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TRANSPORT PROCESSES: GOVERNING EQUATIONS

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Summary: *This paper deals with description of heat and moisture transfer in deforming porous media. The mathematical model consists of balance equations of mass, energy and linear momentum and of the appropriate constitutive equations. The chosen macroscopic field variables are temperature, capillary pressures, gas pressure and displacement. The discretization of governing equation using finite element method leads to the system of non-linear and non-symmetric system of equations. The solution of this system of equations is very precisely shown in the following paper "TRANSPORT PROCESSES: NUMERICAL SOLUTION", authors J. Kruis, T. Krejčí, Z. Bittnar.*

1 Introduction

Materials research in concrete has shown that a correct prediction of the distribution and history of moisture content is inevitable for realistic determination of shrinkage, creep and thermal dilatation. Furthermore, the pore moisture content directly affects strength, thermal conductivity and the rate of hydration or maturing. Numerical analysis of drying and wetting is also indispensable for derivation of the constitutive law from creep, shrinkage and thermal dilatation tests at variable moisture conditions.

Similarly, the pore pressure distribution is necessary to analyze long-term deformations of soils. The moisture and heat transport in porous materials consequently affects both the upper structure and its sub-grade and, therefore, strongly influences interactions between the two subdomains.

This phenomenon is mostly studied under the assumption that both the liquid and gas phases flow through a rigid porous matrix [1]. However, this assumption is implausible, when analyzing consolidation of soils and certain other slow (quasi-static) phenomena. To remedy insufficiency of the aforementioned approaches, the temperature and moisture fields are completed by the displacement field, describing volume changes in a deforming porous material.

The aim of the present study is to explain in a condensed form the nature and theoretical basis of the most widely used mathematical models describing the coupled heat and moisture transport in deforming porous media, to provide a set of governing equations together with the

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finite element method. The theory discussed below is based on porous media theories given in [2].

Customary matrix notation is used throughout the text. Matrices are denoted by uppercase boldface italic letters, e.g. $\boldsymbol{D}$, $\boldsymbol{P}$ etc. Conversely, lowercase boldface italic letters stand for vectors $\boldsymbol{\sigma}$, $\boldsymbol{r}$ etc.

2 Mass and heat transfer in deforming porous media - a review of theory

Constitutive relations

Moisture in materials can be present as moist air, water and ice or in some intermediate state as adsorbed phase on the pore walls, respectively. Since it is in general not possible to distinguish the different aggregate states, the water content w is defined as the ratio of the total moisture weight (kg/kg) to the dry weight of the material. The degree of saturation S_w is a function of capillary pressure p^c and temperature T, which is determined experimentally

$$S_w = S_w(p^c, T). \tag{1}$$

The capillary pressure p^c id defined as

$$p^c = p^g - p^w, \tag{2}$$

where $p^w > 0$ is the pressure of the liquid phase (water).

The pressure of the moist air, $p^g > 0$, in the pore system is usually considered as the pressure in a perfect mixture of two ideal gases - dry air, p^{ga}, and water vapor, p^{gw}, i.e.,

$$p^g = p^{ga} + p^{gw} = \Big(\frac{\rho^{ga}}{M_a} + \frac{\rho^{gw}}{M_w}\Big)TR = \frac{\rho^g}{M_g}TR. \tag{3}$$

In this relation ρ^{ga}, ρ^{gw} and ρ^g stand for the respective intrinsic phase densities, T is the absolute temperature, and R is the universal gas constant.

Identity (3) defining the molar mass of the moist air, M_g, in terms of the molar masses of individual constituents is known as Dalton's law. The capillary pressure is larger the smaller the capillary radius is. It is shown thermodynamically that the capillary pressure can be expressed unambiguously by the relative humidity RH using the Kelvin-Laplace law

$$RH = \frac{p^{gw}}{p^{gws}} = \exp\Big(-\frac{p^c M_w}{\rho^w RT}\Big). \tag{4}$$

The water vapor saturation pressure, p^{gws}, is a function of the temperature only and can be expressed by the Clausius-Clapeyron equation

$$p^{gws}(T) = p^{gws}(T_0)\exp\Big[-\frac{M_w \Delta h_{\mathrm{vap}}}{R}\Big(\frac{1}{T} - \frac{1}{T_0}\Big)\Big], \tag{5}$$

where T_0 is a reference temperature and Δh_{vap} is the specific enthalpy of saturation.

