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Numerical Modeling of Heat and Water Transport with Heat Exchange in Unsaturated-Saturated Porous Media including Heat Influence on Flow

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Abstract **-** We discuss the numerical modelling of heat transport with contaminated water into unsaturated-saturated porous media. We focus on the determination of a heat exchange with the matrix of the porous media and adsorption of a contaminant. Numerical modelling includes the influence of temperature and adsorbed contaminant on hydraulic permeability. We also discuss the water volume extension due to the temperature change. This is motivated by hydrothermal isolation properties of building facades under the influence of external weather conditions. Also, contaminant dissolved in the water could be interpreted, e.g., as the salt which can degrade the quality of concrete and other building elements. Dependence of hydraulic permeability on the temperature, concentration of a contaminant, amount of adsorbed contaminant and saturation is discussed on the base of van Genuchten empirical law for unsaturated porous media. An efficient numerical approximation is proposed by means of which we solve the direct and inverse problems of the complex model. The determination of the model parameters we solve by inverse methods. In our numerical experiments, we show the significant sensitivity of hydraulic permeability on temperature and adsorption and the weak sensitivity on water extensions in the physically relevant temperature change. For the solution of inverse problems in laboratory experiments, we suggest the 3D sample in a cylindrical form which enables many experimental scenarios created by suitable boundary conditions.

Keywords**:** Water and heat transport, Heat energy exchange, Contaminant adsorption, Porous media, Numerical modelling.

1. Introduction

In this contribution, we discuss the heat exchange of infiltrating contaminated water with the porous media matrix assuming the unsaturated-saturated flow with contaminant adsorption. The adsorbed contaminant (e.g. salt) can decrease the quality of concrete and other building elements. Also, the adsorbed contaminant can decrease the porosity and together with transported heat significantly affect the hydraulic permeability. The influence of external weather conditions is included in the considered model. Especially, we focus on the numerical modelling of the heat energy exchange between the water in pores and the matrix with its heat conduction property. Moreover, we discuss contaminant transport and adsorption model. The complex mathematical model is strongly coupled with hydraulic permeability influenced by all transported attributes. Scaling this model is its important part. The mathematical model consists of the coupled system of strongly non-linear PDE of elliptic-parabolic type. The flow of water in unsaturated-saturated porous media is governed by Richard's equation. The heat energy of water is subject to the convection, molecular diffusion, dispersion which are driven by capillary and gravitating forces band also by external forces due to water and heat fluxes arising by weather conditions. The mathematical models are well-known and presented in many monographs, e.g. [1], with a very complex list of quotations in this field. The fundamentals of heat and mass transfer with many applications are discussed in [7]. In our setting the heat energy transmission from water in pores to the porous media matrix is our contribution and we model it analogously to the reversible adsorption of the contaminant in unsaturated porous media, see e.g. [6]. Additionally, we take into account the heat conduction of the porous media matrix itself and the adsorption of the contaminant. The adsorbed contaminant can influence the heat balance energy in the form of the source term. This could be interpreted as a latent heat appearing at the creation of the adsorbed contaminant. But it would be a rather rough approximation of precipitation of salt due to evaporation/condensation. A precise mathematical model for this phenomenon requires multiphase flow in porous media including water, vapour and air phases. Some simplified mathematical model with an application and many quotations can be found in [8]. Our model is only one phase model and the phase of air is neglected. The heat conduction in porous media (without water in pores) is a difficult task and it is modelled by the homogenization method. In our setting, we assume very simple heat conduction in the matrix, where heat conduction is obtained separately by solving a corresponding inverse problem and using practical measurements with the dry matrix. In our original experimental scenario, we determine both transmission coefficient and heat permeability in the matrix via the solution of the inverse problem.

In this scenario, we measure some characteristics strongly depending on this heat exchange avoiding water-matrix temperature jump. The reliability of this scenario supported by correct numerical approximation we demonstrate in our numerical experiments. The additional measurements required in solving the inverse problem are non-invasive based on input/output characteristics in laboratory conditions we realize on a 3D sample which is immersed into a bigger cylinder with infiltrated contaminated water. This setting is sketched in the following figure.

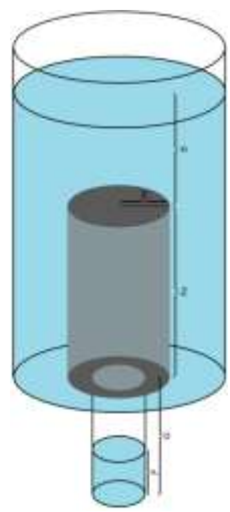

Fig. 1: Setting of the sample in experimental scenarios.

