Mathematical Modelling and Analysis
Volume 23, Issue 4, 554–567, 2018
https://doi.org/10.3846/mma.2018.033

http://mma.vgtu.lt
ISSN: 1392-6292
eISSN: 1648-3510

On Mathematical Modelling of the Solid-Liquid Mixtures Transport in Porous Axial-Symmetrical Container with Henry and Langmuir Sorption Kinetics

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Received October 2, 2017; revised July 20, 2018; accepted August 28, 2018

Abstract. In this paper we study the diffusion and convection filtration problem of one substance through the pores of a porous material which may absorb and immobilize some of the diffusing substances. As an example we consider a round cylinder with filtration process in the axial direction. The cylinder is filled with a sorbent. We derive the system of two partial differential equations (PDEs), one expressing the rate of change of concentration of water in the pores of the sorbent and the other - the rate of change of concentration in the sorbent or kinetical equation for absorption. The approximation of corresponding initial boundary value problem of the system of PDEs is based on the conservative averaging method (CAM). This procedure allows us to reduce the 2-D axisymmetrical mass transfer problem described by a system of PDEs to the initial value problem for a system of ordinary differential equations (ODEs) of the first order. We consider also a 1–D model problem and investigate the dependence of the concentration of water and sorbent on the time.

Keywords: absorption, averaging method, analytical and numerical solution, diffusion problem, sorbents, special splines.

AMS Subject Classification: 76S05; 97N80; 97M50; 65N25; 65M70; 65M99.

1 Introduction

The study of hydrodynamic flow and heat transfer through a porous media becomes much more interesting due to its wide and diverse applications [1], [7]. The numerical algorithms for modelling of liquid polymer injection are considered in the article [14], so that the liquid polymer is flowing through a porous medium. Many mathematical models are developed for the analysis of such processes, for example mathematical models of moisture movement in wood, when the wood is considered as porous media [6].

For the necessary engineering accuracy to solve above mentioned problems the conservative averaging method (CAM) with special integral hyperbolic and exponential type splines is used. The method was proposed by A. Buikis, and it was further developed in several papers [3], [13]. In CAM by applying the special splines with two different functions of the hyperbolic or exponential type the problems of mathematical physics in 3-D with piece-wise coefficients with respect to one coordinate are reduced to problems for system of PDEs in 2-D and 1-D [4]. In this paper we study the linear heat and moisture transfer processes in the porous multilayered media layer by using CAM with special integral hyperbolic type splines. For one layer case a similar process was analysed in [7], [9].

Filtration is the separation process of removing solid particles, microorganisms or droplets from a liquid or a gas by depositing them on a filter medium [15]. In order to evaluate the solute concentration in the solid, several isotherms can be taken into account. In the article [16] the Langmuir expression was considered, correlating it with the saturation concentration and a Langmuir adsorption parameter p (see Langmuir isotherm, Section 2 with $a = \frac{\tilde{u}}{\gamma(1+p\tilde{u})}$).

This paper deals only with filtration processes of solid-liquid mixtures (suspensions, slurries, sludges) [10]. For adsorption kinetics we use the linear Henry ([8]) and the nonlinear Langmuir ([2], [11], [12]) sorptions isotherms. A contaminant transport model with Langmuir sorption under nonequilibrium conditions which is described by two coupled equations – advective-dispersion equation and nonequilibrium sorption equations is considered in [2].

2 The mathematical model

In this paper we study the filtration process with diffusion and convection transport in the domain

$$\Omega = \{(r, z, \phi) : 0 \le r \le R, 0 \le z \le L, 0 \le \phi \le 2\pi\}.$$

Ω consists of porous material, where incompressible liquid pollutants move in z-direction through the pores of filter.

This problem has practical applications and also the theoretical interest in mathematical physics since several small parameters appear in the model. These parameters are connected with some geometrical dimensions in the problem and also with the relations between the coefficients of the given equations.

We derive two equations, the first one describes the adsorbed phase of concentration $a(r,z,t)$ for the pollutants which are absorbed per unit volume and per unit time. The second equation defines the aqueous phase of pollutants concentration $u(r,z,t)$ in sorbent pores. The following non-stationary convection – diffusion PDEs in the cylindrical coordinates are given [5], [17]:

$$\begin{cases} \frac{1}{r}\frac{\partial}{\partial r}\Big(D_r r\frac{\partial u}{\partial r}\Big) + D_z\frac{\partial^2 u}{\partial z^2} + V_0\frac{\partial u}{\partial z} = m\frac{\partial u}{\partial t} + \frac{\partial a}{\partial t}, \\ \frac{\partial a}{\partial t} = \beta(u-\tilde{u}), \ \ r\in[0,R],\ z\in[0,L],\ t>0, \end{cases}$$

where $a=\tilde{u}/\gamma$ is the expression for the linear isotherm of Henry, D_r, D_z are the transversal and tangential diffusion coefficients or the dispersion coefficients, $V_0 = const$ is the pore water velocity in z-direction, m is the fraction of the total volume of the material occupied by pores, $\tilde{u}$ is concentration of pollutants, which is in local equilibrium conditions $\frac{\partial a}{\partial t} = 0$ with the amount of liquid sorbent, t is the time, β is the kinetical coefficients or the sorption rate constant, $1/\gamma$ is the Henry coefficient for the sorbent characteristic. We assume that all coefficients in the PDEs are constant and independent of concentration.