Materials having heat capacities is the term deliberately used to emphasize the similarity to the description of the moisture retention. It is simply expressed as

$$H = H(T), \tag{6}$$

where H is the mass specific enthalpy (J.kg^{-1}), T - temperature (K).

It is not common to write the enthalpy in an absolute way as here. Instead, changes of enthalpy are described in a differential way, which leads to the definition of the specific heat capacity as the slope of the $H-T$ curve, i.e.

$$C_p = \left(\frac{\partial H}{\partial T}\right)_{p=\text{const.}}. \tag{7}$$

The heat capacity varies insignificantly with temperature. It is customary, however, to correct this term for the presence of the fluid phases and to introduce the effective heat capacity as

$$\big(\rho C_p\big)_{\text{eff}} = \rho_s C_{ps} + \rho_w C_{pw} + \rho_g C_{pg}. \tag{8}$$

Transfer equations

The mass averaged relative velocities, $\boldsymbol{v}^\alpha - \boldsymbol{v}^s$, are expressed by the generalized form of ***Darcy's law*** [2]

$$nS_\alpha\big(\boldsymbol{v}^\alpha - \boldsymbol{v}^s\big) = \frac{k^{r\alpha}\boldsymbol{k}_{sat}}{\mu^\alpha}\big(-\operatorname{grad}p^\alpha + \rho^\alpha\boldsymbol{g}\big), \tag{9}$$

where $\alpha = w$ for the liquid phase and $\alpha = g$ for the gaseous phase.

Dimensionless relative permeabilities $k^{r\alpha} \in \langle 0,1\rangle$ are functions of degree of saturation

$$k^{r\alpha} = k^{r\alpha}(S_w) \qquad (\mathrm{m}\cdot\mathrm{s}^{-1}). \tag{10}$$

In Equation (9), $\boldsymbol{k}_{sat}$ (m^2) is the square (3x3) intrinsic permeability matrix and μ^α is the dynamic viscosity (kg.m^{-1}.s^{-1}). The intrinsic mass densities ρ^α are related to the volume averaged mass densities ρ_α through the relation

$$\rho_\alpha = nS_\alpha\rho^\alpha. \tag{11}$$

The relative permeability k^{rw} goes to zero, when water saturation S_w approaches S_{irr}, which is the limiting value of S_w as the suction stress approaches infinity ([3]).

Diffusive-dispersive mass flux (kg.m^{-2}.s^{-1}) of the water vapor (gw) in the gas (g) is the second driving mechanism. It is governed by ***Fick's law***

$$\boldsymbol{J}_g^{gw} = nS_g\rho^{gw}\big(\boldsymbol{v}^{gw} - \boldsymbol{v}^g\big) = -\rho^g\boldsymbol{D}_g^{gw}\operatorname{grad}\Big(\frac{\rho^{gw}}{\rho^g}\Big), \tag{12}$$

where $\boldsymbol{D}_g^{gw}$ (m^2.s^{-1}) is the effective dispersion tensor. It can be shown
[2] that

$$\boldsymbol{J}_g^{gw} = -\rho^g\frac{M_aM_w}{M_g^2}\boldsymbol{D}_g^{gw}\operatorname{grad}\Big(\frac{\rho^{gw}}{\rho^g}\Big) = \rho^g\frac{M_aM_w}{M_g^2}\boldsymbol{D}_g^{ga}\operatorname{grad}\Big(\frac{\rho^{ga}}{\rho^g}\Big) = -\boldsymbol{J}_g^{ga}. \tag{13}$$

Recall that $\boldsymbol{D}_g^{gw} = \boldsymbol{D}_g^{ga} = \boldsymbol{D}_g$. Here, $\boldsymbol{J}_g^{ga}$ is the diffusive-dispersive mass flux of the dry air in the gas.