In the numerical method, we use operator splitting method with flexible time discretization where successively along with the small-time interval we separately solve water flow, transport of the contaminant with adsorption, heat transport by water and then in a matrix including the heat exchange. In the solution of water flow, we follow the approximation strategy introduced in and also used in well-known software Hydrus (see [2]). To control the correctness of our numerical results, we have also developed an approximation scheme (see [6] used only for 1D) based on the reduction of the governing parabolic system to the solution of the stiff system of ordinary differential equations. This approximation simultaneously solves the whole system, but computational time is significantly larger than that one in the present method. The main reason is that the system is stiff and too large when using necessary space discretization. Comparisons justify our method which is significantly quicker and therefore applicable in the solution of inverse problems scaling the model parameters. Moreover, the present method could be efficiently used also for solving 3D problems.

2. Mathematical model

2.1. Water flow model

The flow is modelled by the hydraulic permeability $K = K_s k(h)$, with

$$K_s = \kappa_0 \frac{\rho g}{\mu}, \tag{1}$$

where ρ and μ are the density and the dynamical viscosity of the water, respectively. The function $k(h)$ describes the capillary forces and it is linked with the pressure head h, or on the corresponding effective saturation (see [4]). We note that these parameters depend on water temperature T_w, adsorbed contaminant S and contaminant concentration C_w in infiltrated contaminated water. The coefficient κ_0 depends only on the structure of the porous medium and g is the gravitational acceleration. We consider more general form of hydraulic permeability $K(T_w, C_w, S, h) = K_s(T_w, C_w, S) \cdot k(h)$. Here, $K_s = K(T_w, C_w, S, 0)$ is the hydraulic permeability in fully saturated porous media. We consider k in a van Genuchten/Mualem empirical form (see [4])

$$k(\overline{\theta}) = \overline{\theta}^{\frac{1}{2}}(1 - (1 - \overline{\theta}^{\frac{1}{m}})^m)^2, \tag{2}$$

where by $\overline{\theta}$ we denote the effective saturation defined as

$$\overline{\theta} = (\theta - \theta_r)/(\theta_s - \theta_r) \tag{3}$$

with fully saturated θ_s and residual θ_r water contents, respectively. The capillary pressure vs. saturation (fundamental relation) we consider in the form

$$\overline{\theta} = \frac{1}{(1 + (\alpha h)^n)^m}, \tag{4}$$

where $n > 1$, $m = 1 - \frac{1}{n}$ and $\alpha < 0$ are the soil parameters in the van Genuchten-Mualem (empirical) ansatz. The adsorbed contaminant decreases the volume of poor's and thus, we have $\theta_s - S$ in the place of θ_s and consequently in what follows we consider (for simplicity)

$$K_s(Tw, C_w, S) = \frac{\theta_s - S}{\theta_s} K_s(T_w, C_w, 0). \tag{5}$$

In the saturated zone we have (Darcy's law) $k(h) \equiv 1$ and $\theta \equiv \theta_s$. The influence of dynamical viscosity on C_w, T_w can be found on tables for discrete values of variables and we use a spline interpolation of them in our computations. Richard's equation modelling the contaminated water flow reads as follows

$$\partial_t \theta = \nabla.\left(K(T_w, C_w, S, h)\boldsymbol{A}(x)\nabla(h + z)\right) = \mathrm{div}\left(K(T_w, \rho, S, h)\boldsymbol{A}(x)\nabla(h + z)\right) + \partial_t E, \tag{6}$$

where the matrix A describes the changes in conductivity according to the space structure (in our experiments A = I). The saturation change E due to temperature change is modelled by an ODE

$$\partial_t E = \kappa_w(T_w)\theta \frac{\sigma}{c_w}(T_w - T_m), \tag{7}$$

where c_w is the water heat capacity, κ_w is assumed to be a physical coefficient which measures the extension of unique water volume by unique temperature change. The heat transmission coefficient we denote by σ and T_m is the matrix temperature.

