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# NUMERICAL ANALYSIS OF COUPLED HEAT AND MOISTURE TRANSFER BASED ON KUNZEL MODEL

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**Abstract:** *Coupled heat and moisture transfer is still more often used in many civil engineering problems. In connection with concrete and plasters, the Künzel model is very popular. Unfortunately, very different orders of material parameters have devastating influence on the condition number of matrices obtained after space and time discretization of problems. It results in severe numerical difficulties. This contribution deals with some strategies leading to better numerical behaviour of the coupled transport processes.*

**Keywords:** ***coupled heat and moisture transport, Künzel model, condition number, non-symmetric systems of equations.***

## 1. Introduction

Continuous rapid development of computers enables solution of very complicated and complex problems. Whereas single-physics problems dominated in the past because of limited computer power, multi-physics problems have become a standard in recent years. In civil engineering, the multi-physics problems are usually represented by hydro-thermo-mechanical problems. The coupled heat and moisture transfer is used in connection with concrete ageing, problems in soils and rocks, plaster design, reconstruction of historical buildings, etc.

In the past, the temperature and moisture distribution in structures was estimated and the temperature and relative humidity or the water content were assumed as material parameters of mechanical models. Nowadays, simultaneous analysis of mechanical behaviour together with the temperature and moisture distribution can be performed.

There are several models of heat and moisture transfer depending whether the convection or diffusion phenomena prevails. Comprehensive list of models can be found in reference Černý and Rovnaníková (2002). The coupled heat and moisture transfer in buildings or building components is usually described by the Künzel model which is summarized in section 2.

The material coefficients depend on the actual values of temperature and relative humidity and they are not constant. It means, the conductivity matrix of material has to be computed in every time step. In some configurations, the conductivities are very small and it leads to serious numerical problems because there are zero diagonal matrix entries. In such cases, appropriate degrees of freedom should be removed from the system and they can be returned back when the conductivities become physically important.

## 2. Künzel model of coupled heat and moisture transport

In 1995, Künzel proposed in reference Künzel (1995) a model of coupled heat and moisture transfer suitable for building components.

The Künzel model of coupled heat and moisture transport is based on the relative humidity, $\varphi$, and temperature, $T$. Instead of the relative humidity, water content, $w$, can be also used but it is generally non-continuous variable while the relative humidity is always continuous. The continuity of a variable is

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an advantage in the finite element method. The relative humidity is defined by the relationship

$$\varphi = \frac{p_v}{p_{vs}(T)} \,, \tag{1}$$

where $p_v$ denotes the partial pressure of water vapour and $p_{vs}(T)$ denotes the saturated water vapour pressure which depends on the temperature. The water content, $w$, can be expressed as a function of the relative humidity, $\varphi$. The partial pressure of saturated water vapour in the air has the form

$$p_{vs}(T) = e^{23{,}5771 - \frac{4042{,}9}{T - 37{,}58}} \,. \tag{2}$$

The vapour diffusion flux density has the form

$$\boldsymbol{q}_v = D_m \nabla m + D_T \nabla T \approx D_m \nabla m = -\delta \nabla p_v \,, \tag{3}$$

where $D_m$ (kg/m/s) is the mass-related diffusion coefficient, $m$ (-) is the mass fraction of water vapour related to the total mass of the vapour and air mixture, $D_T$ (kg/m/s/K) is the thermo-diffusion coefficient, $T$ is the temperature, $\delta$ (kg/m/s/Pa) is the water vapour diffusion coefficient in air, $p_v$ (Pa) denotes the water vapour partial pressure. The contribution $D_T \nabla T$ is usually negligible and the mass fraction of water vapour related to the total mass of the vapour and air mixture can be replaced by the water vapour partial pressure. The water vapour diffusion coefficient in air has the form

$$\delta = \frac{2{,}306.10^{-5}}{R_v T} \left( \frac{T}{273{,}15} \right)^{1{,}81} \,, \tag{4}$$

where $R_v = 461{,}5$ J/K/kg. Furthermore, in the case of small capillaries, water vapour diffusion resistance factor, $\mu$, has to be introduced and the vapour diffusion flux density has the form

$$\boldsymbol{q}_v = -\frac{\delta}{\mu} \nabla p_v = -\delta_p \nabla p_v \,, \tag{5}$$

where $\delta_p$ (kg/m/s/Pa) denotes the water vapour permeability. With the help of (1), the vapour diffusion flux density can be written in the form

$$\boldsymbol{q}_v = -\delta_p \nabla p_v = -\delta_p p_{vs} \nabla \varphi - \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T} \nabla T \,. \tag{6}$$

Liquid conduction is described by the liquid flux density (kg/m$^2$/s) in the form

$$\boldsymbol{q}_l = -D_w(w) \nabla w \,, \tag{7}$$

where $D_w(w)$ (m$^2$/s) denotes the capillary transport coefficient. The liquid conduction can be also described by the Darcy's formula

$$\boldsymbol{q}_l = K_1 \nabla p_k \,, \tag{8}$$

where $K_1$ (kg/m/s/Pa) is the permeability coefficient and $p_k$ (Pa) denotes the capillary suction stress. With the help of Kelvin's formula, the capillary suction stress can be written in the form

$$p_k = -\varrho_w R_0 T \ln \varphi \,, \tag{9}$$

where $\rho_w$ (kg/m$^3$) is the density of water and $R_0$ (J/kg/K) denotes the gas constant for water vapour. Equation (8) can be rearranged into new form

$$\boldsymbol{q}_l = -K_1 \varrho_w R_0 \ln \varphi \nabla T - K_1 \varrho_w R_0 T \frac{1}{\varphi} \nabla \varphi \approx -K_1 \varrho_w R_0 \frac{T}{\varphi} \nabla \varphi \,. \tag{10}$$