Conduction of heat in normal sense comprises radiation as well as convective heat transfer on a microscopic level. The generalized version of ***Fourier's law*** is used to describe the conduction heat transfer

$$\boldsymbol{q} = -\boldsymbol{\chi}_{\text{eff}}\operatorname{grad}T, \tag{14}$$

where $\boldsymbol{q}$ is the heat flux (W.m^{-2}), χ_{eff} is the effective thermal conductivity matrix (W.m^{-1}.K^{-1}).

The thermal conductivity increases with increasing temperature due to the non-linear behavior of the microscopic radiation, which depends on difference of temperatures raised to the 4^{th} power. Presence of water also increases the thermal conductivity. A suitable formula reflecting this effect can be found in [2].

Deformation of solid skeleton. Concept of effective stress

The stresses in the grains, $\boldsymbol{\sigma}^s$, can be expressed using a standard averaging technique in terms of the stresses in the liquid phase, $\boldsymbol{\sigma}^w$, the stresses in the gas, $\boldsymbol{\sigma}^g$, and the effective stresses between the grains, $\boldsymbol{\sigma}^{ef}$. The equivalence conditions for the internal stresses and for the total stress $\boldsymbol{\sigma}$ lead to the expression [4].

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{ef} + S_w \boldsymbol{\sigma}^w + S_g \boldsymbol{\sigma}^g + \Delta \boldsymbol{\tau}. \tag{15}$$

Assuming that the shear stress $\boldsymbol{\tau}$ in fluids is negligible converts the latter equation into the form

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}^{ef} - p^s \boldsymbol{m}, \tag{16}$$

where

$$\boldsymbol{\sigma} = \left\{\sigma_x, \sigma_y, \sigma_z, \tau_{yz}, \tau_{zx}, \tau_{xy}\right\}^{\mathrm{T}}, \quad \boldsymbol{m} = \left\{1, 1, 1, 0, 0, 0\right\}^{\mathrm{T}}, \tag{17}$$

and

$$p^s = S_w p^w + S_g p^g. \tag{18}$$

Deformation of a porous skeleton associated with the grain rearrangement can be expressed using the constitutive equation written in the rate form

$$\dot{\boldsymbol{\sigma}}^{ef} = \boldsymbol{D}_{sk} \big(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_0 \big). \tag{19}$$

The dots denote differentiation with respect to time, $\boldsymbol{D}_{sk} = \boldsymbol{D}_{sk}(\dot{\boldsymbol{\varepsilon}}, \boldsymbol{\sigma}^{ef}, T)$ is the tangential matrix of the porous skeleton and $\dot{\boldsymbol{\varepsilon}}_0$ represents the strains that are not directly associated with stress changes (e.g., temperature effects, shrinkage, swelling, creep). It also comprises the strains of the bulk material due to changes of the pore pressure

$$\dot{\boldsymbol{\varepsilon}} = -\boldsymbol{m} \Big(\frac{\dot{p}^s}{3K_s} \Big), \tag{20}$$

where K_s is the bulk modulus of the solid material (matrix).