2.2. Contaminant transport model

The flux of dissolved contaminant with concentration C_w denoted by J_{C_w} is

$$\mathrm{J}_{C_w} = \theta(\mathrm{v}C_w - \mathrm{D}).\nabla C_w. \tag{8}$$

Here, v is the seepage velocity of the contaminated water linked with the flux $\vec{q} = \mathrm{v}\theta$ in flow model

$$\vec{q} = -K(T_w, C_w, S, h)\mathrm{A}(x).\nabla(h + z). \tag{9}$$

Denote by D the dispersion matrix with the components

$$D_{ij} = (D_0 + \alpha_T|\mathrm{v}|)\delta_{ij} + \frac{v_i v_j}{|\mathrm{v}|}(\alpha_L - \alpha_T), \tag{10}$$

where α_L, α_T are longitudinal and transversal dispersivities, respectively, δ_{ij} is the Kronecker delta and D_0 is the molecular diffusion coefficient. Then, the contaminant transport model is

$$\partial_t(\theta C_w) + \mathrm{div}(\vec{q}C_w - \theta\mathrm{D}\nabla C_w) = -\rho_m \partial_t S. \tag{11}$$

where S is adsorbed contaminant by the unique mass of porous media. The adsorption of the contaminant is governed by the ODE

$$\partial_t S = \kappa(\Psi(C_w) - S), \tag{12}$$

where κ is the sorption rate coefficient describing adsorption kinetics and Ψ is a sorption isotherm, which can depend on (T_w, C_w, S) and ρ_m is the matrix density. It belongs to a chosen class of functions with tuning parameters underlying for determination via the solution of the corresponding inverse problem.

2.3. Heat energy transport model

Conservation of water heat energy is expressed in PDE

$$c_v\partial_t(\theta T_w) - \mathrm{div}(-c_v\vec{q}T_w + \theta\mathrm{D}\nabla T_w) = \sigma\theta(T_m - T_w), \tag{13}$$

where σ is a transmission coefficient, $c_v\vec{q}T_w$ being the convective part, and the diffusive part is modelled by dispersion matrix D.

2.4. Heat conduction in porous media matrix

A simple heat conduction model in the matrix is considered in the form

$$c_m\partial_t T_m - \lambda\Delta T_m = \sigma\theta(T_w - T_m), \tag{14}$$

where λ - heat conduction coefficient and c_m- heat capacity of the matrix. In the solution of inverse problems we consider radial symmetric cylindrical sample, and thus we rewrite the considered model in cylindrical coordinates.

3. Mathematical model in cylindrical coordinates

Our sample is with radius R and height Z. We transform the mathematical model using cylindrical coordinates (r; z).

3.1. Water flow

Then the governing PDE for infiltration (in gravitational mode) reads as follows

$$\partial_t\theta(h) = \frac{1}{r}\partial_r(rK(Tw,\rho,S,h)\partial_r h) + \partial_z(K(Tw,\rho,S,h)(\partial_z h - 1)) + \partial_t E, \tag{15}$$

$$\partial_t E = \kappa(T_w)\theta\frac{\sigma}{c_w}(T_w - T_m). \tag{16}$$

The water flux in cylindrical coordinates is of the form

$$\mathbf{q} = -(q^r, q^z)^T, \tag{17}$$

$$q^r = K(T_w, C_w, S, h)\partial_r h,\ \ q^z = K(T_w, h)(\partial_z h - 1). \tag{18}$$

3.2. Heat energy transport by water

D is of the form

$$\mathrm{D} = \begin{pmatrix} D_{1,1} & D_{1,2} \\ D_{2,1} & D_{2,2} \end{pmatrix} = \begin{pmatrix} \alpha_L((q^r)^2 + \alpha_T((q^z)^2 & (\alpha_L - \alpha_T)(q^r q^z) \\ (\alpha_L - \alpha_T)(q^r q^z) & \alpha_L((q^z)^2 + \alpha_T((q^r)^2 \end{pmatrix}\frac{1}{|\vec{q}|} \tag{19}$$

Denote by

$$QT^r = -q_r T_w + \theta(D_{1,1}\partial_r T_w + D_{1,2}\partial_z T_w + D_o\theta \tag{20}$$

$$QT^z = -q_z T_w + \theta(D_{2,1}\partial_r T_w + D_{2,2}\partial_z T_w + D_o\theta. \tag{21}$$

Then, the heat energy transport reads as

$$c_v\partial_t(\theta T_w) - \left(\frac{1}{r}\partial_r(rQT^r) + \partial_z(QT^z\right) = \sigma\theta(T_w - T_m). \tag{22}$$

3.3. Contaminant transport

We define contaminant fluxes QC^r, QC^z in the same way as QT^r, QT^z, where we replace T_w by C_w. Then we rewrite the heat transport equation replacing T_w, QT^r, QT^z by C_w, QC^r, QC^z and obtain contaminant transport equation in cylindrical coordinates.

