion was proposed by [1]. The basic set of equations are:

$$J_B = -D_b \nabla c_b - D_{bT} \nabla T \tag{6}$$

$$D_b = D_b^0 \exp\left(\frac{-E_b}{RT}\right) \tag{7}$$

$$D_{bT} = D_b \frac{c_b E_b}{RT^2} \tag{8}$$

$$E_b = (38.5 - 29m) 1 \times 10^3 \tag{9}$$

$$m = \frac{c_b}{\rho_0} \tag{10}$$

In eqs. (6) – (10), D_b and D_{bT} are diffusion coefficient and thermal coupling bound water diffusion coefficient, R is universal gas constant, E_b the activation energy for bound water diffusion, m moisture content and ρ_0 dry density of wood.

3.2 Free water

The free water flux is described by Darcy's law:

$$J_{FW} = \rho_{FW} v_{FW} \tag{11}$$

$$v_{FW} = \frac{K\, K_{FW}}{\mu_{FW}} \nabla P_{FW} \tag{12}$$

Velocity of free water v_{FW} is defined by specific permeability of dry wood K, relative permeability of water K_{FW}, dynamic viscosity of water μ_{FW} and partial pressure gradient of water ∇P_{FW}.

3.2 Water vapour and air

Water vapour and air fluxes are defined by contribution of diffusion (Fick's law) and convection (Darcy's law).

$$J_A = \varepsilon_G \tilde{\rho}_A v_G - \varepsilon_G \tilde{\rho}_G D_{AV} \nabla \left(\frac{\tilde{\rho}_A}{\tilde{\rho}_G} \right) \tag{13}$$

$$J_V = \varepsilon_G \tilde{\rho}_V v_G - \varepsilon_G \tilde{\rho}_G D_{AV} \nabla \left(\frac{\tilde{\rho}_V}{\tilde{\rho}_G} \right) \tag{14}$$

In the eq. (13) – (14), D_{AV} represents the diffusion of air or vapour in the gaseous mixture. The expression is proposed by [4]:

$$D_{AV} = \xi 1.87 \left(\frac{T^{2.072}}{P_G} \right) \cdot 10^{-5}, \tag{15}$$

where ξ represents the estimated reduction factor due to the hindrance of the diffusion in the cellular structure. ξ is material direction dependent. Velocity of gaseous mixture is defined by Darcy's law.

$$v_G = \frac{K\,K_G}{\mu_G} \nabla P_G\,, \tag{16}$$

where the partial pressure of gaseous mixture is according to Dalton's law the sum of partial pressure of air and partial pressure of water vapour: $P_G = P_V + P_A$. The pressures are assumed to follow thei deal gas law:

$$P_A = R_A \tilde{\rho}_A T\,. \tag{17}$$

$$P_V = R_V \tilde{\rho}_V T\,. \tag{18}$$

3.2 Sorption

Sorption occurs when the driving potentials in the two phases, i.e. water vapour and bound water, are not in equilibrium. Here the Hailwood-Horrobin isotherm is applied:

$$m = \frac{h}{f_1 + f_2 h + f_3 h^2}\,, \tag{19}$$

where h is the humidity, it is defined as ratio between partial pressure of water vapour P_V and saturated vapour pressure P_{SAT}.

$$h = \frac{P_V}{P_{SAT}}\,. \tag{20}$$

The bound water concentration c_b can be compared to the bound water concentration in equilibrium with the vapour pressure P_V, which is denoted as c_{bl}:

$$c_{bl} = m\rho_0 . \tag{21}$$

Model for sorption rate was proposed by [1] and here modified for temperatures above 100°C:

$$\dot{c} = \begin{cases} H_c \left(c_{bl} - c_b\right) & T \leq 100°\mathrm{C} \\ H_c \left(0 - c_b\right) & T > 100°\mathrm{C} \end{cases}, \tag{22}$$

where:

$$H_c = \begin{cases} C_1 \exp\left(-C_2 \left(\frac{c_{bl}}{c_b}\right)^{C_3}\right) + C_4 & c_b < c_{bl} \\ C_1 \exp\left(-C_2 \left(2 - \frac{c_{bl}}{c_b}\right)^{C_3}\right) + C_4 & c_b < c_{bl} \end{cases}, \tag{23}$$

and:

$$C_2 = C_{21} \exp\left(C_2 h\right), \tag{24}$$

4 SYSTEM OF DIFERENTIAL EQUATIONS

By summing eq. (1) and (3) the system of equations is reduced to four. The chosen primary unknown variables are T , P_G , $\tilde{\rho}_V$ and c_b. After some algebraic manipulation, the system of differential equations can be written in a form suitable for a finite element solution.