When admitting only this effect and combining Equations (16), (19) and (20), we get

$$\dot{\boldsymbol{\sigma}} = \dot{\boldsymbol{\sigma}}^{ef} - \dot{p}^s \boldsymbol{m} = \boldsymbol{D}_{sk} \dot{\boldsymbol{\varepsilon}} - \alpha \boldsymbol{m} \dot{p}^s = \dot{\boldsymbol{\sigma}}'' - \alpha \boldsymbol{m} \dot{p}^s, \tag{21}$$

where

$$\alpha = \frac{1}{3} \boldsymbol{m}^{\mathrm{T}} \Big(\boldsymbol{I} - \frac{\boldsymbol{D}_{sk}}{3K_m} \Big) \boldsymbol{m} = 1 - \frac{K_{sk}}{K_s} < 1, \tag{22}$$

and $K_{sk} = \boldsymbol{m}^{\mathrm{T}} \boldsymbol{D}_{sk} \boldsymbol{m}/9$ is the bulk modulus of the porous skeleton. For a material without any pores, $K_{sk} = K_s$. For cohesive soils, $K_{sk} << K_s$ and $\alpha = 1$. The above formulas are also applicable to long-term deformation of rocks, for which $\alpha \leq 0.5$, and this fact strongly affects Equation (21) [5].

Changes of the effective stress along with temperature and pore pressure changes produce change of the solid density $\dot{\rho}^s$. To derive the respective material relation for this quantity, we start from the mass conservation equation for the solid phase. In the second step we introduce the constitutive relationship for the mean effective stress expressed in terms of quantities describing the deformation of the porous skeleton. After some manipulations we arrive at the searched formula

$$(1-n)\frac{\dot{\rho}^s}{\rho^s} = (\alpha - n)\Big(\frac{\dot{p}^s}{K_s} - \beta_s \dot{T}\Big) + (\alpha - 1)\mathrm{div}\boldsymbol{v}^s, \tag{23}$$

where β_s is the thermal expansion coefficient of the solid phase.

Similar approach applied to the mass conservation equation of the liquid phase leads to the following constitutive equation

$$\frac{\dot{\rho}^w}{\rho^w} = \frac{\dot{p}^w}{K_w} - \beta_s \dot{T}, \tag{24}$$

where K_w is the bulk modulus of water and β_w is the thermal expansion coefficient of this phase.

Set of governing equations

The complete set of equations describing the coupled moisture and heat transport in deforming porous media comprises the linear balance (equilibrium) equation formulated for a multi-phase body, the energy balance equation and the continuity equations for the liquid water and gas.

Continuity equation for the dry air

$$\begin{aligned}\frac{\partial}{\partial t}\Big(\varphi(1-S_w)\rho^{ga}\Big) + \alpha(1-S_w)\rho^{ga}\mathrm{div}\dot{\boldsymbol{u}} - \mathrm{div}\Big(\rho^{ga}\frac{k^{rg}\boldsymbol{k}_{sat}}{\mu^g}\mathrm{grad}p^g\Big) + \\ + \mathrm{div}\Big(\rho^g\frac{M_a M_w}{M_g^2}\boldsymbol{D}_{\text{eff}}\mathrm{grad}\Big(\frac{p^{gw}}{p^g}\Big)\Big) = 0,\end{aligned} \tag{25}$$

where $\dot{\boldsymbol{u}}$ ($\dot{\boldsymbol{u}} = \boldsymbol{v}^s$) is the velocity of solid.

Continuity equation for the water species

$$\begin{aligned}\frac{\partial}{\partial t}\Big(\varphi(1-S_w)\rho^{gw}\Big) + \alpha(1-S_w)\rho^{gw}\mathrm{div}\dot{\boldsymbol{u}} - \mathrm{div}\Big(\rho^{gw}\frac{k^{rg}\boldsymbol{k}_{sat}}{\mu^g}\mathrm{grad}p^g\Big) + \\ - \mathrm{div}\Big(\rho^g\frac{M_a M_w}{M_g^2}\boldsymbol{D}_{\text{eff}}\mathrm{grad}\Big(\frac{p^{gw}}{p^g}\Big)\Big) = \\ = -\frac{\partial}{\partial t}\Big(\varphi S_w \rho^w\Big) - \alpha S_w \rho^w \mathrm{div}\dot{\boldsymbol{u}} + \mathrm{div}\Big(\rho^w\frac{k^{rw}\boldsymbol{k}_{sat}}{\mu^w}(\mathrm{grad}p^g - \mathrm{grad}p^c - \rho^w\boldsymbol{g})\Big)\end{aligned} \tag{26}$$