3.4. Heat conduction in the porous media matrix

For heat conduction in the matrix T_m. we obtain

$$c_m\partial_t T_m - \lambda\left(\frac{1}{r}\partial_r(rQT_m) + \partial_z(\partial_z T_m))\right) = \sigma\theta(T_w - T_m). \tag{23}$$

where $QT_m^r = \partial_r T_m$.

These governing equations are completed by corresponding boundary conditions including the external driven forces. For simplicity, we assume that on the boundary there are prescribed fluxes or values of the unknown h, C_w, T_w, T_m and a combination of them. In fact, also water and heat energy transmission from external driven forces into facade could be considered and the corresponding transmission coefficient could be scaled by the solution of the inverse problem.

3.5. Influence of adsorbed contaminant on heat energy equation

Our mathematical model can be easily extended to the case when adsorption process is linked with heat energy gains or loses. The additional heat source term can be modelled by means of HT

$$HT = sign(\partial_t S)H\big(sign(\partial_t S)\big)\partial_t S, \tag{24}$$

where $H(1)$ is heat energy gain and $H(-1)$ is heat energy lose of unite mass of adsorbed contaminant. The term HT we add to the heat transport equation (22).

4. Numerical method

In our approximation scheme we apply operator splitting, flexible time stepping and a finite volume method in space variables. The time derivative we approximate by backwards difference and then we integrate our system over the angular control volume $V_{i,j}$ with the corners $r_{i\pm1/2}, z_{j\pm1/2}$ and with the length $(\Delta r, \Delta z)$ of the edges.Then, our approximation linked with the inner grid point (r_i, z_j) at the time $t = t_k$ (we will use $K(U) := K(T_w^{k-1}, C_w^{k-1}, S^{k-1}, h)$) is

$$\begin{aligned}
\frac{\theta(h)-\theta(h^{k-1})}{\tau}\Delta r\Delta z \quad & -\Delta z\frac{r_{i+1/2}}{r_i}\left[\frac{K(U_{i+1})+K(U)}{2}\left(\frac{h_{i+1}-h}{\Delta r}\right)\right] \\
& +\Delta z\frac{r_{i-1/2}}{r_i}\left[\frac{K(U)+K(U_{i-1})}{2}\left(\frac{h-h_{i-1}}{\Delta r}\right)\right] \\
& -\Delta r\left[\frac{K(U_{j+1})+K(U)}{2}\left(\frac{h_{j+1}-h}{\Delta z}-1\right)\right] \\
& +\Delta r\left[\frac{K(U)+K(U_{j-1})}{2}\left(\frac{h-h_{j-1}}{\Delta z}-1\right)\right] = \frac{E-E^{k-1}}{\tau}\Delta r\Delta z.
\end{aligned} \tag{25}$$

4.1. Quasi-Newton linearization

In each (r_i, z_j) we linearize θ in terms of h iteratively (with iteration parameter l) following [Cellia at all] in the following way

$$\frac{\theta(h^{k,l+1})-\theta(h^{k-1})}{\tau} = R^{k,l}\frac{h^{k,l+1}-h^{k,l}}{\tau} + \frac{\theta^{k,l}-\theta^{k-1}}{\tau}, \tag{26}$$

where

$$R^{k,l} = \frac{\partial\theta^{k,l}}{\partial h^{k,l}} = (\theta_s-\theta_r)(1-n)\alpha(\alpha h^{k,l})^{n-1}(1+(\alpha h^{k,l})^n)^{-(m+1)} \tag{27}$$

for $h^{k,l} < 0$, else $R^{k,l} = 0$. We stop iterations for $= l^*$, when $h^{k,l^*+1} - h^{k,l^*} \leq tollerance$ and then we put $h^k := h^{k,l^*+1}$. Finally we replace the nonlinear term $K(U^k)$ by $K(U^{k,l})$, then our approximation scheme became linear in terms of $h^{k,l+1}$. Generally, we speed the iteration by a special construction of starting point $h^{k,0} \approx h^{k-1}$ and using suitable damping parameter in solving corresponding linearized system. Solution of complex system by **operator splitting method**. To obtain approximate solution for temperature in water and matrix at the time section $t = t_k$ when starting from $t = t_{k-1}$ we use the obtained flow characteristics from $t = t_k$ for θ^k, h^k and $\vec{q}^k$ and for matrix $\overline{D}^k$.