For nonlinear sorption we use $a=\tilde{u}/(\gamma(1+p\tilde{u}))$, referred as the Langmuir isotherm, where p is positive parameter (for $p=0$ we have Henry isotherm).

Initial conditions for $t=0$ are defined as $a(r,z,0)=0, u(r,z,0)=0$ or $u(r,z,0)=U_0$, where U_0 is the initial concentration of liquid solutions. We use following boundary conditions:

$$\frac{\partial u(0,z,t)}{\partial r} = \frac{\partial a(0,z,t)}{\partial r} = 0, \quad u(R,z,t)=a(R,z,t)=0,$$
$$u(r,L,t)=u_0(t)=U_0(1-\tanh(\alpha t)), \quad \frac{\partial u(r,0,t)}{\partial z}=0, \quad \frac{\partial a(r,0,t)}{\partial z}=0,$$

where $\alpha = const > 1, U_0 = const > 0$. The concentration u on the inlet is decreasing with respect to t.

For the normed parameters $u_1 = u/U_0$, $a_1 = a\gamma/U_0$, $\tilde{u}_1 = \tilde{u}/U_0$, $t_1 = t\gamma\beta$ we have the following system:

$$\begin{cases} m\gamma\beta\frac{\partial u_1}{\partial t_1} + \beta\frac{\partial a_1}{\partial t_1} = \frac{1}{r}\frac{\partial}{\partial r}\Big(D_r r\frac{\partial u_1}{\partial r}\Big) + D_z\frac{\partial^2 u_1}{\partial z^2} + V_0\frac{\partial u_1}{\partial z}, \\ \frac{\partial a_1}{\partial t_1} = u_1 - f(a_1), \quad r\in[0,R],\ z\in[0,L],\ t_1>0, \end{cases} \tag{2.1}$$

where $f(a_1) = \frac{a_1}{1-\tilde{p}a_1}, \tilde{p} = p\,U_0, u_1(r,L,t_1) = u_0(t_1) = 1-\tanh(\alpha_1 t_1), \alpha_1 = \frac{\alpha}{\gamma\beta}$. For $\tilde{p}=0$ we have the linear Henry isotherm.

3 The conservative averaging method in z-direction

We consider conservative averaging method (CAM) of the special integral splines with hyperbolic trigonometrical functions for solving the initial boundary-value problem in z-direction [3]. This procedure allows us to reduce the 2-D problem in r, z-directions to a 1–D problem in r-direction. Using CAM in z-direction with parameter a_z we have

$$u_1(r,z,t_1) = u_v(r,t_1) + m_z(r,t_1)0.5L\sinh(a_z(z-L/2))/\sinh(0.5a_zL) + e_z(r,t_1)\Big(\frac{\cosh(a_z(z-L/2)) - A_z}{8\sinh^2(a_zL/4)}\Big),$$

where $u_v(r,t_1) = \frac{1}{L}\int_0^L u_1(r,z,t_1)dz$, $A_z = \sinh(a_zL/2)/(a_zL/2)$. The parameter a_z can be selected for minimizing the maximal error. We can see if the parameters $a_z > 0$ tend to zero then in the limit we get the integral parabolic spline [13]:

$$A_0 \to 1: \quad u_1(r,z,t_1) = u_v + m_z(z-L/2) + e_z\big((z-L/2)/L^2 - 1/12\big).$$

The unknown functions $m_z = m_z(r,t_1), e_z = e_z(r,t_1)$, can be determined from the following conditions:

1. for $z=0:\quad m_zd - e_zk = 0,\quad m_z = e_zp_1,\quad p_1 = k/d,$ $u_1(r,0,t) = u_v - m_zL/2 + e_zb,$
2. for $z = L:\quad u_{0z} = u_v + m_zL/2 + e_zb,\quad e_z = (u_{0z} - u_v)/g_0$, where $d = 0.5La_z\coth(0.5a_zL),\quad k = 0.25a_z\coth(0.25a_zL),\quad b = ((\cosh(a_zL/2) - A_z)/(8\sinh^2(a_zL/4)),\quad g_0 = b + 0.5Lp_1.$