The term $K_1 \varrho_w R_0 \ln \varphi \nabla T$ is significantly smaller than the other and therefore it is usually neglected. The liquid flux density can be also written in the form

$$\boldsymbol{q}_l = -D_\varphi \nabla \varphi \,, \tag{11}$$

where $D_\varphi$ (kg/m/s) is the liquid conduction coefficient. Comparison of (11), (7) and (10) reveals relationships among the particular material parameters

$$D_\varphi = D_w \frac{\mathrm{d}w}{\mathrm{d}\varphi} = K_1 \varrho_w R_0 \frac{T}{\varphi} \,. \tag{12}$$

Balance equation for the moisture has the form

$$\frac{\partial w}{\partial t} = -\mathrm{div}(\boldsymbol{q}_l + \boldsymbol{q}_v) + S_w \,, \tag{13}$$

where $S_w$ (kg/m$^3$/s) denotes the moisture source or sink. Substitution of (11) and (6) into the balance equation (13) results in

$$\begin{aligned} \frac{\partial w}{\partial t} &= \mathrm{div}\left( D_\varphi \nabla\varphi + \delta_p p_{vs} \nabla\varphi + \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T} \nabla T \right) + S_w = \\ &= \mathrm{div}\left( \left(D_\varphi + \delta_p p_{vs}\right) \nabla\varphi + \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T} \nabla T \right) + S_w \,. \end{aligned} \tag{14}$$

The time derivate on the left hand side can be further modified

$$\frac{\partial w}{\partial t} = \frac{\mathrm{d}w}{\mathrm{d}\varphi} \frac{\partial \varphi}{\partial t} = h_{\varphi\varphi} \,. \tag{15}$$

Heat transport is described by the well known balance equation

$$\frac{\partial H}{\partial t} = \frac{\partial (H_s + H_w)}{\partial t} = -\mathrm{div}\boldsymbol{q}_T + S_h \,, \tag{16}$$

where $H$ (J/m$^3$) denotes the total enthalpy, $H_s$ (J/m$^3$) denotes the enthalpy of dry material, $H_w$ (J/m$^3$) denotes the enthalpy of material moisture, $\boldsymbol{q}_T$ (J/m$^2$/s=W/m$^2$) denotes the heat flux density and $S_h$ (W/m$^3$) denotes the heat source or sink. The Fourier law has the form

$$\boldsymbol{q}_T = -\lambda \nabla T \,, \tag{17}$$

where $\lambda$ (W/m/K) denotes the thermal conductivity of the moist material and $T$ (K) denotes the temperature. The source or sink of heat can be written in the form

$$S_h = -h_v \mathrm{div}\boldsymbol{q}_v \,, \tag{18}$$

where $h_v$ (J/kg) denotes the latent heat of phase change and $\boldsymbol{q}_v$ (kg/m$^2$/s) denotes the vapour diffusion flux density.

With respect to (6), the balance equation has the form

$$\begin{aligned} \frac{\partial H}{\partial t} &= -\mathrm{div}\boldsymbol{q}_T + S_h = \mathrm{div}(\lambda \nabla T) + h_v \mathrm{div}\left( \delta_p p_{vs} \nabla\varphi + \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T} \nabla T \right) = \\ &= \mathrm{div}\left( \lambda \nabla T + h_v \delta_p p_{vs} \nabla\varphi + h_v \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T} \nabla T \right) = \\ &= \mathrm{div}\left( h_v \delta_p p_{vs} \nabla\varphi + \left( \lambda + h_v \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T} \right) \nabla T \right) \,. \end{aligned} \tag{19}$$

Similarly to the mass balance equation, the left hand side can be written in the form

$$\frac{\partial H}{\partial t} = \left( \frac{\mathrm{d}H_s}{\mathrm{d}T} + \frac{\mathrm{d}H_w}{\mathrm{d}T} \right) \frac{\partial T}{\partial t} = \left( \varrho C + \frac{\mathrm{d}H_w}{\mathrm{d}T} \right) \frac{\partial T}{\partial t} = h_{TT} \,, \tag{20}$$

where $\varrho$ (kg/m$^3$) denotes the density of material and $C$ (J/kg/K) is the heat capacity coefficient.

Let new notation be introduced in the form

$$\begin{pmatrix} \boldsymbol{q}_\varphi \\ \boldsymbol{q}_T \end{pmatrix} = \begin{pmatrix} \boldsymbol{D}_{\varphi\varphi} & \boldsymbol{D}_{\varphi T} \\ \boldsymbol{D}_{T\varphi} & \boldsymbol{D}_{TT} \end{pmatrix} \begin{pmatrix} \boldsymbol{g}_\varphi \\ \boldsymbol{g}_T \end{pmatrix} = \\ = \begin{pmatrix} D_\varphi + \delta_p p_{vs} & \delta_p \varphi \dfrac{\mathrm{d}p_{vs}}{\mathrm{d}T} \\ h_v \delta_p p_{vs} & \lambda + h_v \delta_p \varphi \dfrac{\mathrm{d}p_{vs}}{\mathrm{d}T} \end{pmatrix} \begin{pmatrix} \nabla\varphi \\ \nabla T \end{pmatrix} . \tag{21}$$

With the new notation, the balance equations have the form

$$h_{\varphi\varphi} \frac{\partial \varphi}{\partial t} = \operatorname{div} \left( \boldsymbol{D}_{\varphi\varphi} \nabla\varphi + \boldsymbol{D}_{\varphi T} \nabla T \right) , \tag{22}$$

$$h_{TT} \frac{\partial T}{\partial t} = \operatorname{div} \left( \boldsymbol{D}_{T\varphi} \nabla\varphi + \boldsymbol{D}_{TT} \nabla T \right) . \tag{23}$$

## 3. Initial and boundary conditions

The balance equations (22) and (23) are valid in domain $\Omega$ which has boundary $\Gamma$. The boundary of the domain $\Omega$ is split into parts $\Gamma_T$, $\Gamma_\varphi$, where the Dirichlet boundary conditions are prescribed (prescribed values), $\Gamma_{qT}$, $\Gamma_{q\varphi}$, where the Neumann boundary conditions are prescribed (prescribed fluxes) and $\Gamma_{NT}$ and $\Gamma_{N\varphi}$, where the Newton (Cauchy) boundary conditions are prescribed. The parts $\Gamma_T$, $\Gamma_{qT}$ and $\Gamma_{NT}$ are disjoint and their union is the whole boundary $\Gamma$. The same is valid for the parts $\Gamma_\varphi$, $\Gamma_{q\varphi}$ and $\Gamma_{N\varphi}$.