To obtain approximation linked with the boundary points we apply the same strategy of FVM where the control volume $V_{i,j}$ is only half or quoter of the $\Delta r\Delta z$ corresponding to the inner grid points. All iterations we realize in flow part of the model thanks to the operator splitting strategy. The other model variables are taken from the time section $k-1$. The approximation of other model equation is very similar and must be done carefully for flux $\vec{q}$ and matrix $\vec{D}$.

5. Inverse problems

We choose the optimal experimental scenarios for determination of all model parameters which we restore successively. The determination of parameters K_s, n, α, α_L and α_T we have discussed in our previous contributions (see [5],[6]). We shortly discuss the determination of transmission coefficient σ and matrix heat conduction λ, where we discuss the influence of T_w, C_w, S which was neglected (because of a reduced model) in our previous contributions. By means of our $3D$ sample we can choose a suitable input/output boundary conditions to create not invasive and relative simple measurements for determination of required model parameters via the solution of inverse problems. To validate the reliability of the used scenario we compute the corresponding direct problem (when model parameters are given) and we create the data (original) corresponding to chosen characteristics. Then, we apply some noise (generated by random function) to the original data and these will represent our measurements of corresponding characteristics. Finally, we forget the original model data and iteratively we construct the new (optimal) model data, minimizing the distance of computed characteristics with the original ones. We successively determine the required model data (flow, dispersion, adsorption, heat transmission). Also we test the reliability of the obtained model parameters by choosing different starting parameters in the iteration procedure and changing the level of added noise. These facts and the sensitivity of characteristics on model parameters create the ground for suitability of suggested experimental scenario.

5.1. Model data and solution

In our numerical experiments we assume the following model data ([CGS])

$\theta_0 = 0.38,\ \theta_r = 0,\ K_s = 2.4 \times 10^{-4},\ \alpha = 0.0189,\ n = 2.81,\ H(0) = 5, g = 981,\ \lambda_v = 0.03,\ \lambda = 0.1, D_0 = 0.01,$ $\alpha_L = 1, \alpha_T = \frac{1}{10}, c_v = c_m = 1, \rho_m = 1, \sigma = 1$ and $\kappa = 0.05$.

To determine the transmission coefficients σ and λ, we consider the original temperature of sample $90°\mathrm{C}$ and the temperature of infiltrated water $10°\mathrm{C}$. The water infiltrates through the mantel and we measure the temperature in the center on the top of the sample, which is (together with the bottom) flow and temperature isolated. Original sample is almost dry $(h = -200)$. The example of original and perturbed characteristic used for determination of σ, λ is drawn below.

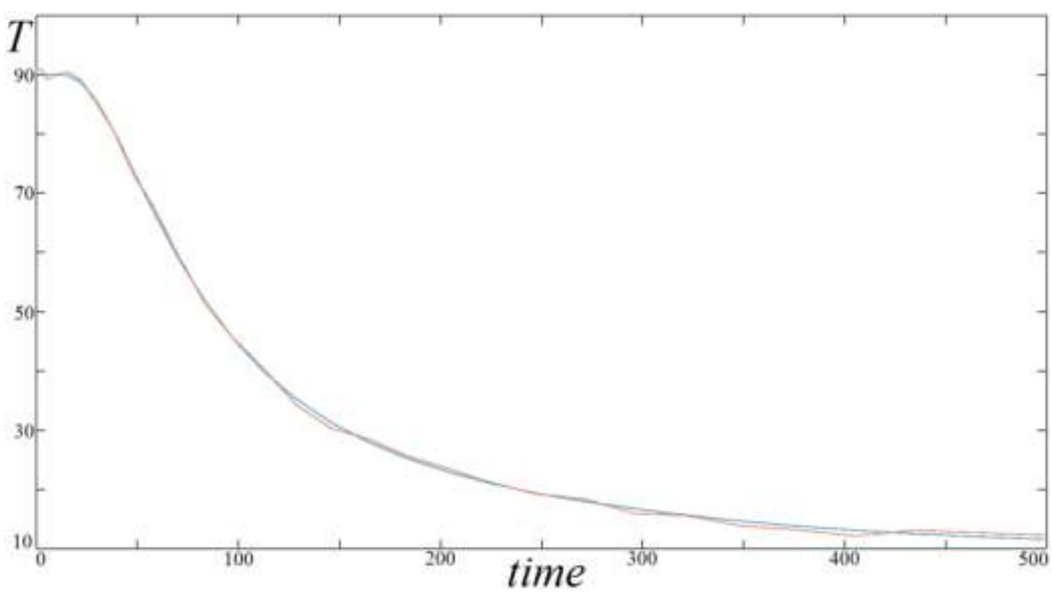

Fig. 2: Time evolution of the temperature in the center of the sample top (blue) and with random noise (red).