Energy balance equation

$$\begin{aligned}\big(\rho C_p\big)_{\text{eff}}\frac{\partial T}{\partial t} - \mathrm{div}\big(\lambda_{\text{eff}}\mathrm{grad}T\big) + \\ -\Big(C_{pw}\rho^w\frac{k^{rw}\boldsymbol{k}_{sat}}{\mu^w}(\mathrm{grad}p^g - \mathrm{grad}p^c - \rho^w\boldsymbol{g}) + C_{pg}\rho^{gw}\frac{k^{rg}\boldsymbol{k}_{sat}}{\mu^g}\mathrm{grad}p^g\Big)\mathrm{grad}T = \\ = \Delta h_{\text{vap}}\Big[\frac{\partial}{\partial t}\Big(\varphi S_w \rho^w\Big) + \alpha S_w \rho^w \mathrm{div}\dot{\boldsymbol{u}} - \mathrm{div}\Big(\rho^w\frac{k^{rw}\boldsymbol{k}_{sat}}{\mu^w}(\mathrm{grad}p^g - \mathrm{grad}p^c - \rho^w\boldsymbol{g})\Big)\Big]\end{aligned} \tag{27}$$

The *equilibrium equation* (the linear balance equation) must yet be introduced to complete a set of governing equations

$$\operatorname{div}\big(\boldsymbol{\sigma} - \boldsymbol{m}(p^g - S_w p^c)\big) + \rho \boldsymbol{g} = \boldsymbol{0} \tag{28}$$

with density of the multi-phase medium defined as

$$\rho = (1-n)\rho^s + nS_w\rho^w + nS_g\rho^g = \rho_s + \rho_w + \rho_g. \tag{29}$$

Initial and boundary conditions

The initial conditions specify the full fields of gas pressure, capillary or water pressure, temperature and displacement and velocities:

$$p^g = p^g_0, \qquad p^c = p^c_0, \qquad T = T_0, \qquad \boldsymbol{u} = \boldsymbol{u}_0, \quad \text{and} \quad \dot{\boldsymbol{u}} = \dot{\boldsymbol{u}}_0, \quad \text{at} \quad t = 0. \tag{30}$$

The boundary conditions can be imposed values on Γ^1_π or fluxes on Γ^2_π, where the boundary $\Gamma = \Gamma^1_\pi + \Gamma^2_\pi$.

$$p^g = \overline{p}^g \quad \text{on} \quad \Gamma^1_g, \quad p^c = \overline{p}^c \quad \text{on} \quad \Gamma^1_c, \quad T = \overline{T} \quad \text{on} \quad \Gamma^1_T, \quad \boldsymbol{u} = \overline{\boldsymbol{u}} \quad \text{on} \quad \Gamma^1_u. \tag{31}$$

The volume averaged flux boundary conditions for water species and dry air conservation equations and energy equation to be imposed at the interface between the porous medium and the surrounding fluid are as follows

$$\begin{array}{rcl} \big(\rho^{ga}\boldsymbol{J}^{ga} - \rho^g\boldsymbol{J}^{gw}\big)\cdot\boldsymbol{n} & = & q_{ga} \quad \text{on} \quad \Gamma^2_g \\ \big(\rho^{gw}\boldsymbol{J}^{ga} + \rho^w\boldsymbol{J}^w + \rho^g\boldsymbol{J}^{gw}\big)\cdot\boldsymbol{n} & = & \beta_c(\rho^{gw} - \rho^{gw}_\infty) + q_{gw} + q_w \quad \text{on} \quad \Gamma^2_c \\ -\big(\rho^w\boldsymbol{J}^w\Delta h_{\text{vap}} - \lambda_{\text{eff}}\operatorname{grad}T\big)\cdot\boldsymbol{n} & = & \alpha_c(T - T_\infty) + q_T \quad \text{on} \quad \Gamma^2_T \end{array} \tag{32}$$

where $\boldsymbol{n}$ is the unit normal vector of the surface of the porous medium, ρ^{gw}_∞ and T_∞ are the mass concentration of water vapor and temperature in the undisturbed gas phase far away from the interface, and q_{ga}, q_{gw}, q_w and q_T are the imposed air flux, the imposed vapor flux, the imposed liquid flux and the imposed heat flux, respectively.