$$C_{TT} \frac{\partial T}{\partial t} + C_{TP} \frac{\partial P_G}{\partial t} + C_{TV} \frac{\partial \tilde{\rho}_V}{\partial t} + C_{TB} \frac{\partial c_b}{\partial t} = \nabla\left(K_{TT} \nabla T + K_{TP} \nabla P_G + K_{TV} \nabla \tilde{\rho}_V + K_{TB} \nabla c_b\right) - \\ - K_{TVV} \nabla T . \tag{25}$$

$$C_{PT} \frac{\partial T}{\partial t} + C_{PP} \frac{\partial P_G}{\partial t} + C_{PV} \frac{\partial \tilde{\rho}_V}{\partial t} + C_{PB} \frac{\partial c_b}{\partial t} = \nabla\left(K_{PT} \nabla T + K_{PP} \nabla P_G + K_{PV} \nabla \tilde{\rho}_V + K_{PB} \nabla c_b\right). \tag{26}$$

$$C_{VT} \frac{\partial T}{\partial t} + C_{VP} \frac{\partial P_G}{\partial t} + C_{VV} \frac{\partial \tilde{\rho}_V}{\partial t} + C_{VB} \frac{\partial c_b}{\partial t} = \nabla\left(K_{VT} \nabla T + K_{VP} \nabla P_G + K_{VV} \nabla \tilde{\rho}_V + K_{VB} \nabla c_b\right). \tag{27}$$

$$C_{BT} \frac{\partial T}{\partial t} + C_{BP} \frac{\partial P_G}{\partial t} + C_{BV} \frac{\partial \tilde{\rho}_V}{\partial t} + C_{BB} \frac{\partial c_b}{\partial t} = \nabla\left(K_{BT} \nabla T + K_{BP} \nabla P_G + K_{BV} \nabla \tilde{\rho}_V + K_{BB} \nabla c_b\right). \tag{28}$$

Comparing to the other equations, the eq. (25) is additionally accounted by $K_{TVV} \nabla T$. In this term energy transport by fluid convection is considered.

4.1 Boundary conditions

It is assumed that the water vapor concentration at the (imaginary) boundary between surrounding air and pores (lumens) at a macroscopic surface is identical to the partial vapor pressure of ambient air. Dirichlet boundary condition is applied:

$$\tilde{\rho}_V = \tilde{\rho}_{V,\infty} . \tag{29}$$

Also the pressure on the boundary surface is equal to the atmospheric pressure:

$$P_G = P_{G,\infty} . \tag{30}$$

The bound water is restricted to the wood cell wall and is only exchanged by sorption, therefore the Neumann boundary condition is applied, accordingly to:

$$\mathrm{n} \cdot J_b = 0 . \tag{31}$$

Boundary condition for heat transfer:

$$k \frac{\partial T}{\partial n} = -h_{qr} \left(T - T_\infty \right) . \tag{32}$$

5 FINITE ELEMENT FORMULATION

In the matrix form the system of eqs. (25) – (28) can be written:

$$C \frac{\partial u}{\partial t} - \nabla \left(K \nabla u \right) + K_V \nabla u = 0 , \tag{33}$$

with boundary conditions:

$$\frac{\partial u}{\partial n} = R_\infty - R_k u , \tag{34}$$

In the above eq., u is vector of basic unknowns $\left[T, P_G, \tilde{\rho}_V, c_b \right]$, matrices C and K contains coefficients C_{ij} and K_{ij} (i,j = T, P, V, b), matrix K_V contain only coefficient K_{VTT}, other components of matrix are equal to zero.