The obtained determination results are collected in the following table.

Table 1: Starting points and different optimal values of σ, λ for different random noises up to 1°C.

σ_{start}	2	2	0.5	0.5	2	2	0.5	0.5
λ_{start}	0.5	0.5	0.5	0.5	0.05	0.05	0.05	0.05
$\sigma_{optimal}$	0.9498	0.9684	1.0515	1.0529	1.0396	1.0581	0.9407	1.0575
$\lambda_{optimal}$	0.09954	0.10089	0.10119	0.09949	0.10210	0.09933	0.09897	0.09972

The noise 1°C causes defect up to 6%. The flow, temperature and adsorption influence at the infiltration time $t = 100s$ with same boundary conditions as before with $C_w = 0.035$ in inflow water are drawn in the figure below.

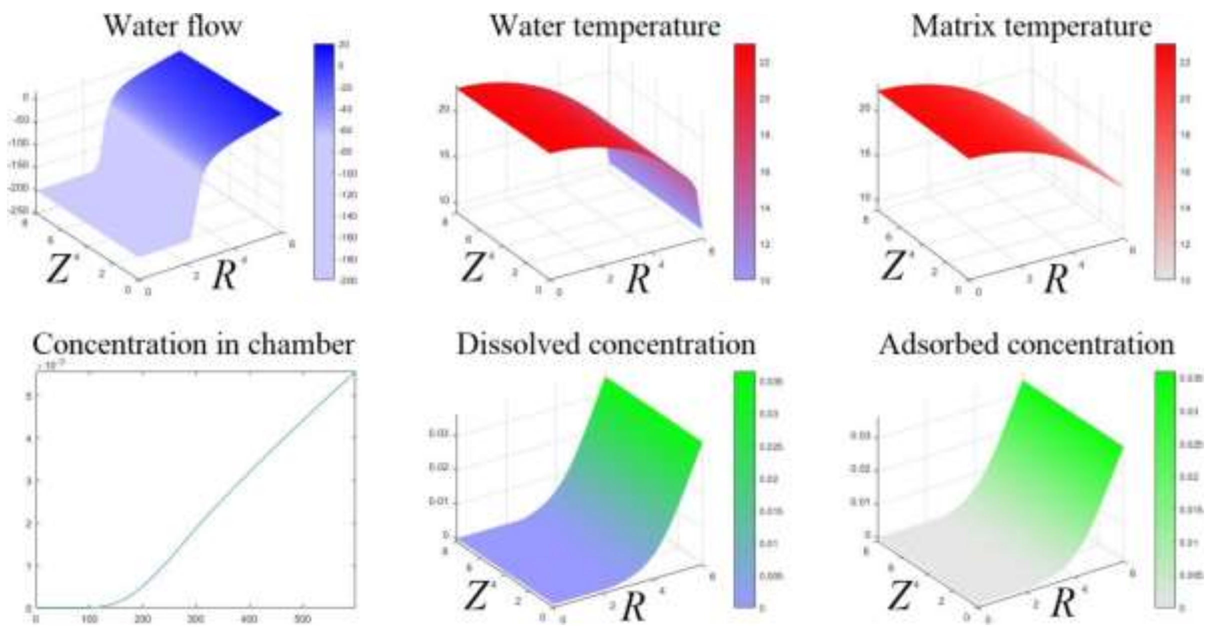

Fig. 3: Water flow, water temperature, matrix temperature, dissolved concentration in the water and adsorbed concentration in the matrix at $t = 100s$ and time evolution of concentration of the outflowed water in the collector chamber.

6. Conclusion

Numerical modelling of heat and mass transport into unsaturated porous media is discussed. The mathematical model includes heat and contaminant transport with heat exchange and adsorption. The adsorbed contaminant and the temperature influence the hydraulic permeability and the change of the porosity. Efficient numerical method is developed on the base of operator splitting, flexible time discretization and finite volume method.

A laboratory experiment scenario is proposed to determine the heat transmission coefficient and heat conductivity in porous media matrix. In numerical experiments, the efficiency of the numerical method is demonstrated.

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