The Dirichlet boundary conditions have the form

$$\varphi(\boldsymbol{x}, t) = \overline{\varphi}(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_\varphi , \tag{24}$$
$$T(\boldsymbol{x}, t) = \overline{T}(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_T , \tag{25}$$

where $\overline{T}(\boldsymbol{x}, t)$ denotes the prescribed temperature on the part $\Gamma_T$ and $\overline{\varphi}(\boldsymbol{x}, t)$ denotes the prescribed relative humidity on the part $\Gamma_\varphi$. The Neumann boundary conditions have the form

$$\boldsymbol{q}_\varphi(\boldsymbol{x}, t) = \overline{\boldsymbol{q}}_\varphi(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_{q\varphi} , \tag{26}$$
$$\boldsymbol{q}_T(\boldsymbol{x}, t) = \overline{\boldsymbol{q}}_T(\boldsymbol{x}, t), \qquad \boldsymbol{x} \in \Gamma_{qT} , \tag{27}$$

where $\overline{\boldsymbol{q}}_\varphi(\boldsymbol{x}, t)$ denotes the prescribed moisture flux on the part $\Gamma_{q\varphi}$ of the boundary and $\overline{\boldsymbol{q}}_T(\boldsymbol{x}, t)$ denotes the prescribed heat flux on the Cauchy boundary conditions part $\Gamma_{qT}$. The Newton (Cauchy) boundary conditions have the form

$$\boldsymbol{q}_\varphi(\boldsymbol{x}, t) = \beta_\varphi(p(\boldsymbol{x}, t) - p_\infty(\boldsymbol{x}, t))\boldsymbol{n}, \qquad \boldsymbol{x} \in \Gamma_{N\varphi} , \tag{28}$$
$$\boldsymbol{q}_T(\boldsymbol{x}, t) = \beta_T(T(\boldsymbol{x}, t) - T_\infty(\boldsymbol{x}, t))\boldsymbol{n}, \qquad \boldsymbol{x} \in \Gamma_{NT} , \tag{29}$$

where $p_\infty(\boldsymbol{x}, t)$ denotes the ambient water vapour pressure and $\beta_\varphi$ is the mass transfer coefficient, both defined in the part $\Gamma_{N\varphi}$. The pressures are transformed to the relative humidity with the help of relationship (1). $T_\infty(\boldsymbol{x}, t)$ is the ambient temperature and $\beta_T$ is the heat transfer coefficient, both defined in the part $\Gamma_{NT}$.

Besides the boundary conditions, the initial conditions are prescribed in the form

$$\varphi(\boldsymbol{x}, 0) = \varphi_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \tag{30}$$
$$T(\boldsymbol{x}, 0) = T_0(\boldsymbol{x}), \qquad \boldsymbol{x} \in \Omega, \tag{31}$$

where $\varphi_0(\boldsymbol{x})$ denotes the initial relative humidity and $T_0(\boldsymbol{x})$ denotes the initial temperature.

## 4. Discretization of the differential equations

The finite element method is used for spatial discretization of the partial differential equations (22) and (23). The weighted residual statement is applied to the mass balance equation assuming $(\delta\varphi) = 0$ on $\Gamma_\varphi$ and $(\delta T) = 0$ on $\Gamma_T$. The brackets are used for weight functions $(\delta\varphi)$ and $(\delta T)$ because there are some material parameters denoted by $\delta$.

The mass balance equation multiplied by the test function $(\delta\varphi)$ has the form

$$\int_\Omega (\delta\varphi)\Big(h_{\varphi\varphi}\frac{\partial\varphi}{\partial t} - \operatorname{div}\big(\boldsymbol{D}_{\varphi\varphi}\nabla\varphi + \boldsymbol{D}_{\varphi T}\nabla T\big)\Big)\mathrm{d}\Omega = 0 \tag{32}$$

and the energy balance equation multiplied by the test function $(\delta T)$ has the form

$$\int_\Omega (\delta T)\Big(h_{TT}\frac{\partial T}{\partial t} - \operatorname{div}\big(\boldsymbol{D}_{T\varphi}\nabla\varphi + \boldsymbol{D}_{TT}\nabla T\big)\Big)\mathrm{d}\Omega = 0\,. \tag{33}$$

Applying Green's theorem, the weak formulation for the mass transfer yields

$$\begin{aligned}\int_\Omega (\delta\varphi)h_{\varphi\varphi}\frac{\partial\varphi}{\partial t}\mathrm{d}\Omega + \int_\Omega \nabla(\delta\varphi)\boldsymbol{D}_{\varphi\varphi}\nabla\varphi\mathrm{d}\Omega + \int_\Omega \nabla(\delta\varphi)\boldsymbol{D}_{\varphi T}\nabla T\mathrm{d}\Omega + \\ - \int_{\Gamma_{q\varphi}\cup\Gamma_{N\varphi}} (\delta\varphi)\boldsymbol{D}_{\varphi\varphi}\frac{\mathrm{d}\varphi}{\mathrm{d}\boldsymbol{n}}\mathrm{d}\Gamma - \int_{\Gamma_{qT}\cup\Gamma_{NT}} (\delta\varphi)\boldsymbol{D}_{\varphi T}\frac{\mathrm{d}T}{\mathrm{d}\boldsymbol{n}}\mathrm{d}\Gamma = 0\end{aligned} \tag{34}$$