The finite element solution is based on approximation of the unknown vector function:

$$u = \sum_{i=1}^{n_{node}} N y^i , \tag{35}$$

where N denotes a matrix of polynomial shape functions, y is vector of discrete node unknowns. Using Galerkin method and integration by parts, the system (33) can be rewritten on the equivalent system of differential equation of first order:

$$\hat{C} \frac{\partial y}{\partial t} - \hat{K} y = \hat{F} , \tag{36}$$

where

$$\hat{C} = \sum_{e=1}^{n_{el}} \hat{C}^e ; \qquad \hat{K} = \sum_{e=1}^{n_{el}} \hat{K}^e + \hat{K}_V^e + \hat{K}_R^e ; \qquad \hat{R} = \sum_{e=1}^{n_{el}} \hat{R}^e ; \qquad u = \sum_{e=1}^{n_{el}} u^e , \tag{37}$$

$$\hat{C}^e = \int_{\Omega_e} N^T C^e N d\Omega; \quad \hat{K}^e = \int_{\Omega_e} \nabla N^T K^e \nabla N d\Omega; \quad \hat{K}_V^e = \int_{\Omega_e} N^T K_V^e \nabla N d\Omega; \tag{38}$$

$$\hat{K}_R^e = \int_{\Gamma_e} N^T K^e R_k^e N d\Gamma; \qquad \hat{R}^e = \int_{\Gamma_e} N^T K^e R_\infty^e d\Gamma\,, \tag{39}$$

A finite difference scheme is used for the time discretisation. The calculation time is divided on time increments $\left[t^{k-1}, t^k\right]$, within each time interval linear variation of nodal quantities is assumed. The eq. (30) has to be satisfied in each time step, i.e., at the time $t^k = t^{k-1} + \mu\Delta t$. Δt is the magnitude of time step and μ is predefined time step: $\mu = 0$ (explicit method), $\mu = 1/2$ (Crank-Nicolson method), $\mu = 2/3$ (Galerkin method), $\mu = 1$ (implicit method). Considering time discretisation leads system (36) to:

$$\tilde{C}^k y^k = \tilde{F}^k, \tag{40}$$

$$\tilde{C}^k = \mu\hat{K} + \tfrac{1}{\delta t}\hat{C} \quad \text{and} \quad \tilde{F}^k = \left[\tfrac{1}{\delta t}\hat{C} - (1-\mu)\hat{K}\right] y^{k-1} + (1-\mu)\hat{F}^k + \mu\hat{F}^{k-1}. \tag{41}$$

The system is solved iteratively in each time step. Implicit method is applied.

6 EXAMPLE

The example presents the spatial and time development of temperature and moisture state of timber specimen exposed to varying outside conditions. Size of timber specimen is b/L = 1/5 cm, it is modeled with 200 four-node quadrilateral finite elements. Temperature and water vapour boundary condition are shown in Fig.1. On the exposed side the emissivity of timber surface and convection factor are $\varepsilon = 0.7$ and $h_q = 25$ W/m^{2}K. Thermal conductivity of timber is taken in accordance with [5]. Other parameters are shown in table 1.It should be noted that in this case free water within the specimen was not taken into account.

Table 1: Input data

$\rho_0 = 500\,\text{kg/m}^3$	$\rho_{FW} = 1000\,\text{kg/m}^3$	$R = 8.3144\,\text{J/molK}$	$K = 1\cdot 10^{-16}$
$K_G = 1$	$R_A = 287\cdot 10^{-16}\,\text{J/kgK}$	$R_V = 461.5\cdot 10^{-16}\,\text{J/kgK}$	$\xi = 0.03$ (tangential direction)
$D_b^0 = 7\cdot 10^{-6}\,\text{m}^2/\text{s}$			
Initial values are:			
$c_{b0} = 4.15\,\text{kg/m}^3$	$\tilde{\rho}_{V,0} = 0.0113\,\text{kg/m}^3$	$P_{G,0} = 0.1\,\text{MPa}$	$T_0 = 23°\text{C}$
Sorption parameters:			
$f_1 = 2.22$	$f_2 = 15.7$	$f_3 = -14.7$	$C_1 = 2.7\cdot 10^{-4}$
$C_{21} = 2.74\cdot 10^{-5}$	$C_{22} = 19$	$C_3 = 60$	$C_4 = 1\cdot 10^{-7}$