Now the 1–D initial-value problem (2.1) is given in the following form

$$\begin{cases} m\gamma\beta\dfrac{\partial u_v}{\partial t_1} + \beta\dfrac{\partial a_v}{\partial t_1} = \dfrac{1}{r}\dfrac{\partial}{\partial r}\Big(D_r r\dfrac{\partial u_v}{\partial r}\Big) + a_0^2(u_{0z} - u_v), \\ \dfrac{\partial a_v}{\partial t_1} = u_v - f(a_v), \quad r\in[0,R],\ \ t_1 > 0, \\ \dfrac{\partial u_v(0,t_1)}{\partial r} = 0, \quad \dfrac{\partial a_v(0,t_1)}{\partial r} = 0, \quad u_v(R,t_1) = a_v(R,t_1) = 0, \\ u_v(r,0) = a_v(r,0) = 0, \end{cases} \tag{3.1}$$

where $a_v(r,t_1) = \frac{1}{L}\int_0^L a_1(r,z,t_1)dz$, $a_0^2 = (2D_z\frac{k}{L} + V_0p_1)/g_0$, $f(a_v) = \frac{a_v}{1-\tilde{p}a_v}$, here we use the averaging of the nonlinear term with the remaining form.

4 CAM in r-direction

Using averaged method in r-direction with parameters a_r we have

$$u_v(r,t_1) = u_{vv}(t_1) + m_r(t_1)f_m(r) + e_r(t_1)f_e(r),$$

where $f_m(r) = (\frac{0.25R^2(a_r)^2\sinh(a_r(r-0.5R))}{\sinh(0.5a_rR)(d_1-1)} - 1)$, $f_e(r) = (\frac{\cosh(a_r(r-0.5R))-A_r}{8\sinh^2(a_rR/4)})$, $u_{vv}(t_1) = \frac{2}{R^2}\int_0^R ru_v(r,t_1)dr$, $\frac{2}{R^2}\int_0^R rf_m(r)dr = \frac{2}{R^2}\int_0^R rf_e(r)dr = 0$, $A_r = \frac{sinh(a_rR/2)}{a_rR/2}$, $d_1 = 0.5Ra_r\coth(0.5a_rR)$. We use the following values of parameters $a_r = a_0\sqrt{1/D_r}$. If the parameters $a_r > 0$ tend to zero, then in the limit we get the integral parabolic spline:

$$u_v(r,t_1) = u_{vv} + m_r\Big(\frac{6}{R}(r-0.5R) - 1\Big) + e_r\Big(\frac{(r-0.5R)^2}{R^2} - \frac{1}{12}\Big).$$

From boundary conditions (3.1) the unknown coefficients-functions are obtained:

1. for $r = 0$, $m_r d_r - e_r k_r = 0$ or $m_r = e_r p_r$,
2. for $r = R$, $0 = u_{vv} + m_r b_m + e_r b_e$ or $e_r = -u_{vv}/g_r$, where
   $d_r = \frac{0.5 d_1 R (a_r)^2}{d_1 - 1}$, $k_r = 0.25 a_r \coth(0.25 a_r R)$, $p_r = k_r/d_r$,
   $b_e = ((\cosh(a_r R/2) - A_r)/(8\sinh^2(a_r R/4))$, $b_m = \frac{0.25 R^2 (a_r)^2}{d_1 - 1} - 1$,
   $g_r = b_e + p_r b_m$.

Now the 1–D initial-value problem (3.1) is defined as the ODEs system:

$$\begin{cases} m\gamma\beta \dfrac{\partial u_{vv}}{\partial t_1} + \beta \dfrac{\partial a_{vv}}{\partial t_1} = -b_0^2 u_{vv}(t_1) + a_0^2 \big(u_{0z}(t_1) - u_{vv}(t_1)\big), \\ \dfrac{\partial a_{vv}(t_1)}{\partial t_1} = u_{vv}(t_1) - f(a_{vv}), \;\; t_1 > 0, \\ u_{vv}(0) = 0, a_{vv}(0) = 0, \end{cases} \tag{4.1}$$

where $f(a_{vv}) = \frac{a_{vv}(t_1)}{1 - \tilde{p} a_{vv}(t_1)}$, $a_{vv}(t_1) = \frac{2}{R^2}\int_0^R r a_v(r, t_1) dr$, $b_0^2 = 4 D_r k_r / R g_r$.