and the weak formulation for heat transfer

$$\begin{aligned}\int_\Omega (\delta T)h_{TT}\frac{\partial T}{\partial t}\mathrm{d}\Omega + \int_\Omega \nabla(\delta T)\boldsymbol{D}_{T\varphi}\nabla\varphi\mathrm{d}\Omega + \int_\Omega \nabla(\delta T)\boldsymbol{D}_{TT}\nabla T\mathrm{d}\Omega - \\ - \int_{\Gamma_{q\varphi}\cup\Gamma_{N\varphi}} (\delta T)\boldsymbol{D}_{T\varphi}\frac{\mathrm{d}\varphi}{\mathrm{d}\boldsymbol{n}}\mathrm{d}\Gamma - \int_{\Gamma_{qT}\cup\Gamma_{NT}} (\delta T)\boldsymbol{D}_{TT}\frac{\mathrm{d}T}{\mathrm{d}\boldsymbol{n}}\mathrm{d}\Gamma = 0\,.\end{aligned} \tag{35}$$

In the finite element method, the temperature $T$ and relative humidity $\varphi$ are approximated in the form

$$\varphi = \boldsymbol{N}_\varphi(\boldsymbol{x})\boldsymbol{d}_\varphi\,, \tag{36}$$

$$T = \boldsymbol{N}_T(\boldsymbol{x})\boldsymbol{d}_T\,, \tag{37}$$

and the gradients of the temperature and relative humidity are also needed

$$\nabla\varphi = \boldsymbol{B}_\varphi(\boldsymbol{x})\boldsymbol{d}_\varphi\,, \tag{38}$$

$$\nabla T = \boldsymbol{B}_T(\boldsymbol{x})\boldsymbol{d}_T\,. \tag{39}$$

In the previous equations, $\boldsymbol{N}_\varphi(\boldsymbol{x})$ denotes the matrix of approximation functions for the relative humidity, $\boldsymbol{N}_T(\boldsymbol{x})$ denotes the matrix of approximation functions for the temperature, $\boldsymbol{B}_\varphi(\boldsymbol{x})$ is the matrix of gradients of the approximation functions collected in the matrix $\boldsymbol{N}_\varphi(\boldsymbol{x})$, $\boldsymbol{B}_T(\boldsymbol{x})$ is the matrix of gradients of the approximation functions collected in the matrix $\boldsymbol{N}_T(\boldsymbol{x})$, $\boldsymbol{d}_\varphi$ denotes the vector of nodal relative humidities and $\boldsymbol{d}_T$ denotes the vector of nodal temperatures. The approximations of weight functions have the form

$$(\delta\varphi) = \boldsymbol{N}_{(\delta\varphi)}(\boldsymbol{x})\boldsymbol{d}_{(\delta\varphi)}\,, \tag{40}$$

$$(\delta T) = \boldsymbol{N}_{(\delta T)}(\boldsymbol{x})\boldsymbol{d}_{(\delta T)}\,, \tag{41}$$

where the notation is similar to the previous one.

Using approximations (36)–(39) in equations (34) and (35), a set of the first order differential equations is obtained in the matrix form

$$\begin{pmatrix} \boldsymbol{K}_{\varphi\varphi} & \boldsymbol{K}_{\varphi T} \\ \boldsymbol{K}_{T\varphi} & \boldsymbol{K}_{TT} \end{pmatrix}\begin{pmatrix} \boldsymbol{d}_\varphi \\ \boldsymbol{d}_T \end{pmatrix} + \begin{pmatrix} \boldsymbol{C}_{\varphi\varphi} & \boldsymbol{C}_{\varphi T} \\ \boldsymbol{C}_{T\varphi} & \boldsymbol{C}_{TT} \end{pmatrix}\begin{pmatrix} \dot{\boldsymbol{d}}_\varphi \\ \dot{\boldsymbol{d}}_T \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_\varphi \\ \boldsymbol{f}_T \end{pmatrix}\,. \tag{42}$$

The matrices $\boldsymbol{K}_{\varphi\varphi}$, $\boldsymbol{K}_{\varphi T}$, $\boldsymbol{K}_{T\varphi}$ and $\boldsymbol{K}_{TT}$ create the conductivity matrix of the problem and they have the form

$$\boldsymbol{K}_{\varphi\varphi} = \int_\Omega \boldsymbol{B}^T_{(\delta\varphi)} \boldsymbol{D}_{\varphi\varphi} \boldsymbol{B}_\varphi \mathrm{d}\Omega, \quad \boldsymbol{K}_{\varphi T} = \int_\Omega \boldsymbol{B}^T_{(\delta\varphi)} \boldsymbol{D}_{\varphi T} \boldsymbol{B}_T \mathrm{d}\Omega, \tag{43}$$

$$\boldsymbol{K}_{T\varphi} = \int_\Omega \boldsymbol{B}^T_{(\delta T)} \boldsymbol{D}_{T\varphi} \boldsymbol{B}_\varphi \mathrm{d}\Omega, \quad \boldsymbol{K}_{TT} = \int_\Omega \boldsymbol{B}^T_{(\delta T)} \boldsymbol{D}_{TT} \boldsymbol{B}_T \mathrm{d}\Omega\,, \tag{44}$$

where the conductivity matrices of material $\boldsymbol{D}_{\varphi\varphi}$, $\boldsymbol{D}_{\varphi T}$, $\boldsymbol{D}_{T\varphi}$ and $\boldsymbol{D}_{TT}$ are diagonal matrices and the diagonal entries are equal to appropriate conductivities

$$d_{\varphi\varphi} = D_w \frac{\mathrm{d}w}{\mathrm{d}\varphi} + \delta_p p_{vs}, \quad d_{\varphi T} = \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T}, \tag{45}$$

$$d_{T\varphi} = h_v \delta_p p_{vs}, \quad d_{TT} = \lambda + h_v \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T}\,. \tag{46}$$