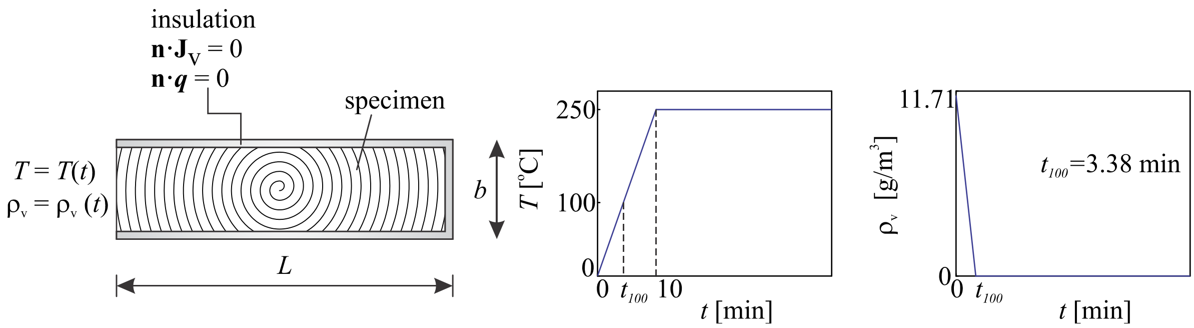

Figure 1: Boundary conditions

The results at different specimen location are show in Fig.2

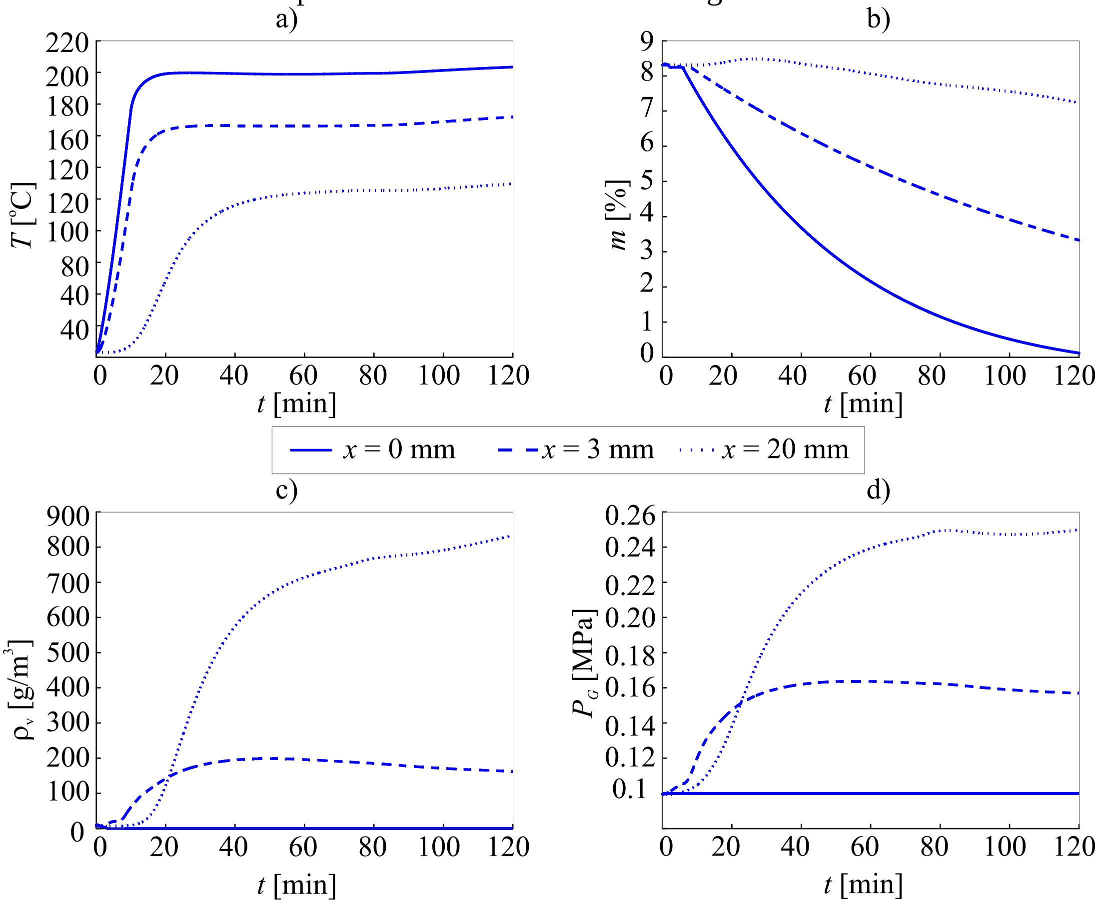

Figure 2: Temperature, moisture content, water vapour and pore pressures distribution over time in different specimen location