The traction boundary conditions for displacement field are:

$$\sigma\cdot\boldsymbol{n} = \boldsymbol{t} \quad \text{on} \quad \Gamma^2_u \tag{33}$$

where $\boldsymbol{t}$ is the imposed traction.

3 Discretization of governing equations

A weak formulation of the governing equations (25) to (28) is obtained by applying Galerkin's method of weighted residuals. For the numerical solution, the governing equations are discretized in space by means of the finite element method, yielding a non-symmetric and nonlinear system of partial differential equations:

$$\begin{array}{rcl} \boldsymbol{K}_{uu}\boldsymbol{u} + \boldsymbol{K}_{ug}\boldsymbol{p}_g + \boldsymbol{K}_{uc}\boldsymbol{p}_c + \boldsymbol{K}_{ut}\boldsymbol{T} & = & \boldsymbol{F}_u, \\ \boldsymbol{C}_{gg}\dot{\boldsymbol{p}}_g + \boldsymbol{C}_{gc}\dot{\boldsymbol{p}}_c + \boldsymbol{C}_{gt}\dot{\boldsymbol{T}} + \boldsymbol{C}_{gu}\dot{\boldsymbol{u}} + \boldsymbol{K}_{gg}\boldsymbol{p}_g + \boldsymbol{K}_{gc}\boldsymbol{p}_c + \boldsymbol{K}_{gt}\boldsymbol{T} & = & \boldsymbol{F}_g, \\ \boldsymbol{C}_{cg}\dot{\boldsymbol{p}}_g + \boldsymbol{C}_{cc}\dot{\boldsymbol{p}}_c + \boldsymbol{C}_{ct}\dot{\boldsymbol{T}} + \boldsymbol{C}_{cu}\dot{\boldsymbol{u}} + \boldsymbol{K}_{cg}\boldsymbol{p}_g + \boldsymbol{K}_{cc}\boldsymbol{p}_c + \boldsymbol{K}_{ct}\boldsymbol{T} & = & \boldsymbol{F}_c, \\ \boldsymbol{C}_{tg}\dot{\boldsymbol{p}}_g + \boldsymbol{C}_{tc}\dot{\boldsymbol{p}}_c + \boldsymbol{C}_{tt}\dot{\boldsymbol{T}} + \boldsymbol{C}_{tu}\dot{\boldsymbol{u}} + \boldsymbol{K}_{tg}\boldsymbol{p}_g + \boldsymbol{K}_{tc}\boldsymbol{p}_c + \boldsymbol{K}_{tt}\boldsymbol{T} & = & \boldsymbol{F}_t. \end{array} \tag{34}$$

The equations (34) can be rewritten in concise form as

$$\boldsymbol{K}(\boldsymbol{X})\boldsymbol{X} + \boldsymbol{C}(\boldsymbol{X})\dot{\boldsymbol{X}} = \boldsymbol{F}(\boldsymbol{X}), \tag{35}$$

where $\boldsymbol{X}^{\mathrm{T}} = \{\boldsymbol{p}^g, \boldsymbol{p}^c, \boldsymbol{T}, \boldsymbol{u}\}$, $\boldsymbol{C}(\boldsymbol{X})$ is “the general capacity matrix”, $\boldsymbol{K}(\boldsymbol{X})$ is “the general conductivity matrix” and are obtained together with $\boldsymbol{F}(\boldsymbol{X})$ by assembling the sub-matrices indicated in equations (34). The dot denotes the time derivative.

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