The matrices $\boldsymbol{C}_{\varphi\varphi}$, $\boldsymbol{C}_{\varphi T}$, $\boldsymbol{C}_{T\varphi}$ and $\boldsymbol{C}_{TT}$ create the capacity matrix of the problem and they have the form

$$\boldsymbol{C}_{\varphi\varphi} = \int_\Omega \boldsymbol{N}^T_{(\delta\varphi)} \boldsymbol{H}_{\varphi\varphi} \boldsymbol{N}_\varphi \mathrm{d}\Omega, \quad \boldsymbol{C}_{\varphi T} = \int_\Omega \boldsymbol{N}^T_{(\delta\varphi)} \boldsymbol{H}_{\varphi T} \boldsymbol{N}_T \mathrm{d}\Omega, \tag{47}$$

$$\boldsymbol{C}_{T\varphi} = \int_\Omega \boldsymbol{N}^T_{(\delta T)} \boldsymbol{H}_{T\varphi} \boldsymbol{N}_\varphi \mathrm{d}\Omega, \quad \boldsymbol{C}_{TT} = \int_\Omega \boldsymbol{N}^T_{(\delta T)} \boldsymbol{H}_{TT} \boldsymbol{N}_T \mathrm{d}\Omega, \tag{48}$$

where the capacity matrices of material $\boldsymbol{H}_{\varphi\varphi}$, $\boldsymbol{H}_{\varphi T}$, $\boldsymbol{H}_{T\varphi}$ and $\boldsymbol{H}_{TT}$ are diagonal matrices and the diagonal entries are equal to appropriate capacities

$$h_{\varphi\varphi} = \frac{\mathrm{d}w}{\mathrm{d}\varphi}, \quad h_{\varphi T} = 0, \tag{49}$$

$$h_{T\varphi} = 0, \quad h_{TT} = \rho C + \frac{\mathrm{d}H_w}{\mathrm{d}T}\,. \tag{50}$$

The vectors $\boldsymbol{f}_\varphi$ and $\boldsymbol{f}_T$ contain prescribed nodal fluxes and have the form

$$\boldsymbol{f}_\varphi = \int_{\Gamma_{qT} \cup \Gamma_{NT}} \boldsymbol{N}^T_{(\delta\varphi)} \hat{q}_\varphi \mathrm{d}\Gamma, \quad \boldsymbol{f}_T = \int_{\Gamma_{q\varphi} \cup \Gamma_{N\varphi}} \boldsymbol{N}^T_{(\delta T)} \hat{q}_T \mathrm{d}\Gamma\,, \tag{51}$$

where $\hat{q}_\varphi$ denotes the mass boundary fluxes and $\hat{q}_T$ denotes the heat boundary fluxes.

## 5. Numerical solution

From the numerical point of view, coupled problems are described by balance equations which have the form of partial differential equations. The exact solution cannot be obtained with respect to non-linearities hidden in the material models. Another obstacle is caused by very general domains which are solved in real engineering problems. Therefore, numerical methods have to be used.

The balance equations (42) can be written in the form

$$\begin{pmatrix} \boldsymbol{C}_{\varphi\varphi} & \boldsymbol{C}_{\varphi T} \\ \boldsymbol{C}_{T\varphi} & \boldsymbol{C}_{TT} \end{pmatrix} \begin{pmatrix} \dot{\boldsymbol{d}}_\varphi \\ \dot{\boldsymbol{d}}_T \end{pmatrix} + \begin{pmatrix} \boldsymbol{K}_{\varphi\varphi} & \boldsymbol{K}_{\varphi T} \\ \boldsymbol{K}_{T\varphi} & \boldsymbol{K}_{TT} \end{pmatrix} \begin{pmatrix} \boldsymbol{d}_\varphi \\ \boldsymbol{d}_T \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_\varphi \\ \boldsymbol{f}_T \end{pmatrix} = \begin{pmatrix} \boldsymbol{f}_{\varphi\varphi} + \boldsymbol{f}_{\varphi T} \\ \boldsymbol{f}_{T\varphi} + \boldsymbol{f}_{TT} \end{pmatrix}, \tag{52}$$

where the vectors $\boldsymbol{f}_T$ and $\boldsymbol{f}_\varphi$ denote prescribed nodal fluxes and they can be further split to two contributions. The vector $\boldsymbol{f}_\varphi$ is the sum of vectors $\boldsymbol{f}_{\varphi\varphi}$ and $\boldsymbol{f}_{\varphi T}$ which represent contributions to the nodal fluxes caused by temperature changes and humidity changes. The meaning of other contributions is similar.

The system of differential equations (52) can be written more compactly in the form

$$\boldsymbol{C}(\boldsymbol{d})\dot{\boldsymbol{d}} + \boldsymbol{K}(\boldsymbol{d})\boldsymbol{d} = \boldsymbol{f}\,, \tag{53}$$

where the dependency of the stiffness, conductivity, capacity and coupling matrices on the attained values of variables is explicitly denoted. $\Delta \boldsymbol{d}$ and $\Delta \dot{\boldsymbol{d}}$ denote increments of nodal variables and their time derivatives.

The system (53) has to be solved by an incremental method. Time discretization is based on the $\boldsymbol{v}$-form of the generalized trapezoidal method Hughes (1987) defined by the relationships

$$\boldsymbol{d}_{n+1} = \boldsymbol{d}_n + \Delta t \boldsymbol{v}_{n+\gamma} \,, \tag{54}$$

$$\boldsymbol{v}_{n+\gamma} = (1-\gamma)\boldsymbol{v}_n + \gamma \boldsymbol{v}_{n+1} \,, \tag{55}$$

where $\boldsymbol{v}$ denotes the first derivatives of nodal values with respect to time and $\gamma$ is a parameter from the range $[0, 1]$. The subscript $n$ denotes the time step and it serves also as an index in the incremental method, called the outer iteration loop. It is assumed that all variables are known at the time $t_n$ and variables at the time $t_{n+1}$ are searched.