The increase of temperatures inside of specimen is expected. Maximum observed temperatures at points 1, 2 and 3 (x=0 mm, x=3 mm and x=20 mm) are 200°C, 160°C and 120°C. The increase is faster for point 1. Partial pressure of gaseous mixture is approximated by the ideal gas law, and it is directly correlated to the temperature. This correlation is well observed in Fig.2(d) where the increase of temperatures results in the increase of pressure inside the specimen. As mentioned, sorption occurs where driving potentials in the two phases are not in equilibrium. At elevated temperatures, the water vapour migrates much faster than bound water, consequently the driving potential between the two phases and sorption increases. In eq.(22) it is assumed that for temperatures above 100°C, only desorption can occur. It is considered that the pressure does not have any impact on sorption. The result of all phenomenons is phase change of bound water into water vapour. Fig.2(b) and Fig.2(c) present all this processes described. As the moisture content decreases with time, the concentration of water vapour increases. Fig.(3) present the variables distribution along the specimen for different times.

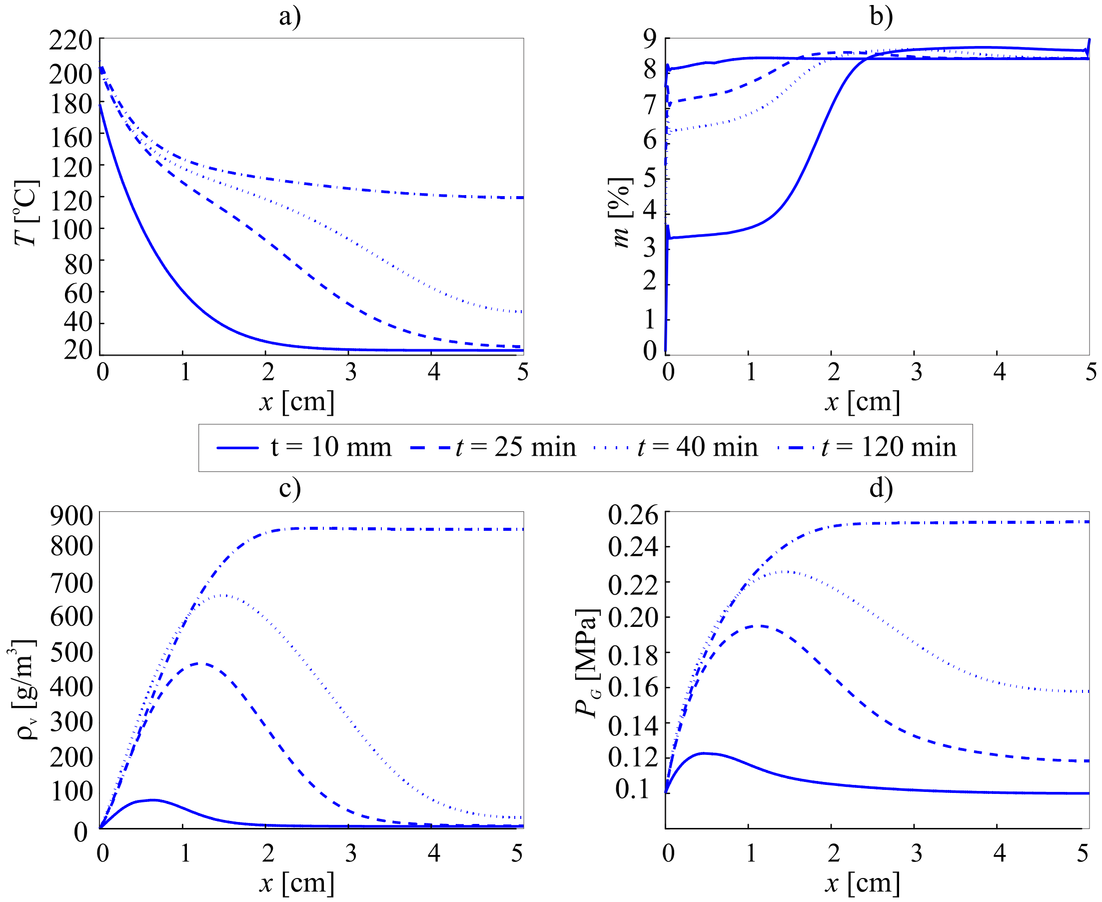

Figure 3: Temperature, moisture content, water vapour and pore pressures distribution along the specimen for different times

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