Substitution of expressions defined in equations (54) and (55) to the system of differential equations (53) leads to relationship

$$\left(\boldsymbol{C}_n + \Delta t \gamma \boldsymbol{K}_n\right) \boldsymbol{v}_{n+1} = \boldsymbol{f}_{n+1} - \boldsymbol{K}_n \left(\boldsymbol{d}_n + \Delta t (1-\gamma) \boldsymbol{v}_n\right) \,, \tag{56}$$

where $\boldsymbol{C}_n$ and $\boldsymbol{K}_n$ denote the capacity and stiffness/conductivity matrices evaluated with the help of values $\boldsymbol{d}_n$. The system of algebraic equations (56) is generally non-linear and the Newton-Raphson method Bittnar and Šejnoha (1996) has to be used at each time step.

The trial solution $\boldsymbol{v}_{n+1,0}$ of the system of equations (56) is used for computation of the trial nodal values $\boldsymbol{d}_{n+1,0}$ which are obtained from equations (55) and (54). Substitution of the trial solution back to the system of equations (56) with modified matrices does not generally lead to equality. An iteration loop, called the inner iteration loop, in every time step is based on residual which is computed from the relationship

$$\begin{aligned} \boldsymbol{r}_{n+1,j} &= \boldsymbol{f}_{n+1} - \boldsymbol{K}_n \left(\boldsymbol{d}_n + \Delta t (1-\gamma) \boldsymbol{v}_n\right) \\ &- \left(\boldsymbol{C}_{n+1,j} + \Delta t \gamma \boldsymbol{K}_{n+1,j}\right) \boldsymbol{v}_{n+1,j} \,, \end{aligned} \tag{57}$$

where $\boldsymbol{C}_{n+1,j}$ and $\boldsymbol{K}_{n+1,j}$ denote the matrices evaluated for $\boldsymbol{d}_{n+1,j}$ and $j$ is the index in the inner loop. Correction of nodal time derivatives are computed from the equation

$$\left(\boldsymbol{C}_{n+1,j} + \Delta t \gamma \boldsymbol{K}_{n+1,j}\right) \Delta \boldsymbol{v}_{n+1,j+1} = \boldsymbol{r}_{n+1,j} \tag{58}$$

and new time derivatives are in the form

$$\boldsymbol{v}_{n+1,j+1} = \boldsymbol{v}_{n+1,j} + \Delta \boldsymbol{v}_{n+1,j+1} \,. \tag{59}$$

It has to be noted that the permanent recalculation of matrices $\boldsymbol{K}$ and $\boldsymbol{C}$ with respect to actual nodal values is very computationally demanding. In such a case, the matrix of the system of equations $\boldsymbol{C}(\boldsymbol{d}) + \Delta t \gamma \boldsymbol{K}(\boldsymbol{d})$ has to be always factorized and it requires additional computational time. The numerical examples show that the modified Newton method, which changes the system matrix only at the beginning of a new time step is the best choice. More details can be found in references Kruis and Koudelka and Krejčí (2010) and Kruis and Koudelka and Krejčí (2012).

## 6. Numerical experiments

In order to show possible difficulties, coupled heat and moisture transfer described by the Künzel model on a rectangular two-dimensional domain is assumed. Rectangular finite elements with bi-linear basis functions are used. The quadrilateral element contains four nodes and therefore there are eight degrees of freedom in the case of heat and moisture transfer on each element. The degrees of freedom are located in vector

$$\boldsymbol{d}_e^T = (\varphi_1, \varphi_2, \varphi_3, \varphi_4, T_1, T_2, T_3, T_4) \,. \tag{60}$$

*Tab. 1: Material parameters.*

| | |
|---|---|
| density of material | $\varrho$=16.5 kg/m$^3$ |
| water vapour diffusion resistance factor | $\mu$=58 (-) |
| capillary transport coefficient | $D_w = 6.2 \times 10^{-12}$ m$^2$/s |
| | $\dfrac{\mathrm{d}H}{\mathrm{d}T} = \varrho c$ |
| heat capacity coefficient | $c = 1567$ |

*Tab. 2: Thermal conductivity.*

| | |
|---|---|
| 0.00000 | 0.0393 |
| 0.00219 | 0.0423 |
| 0.03040 | 0.0443 |
| 0.03968 | 0.0484 |
| 0.06349 | 0.5130 |

With respect to the ordering of degrees of freedom in the vector $\boldsymbol{d}$, the matrix of basis functions has the form

$$\boldsymbol{N} = \begin{pmatrix} \boldsymbol{N}_\varphi & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{N}_T \end{pmatrix} = \begin{pmatrix} N_1 & N_2 & N_3 & N_4 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & N_1 & N_2 & N_3 & N_4 \end{pmatrix} . \tag{61}$$

The matrix of partial derivatives has the form

$$\boldsymbol{B} = \begin{pmatrix} \dfrac{\partial \varphi}{\partial x} \\ \dfrac{\partial \varphi}{\partial y} \\ \dfrac{\partial T}{\partial x} \\ \dfrac{\partial T}{\partial y} \end{pmatrix} = \begin{pmatrix} \dfrac{\partial \boldsymbol{N}_\varphi}{\partial x} & \boldsymbol{0} \\ \dfrac{\partial \boldsymbol{N}_\varphi}{\partial y} & \boldsymbol{0} \\ \boldsymbol{0} & \dfrac{\partial \boldsymbol{N}_T}{\partial x} \\ \boldsymbol{0} & \dfrac{\partial \boldsymbol{N}_T}{\partial y} \end{pmatrix} = \begin{pmatrix} \boldsymbol{B}_\varphi & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}_T \end{pmatrix} . \tag{62}$$

The conductivity matrix of an element has the form

$$\boldsymbol{K} = \int_{\Omega_e} \boldsymbol{B}^T \boldsymbol{D} \boldsymbol{B} \, \mathrm{d}\Omega \, , \tag{63}$$

where the matrices $\boldsymbol{B}$ and $\boldsymbol{D}$ are defined by relationships (62) and (21) respectively. $\Omega_e$ denotes the element area. The conductivity matrix is assembled from four blocks in the form

$$\begin{pmatrix} \boldsymbol{B}_\varphi & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}_T \end{pmatrix}^T \begin{pmatrix} \boldsymbol{D}_{\varphi\varphi} & \boldsymbol{D}_{\varphi T} \\ \boldsymbol{D}_{T\varphi} & \boldsymbol{D}_{TT} \end{pmatrix} \begin{pmatrix} \boldsymbol{B}_\varphi & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{B}_T \end{pmatrix} = \begin{pmatrix} \boldsymbol{B}_\varphi^T \boldsymbol{D}_{\varphi\varphi} \boldsymbol{B}_\varphi & \boldsymbol{B}_\varphi^T \boldsymbol{D}_{\varphi T} \boldsymbol{B}_T \\ \boldsymbol{B}_T^T \boldsymbol{D}_{T\varphi} \boldsymbol{B}_\varphi & \boldsymbol{B}_T^T \boldsymbol{D}_{TT} \boldsymbol{B}_T \end{pmatrix} . \tag{64}$$

If the diagonal conductivity matrices of material, $\boldsymbol{D}_{\varphi\varphi}, \boldsymbol{D}_{TT}$, are zero or very close to zero, zero or nearly zero entries appear on the main diagonal of the conductivity matrix of an element and on the main diagonal of the conductivity matrix of problem.

Let the material parameters summarized in table 1 be used. Table 2 contains the thermal conductivity which is given by measured data.

The conductivity matrix of material, $\boldsymbol{D}$, in the Künzel model is defined in (21). The matrix evaluated at the beginning of the analysis has the form

$$\boldsymbol{D}_K = \begin{pmatrix} D_\varphi + \delta_p p_{vs} & \delta_p \varphi \dfrac{\mathrm{d}p_{vs}}{\mathrm{d}T} \\ L_v \delta_p p_{vs} & (\lambda + L_v \delta_p \varphi \dfrac{\mathrm{d}p_{vs}}{\mathrm{d}T}) \end{pmatrix} = \begin{pmatrix} 9.895512 \times 10^{-9} & 2.68344 \times 10^{-10} \\ 2.418454 \times 10^{-2} & 4.013119 \times 10^{-2} \end{pmatrix} . \quad (65)$$

There are obvious differences in orders of particular matrix entries. The eigenvalues of the matrix are

$$\lambda_1 = 9.733798 \times 10^{-9} , \quad (66)$$
$$\lambda_2 = 4.013119 \times 10^{-2} , \quad (67)$$

and their ratio is

$$\kappa = 4.123 \times 10^{6} . \quad (68)$$

In order to fix ideas, a plane stress problem is analyzed and compared with the coupled heat and moisture transport. Let the Young modulus be $E = 50$ GPa and the Poisson ratio $\nu = 0.2$. The stiffness matrix of elastic material subjected to plane stress conditions has the form

$$\boldsymbol{D}_{ps} = \begin{pmatrix} \frac{E}{1-\nu^2} & \frac{E\nu}{1-\nu^2} & 0 \\ \frac{E\nu}{1-\nu^2} & \frac{E}{1-\nu^2} & 0 \\ 0 & 0 & \frac{E}{2(1+\nu)} \end{pmatrix} = 10^6 \begin{pmatrix} 52\,083 & 10\,417 & 0 \\ 10\,417 & 52\,083 & 0 \\ 0 & 0 & 20\,833 \end{pmatrix} . \quad (69)$$

The eigenvalues of the stiffness matrix of the material are

$$\lambda_1 = 20833 \times 10^6 , \quad (70)$$
$$\lambda_2 = 41666 \times 10^6 , \quad (71)$$
$$\lambda_3 = 62500 \times 10^6 \quad (72)$$

and the ratio of the largest and smallest eigenvalues results in the condition number

$$\kappa = 3 . \quad (73)$$

The larger condition number, the worse behaviour of many iterative method and greater cancellation errors. Comparison of the condition numbers (73) for plane stress and (68) for the coupled heat and moisture transfer reveals that the transport problem behaves much worse than the plane stress problem.

The conductivity matrix of the whole problem has the following smallest and largest eigenvalues

$$\lambda = \begin{pmatrix} 0.000000001366664 \\ \vdots \\ 0.085677899281368 \end{pmatrix} \quad (74)$$

and the condition number is

$$\kappa = 6.269 \times 10^{7} . \quad (75)$$

The conductivity matrix of the whole problem has no kernel because there have to be Dirichlet boundary conditions somewhere on domain boundary.

The generalized trapezoidal rule generates the following matrix $\boldsymbol{C}_n + \Delta t \gamma \boldsymbol{K}_n$. The smallest and largest eigenvalues are

$$\lambda = \begin{pmatrix} 0.0000669816805 \\ \vdots \\ 132.3215121202840 \end{pmatrix} \quad (76)$$

and the condition number is

$$\kappa = 1.975 \times 10^6 \,. \tag{77}$$

It is slightly better than the condition number of the conductivity matrix of the whole problem $\boldsymbol{K}$ because the capacity matrix is non-singular and positive definite.

The conductivity matrix of material $\boldsymbol{D}_K$ based on the Künzel assumption is populated by entries with very different order of magnitude. The better moisture insulation, the larger difference in orders of magnitude. Theoretically, a perfect hydrophobic material leads to zero term $d_{\varphi\varphi} = D_\varphi + \delta_p p_{vs}$ which results in a zero row and column in the conductivity matrix of a finite element $\boldsymbol{K}$. Moreover, there could be a zero column and row in the matrix of the whole problem which make difficulties for solvers of linear algebraic systems of equations. In the case of real materials, the diagonal term $D_\varphi + \delta_p p_{vs}$ is not exactly equal to zero but it could be very small and rows and columns in the global matrix could be nearly zero. The condition number of the global matrix is very large in such cases. It causes severe problems to iterative solvers because the rate of convergence usually depends on the condition number. If a direct solver is used for such systems of equations, significant cancellation errors could occur.

If materials with extremely small moisture conductivities are used, numerical difficulties may occur when significant moisture fluxes are presents. Such situation emerges e.g. near boundary where moisture flux is defined by external conditions. If an insulation material is close to the structure surface, the model is unable to transport the moisture flux from the exterior into structure. It results in non-balanced fluxes and the non-linear solver tends to reduce the length of time step. When the time step length is smaller than reasonable threshold, e.g. $10^{-3}$ s, the solver announces problems and it stops. This phenomena is illustrated in figures 1 and 2. The distribution of relative humidity along the coordinate axis is depicted in figure 1 while the time behaviour of the relative humidity at point near the external surface is visible in figure 2. The red line represents the relative humidity for structure with insulation near the surface. It means, there are extremely small moisture conductivities. On the other hand, the blue curve shows the relative humidity for structure without an insulation. Another examples can be found in references Kočí et al (2012) and Kočí et al (2010).

Zero columns and rows can be removed from the system of equations but it is not easy in real world problems. It is difficult to recognize small value nearly equal to zero because of a hydrophobic material with extremely small conductivity and small matrix entries caused by inappropriate scale of variables. The decision which numbers could be removed from the system of equations has to be based on evaluation of the heat and moisture fluxes. Contributions to the fluxes from particular gradients are evaluated and they are compared. The moisture flux contains two contributions

$$\boldsymbol{q}_\varphi = \boldsymbol{q}_{\varphi\varphi} + \boldsymbol{q}_{\varphi T} \,, \tag{78}$$

where

$$\boldsymbol{q}_{\varphi\varphi} = (D_\phi + \delta_p p_{vs})\nabla\varphi \,, \tag{79}$$

$$\boldsymbol{q}_{\varphi T} = \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T}\nabla T \,. \tag{80}$$

Similarly for the heat flux

$$\boldsymbol{q}_T = \boldsymbol{q}_{T\varphi} + \boldsymbol{q}_{TT} \,, \tag{81}$$

where

$$\boldsymbol{q}_{T\varphi} = h_v \delta_p p_{vs} \nabla\varphi \,, \tag{82}$$

$$\boldsymbol{q}_{TT} = (\lambda + h_v \delta_p \varphi \frac{\mathrm{d}p_{vs}}{\mathrm{d}T})\nabla T \,. \tag{83}$$

If some of the contributions $\boldsymbol{q}_{\varphi\varphi}, \boldsymbol{q}_{\varphi T}, \boldsymbol{q}_{T\varphi}, \boldsymbol{q}_{TT}$ are significantly smaller than others in the vicinity of a node, the appropriate variable (temperature or relative humidity) is removed from the node and the appropriate degree of freedom is removed from the discrete system. This operation represents perfect barrier and no flux is possible there.

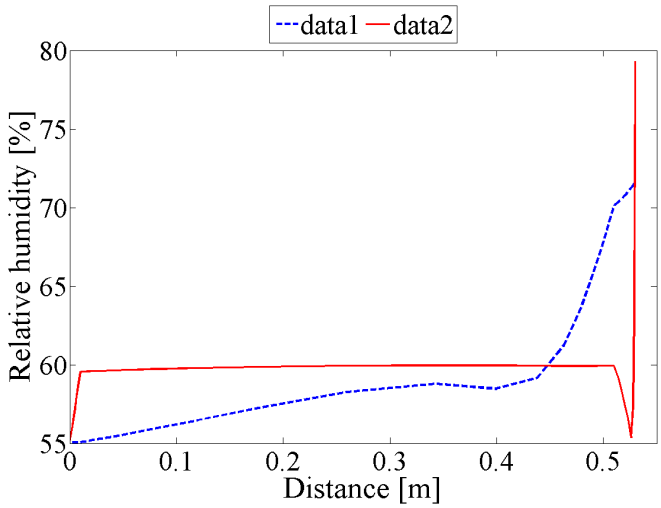


*Fig. 1: Distribution of the relative humidity along the thickness.*

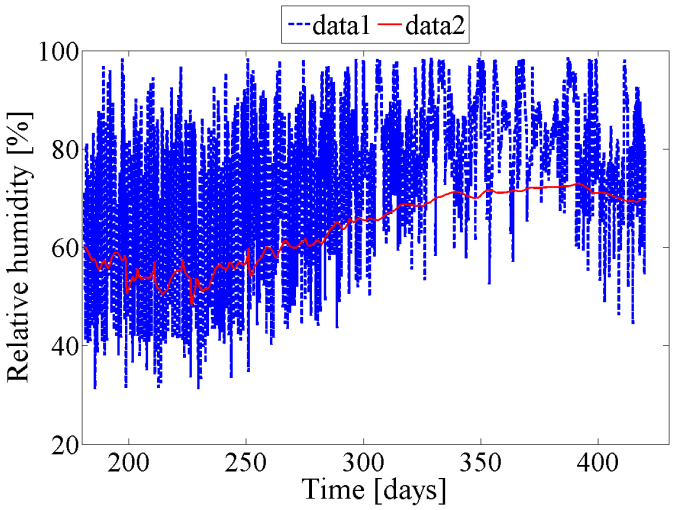


*Fig. 2: Behaviour of the relative humidity in time at point near external boundary.*

## 7. Conclusions

Modification of the algorithm for solution of coupled heat and moisture transfer based on the Künzel model was introduced. It evaluates contributions to the moisture and heat fluxes and it adaptively deals with the degrees of freedom defined in nodes of finite element mesh. If some fluxes are smaller than the others, the appropriate degrees of freedom are removed from the system and perfect insulation is obtained. When material parameters change their values, the degrees of freedom are returned to the system.

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