We rewrite the 1–D initial-value problem for system ODEs (4.1) in the following normal form:

$$\begin{cases} \dot{u}_{vv}(t_1) = b_{11} u_{vv}(t_1) + b_{12} f(a_{vv}) + f_1 U_{0z}(t_1), \\ \dot{a}_{vv}(t_1) = b_{21} u_{vv}(t_1) + b_{22} f(a_{vv}), \;\; t_1 > 0, \\ u_{vv}(0) = 0, \quad a_{vv}(0) = 0, \end{cases}$$

where $b_{11} = -\frac{\beta + b_0^2 + a_0^2}{m\gamma\beta}$, $b_{12} = 1/m\gamma$, $b_{21} = 1$, $b_{22} = -1$, $f_1 = -\frac{a_0^2}{m\gamma\beta}$. If $\tilde{p} = 0$ then we have the following vector form of linear ODEs system:

$$\dot{W}(t_1) = A W(t_1) + F, \quad W(0) = 0,$$

where $W(t_1)$, $F(t_1)$ are the 2-order vector-column with elements $(u_{vv}(t_1), a_{vv}(t_1))$, $(f_1 U_{0z}(t_1), 0)$. A is the 2-order matrix

$$A = \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}.$$

The averaged linear and nonlinear ($\tilde{p} \neq 0$) solutions are obtained with the Matlab solver "ode15s".

5 Backward orientation for CAM

To estimate the parameters a_z, a_r we use the backward version of CAM: first the CAM is used in r-direction and then in z-direction. Then we get in r-direction the solution

$$u_1(r, z, t_1) = u_v(z, t_1) + m_r(z, t_1) f_m(r) + e_r(z, t_1) f_e(r),$$

where $u_v(z, t_1) = \frac{2}{R^2}\int_0^R r u_1(r, z, t_1) dr$, and a_r is a fixed parameter. For boundary conditions we get $e_r = -u_v/g_r$, $m_r = e_r p_r$ and the problem (2.1) is reduced to

$$\begin{cases} m\gamma\beta \dfrac{\partial u_v}{\partial t_1} + \beta \dfrac{\partial a_v}{\partial t_1} = D_z \dfrac{\partial^2 u_v}{\partial z^2} + V_0 \dfrac{\partial u_v}{\partial z} - b_0^2 u_v, \\ \dfrac{\partial a_v}{\partial t_1} = u_v - f(a_v), \;\; z \in [0, L], \; t_1 > 0, \end{cases} \tag{5.1}$$

$$\begin{cases} \dfrac{\partial u_v(0,t_1)}{\partial z} = 0, \ \dfrac{\partial a_v(0,t_1)}{\partial z} = 0, \ u_v(L,t_1) = a_v(L,t_1) = u_{0z}, \\ u_v(z,0) = a_v(z,0) = 0, \end{cases}$$

where $a_v(z,t_1) = \frac{2}{R^2}\int_0^R r a_1(r,z,t_1)dr$, $b_0^2 = \frac{4D_r k_r}{R g_r}$, $f(a_v) = \frac{a_v}{1-\tilde{p}a_v}$.

Next we use CAM in z-direction

$$u_v(z,t_1) = u_{vv}(t_1) + m_z(t_1)\frac{0.5L\sinh(a_z(z-L/2))}{\sinh(0.5a_zL)} + e_z(t_1)\Big(\frac{\cosh(a_z(z-L/2)) - A_z}{8\sinh^2(a_zL/4)}\Big),$$

where $u_{vv}(t_1) = \frac{1}{L}\int_0^L u_v(z,t_1)dz$, $a_z = b_0\sqrt{1/D_z}$. We get from boundary conditions that $e_z = (u_{0z} - u_{vv})/g_0$, $m_z = e_z p_1$ and then problem (5.1) is given in the form of (4.1), where $a_{vv}(t_1) = \frac{1}{L}\int_0^L a_v(z,t_1)dz$, $a_0^2 = (2D_z\frac{k}{L} + V_0p_1)/g_0$. Therefore in every CAM orientation we have obtained two algebraic equations to determine the spline parameters $a_r = f_1(a_z) = a_0\sqrt{1/D_r}, a_z = f_2(a_r) = b_0\sqrt{1/D_z}$.

The optimal parameters can be obtained by solution of these equations with the method of iteration. For $V_0 \neq 0$, for CAM of equations (5.1) we also can use the exponential type spline [4].

6 CAM for model equations

For approbation of CAM in r-direction and estimate of the parameter a_r we consider a model – stationary 1-D boundary-value problem:

$$\begin{cases} D\frac{1}{r}\big(ru'(r)\big)' - a_0^2u(r) = F_0, \quad r\in[0,R], \\ u'(0) = 0, \quad u(R) = u_0, \end{cases}$$

where $u_0, F_0, a_0 > 0, D > 0$ are given constants. The analytical solution is defined as $u(r) = C_1I_0(a_1r) - f_1, \quad C_1 = (u_0+f_1)/I_0(a_1R)$, where $I_0'(0) = I_1(0) = 0$, I_0, I_1 are the modified Bessel functions, $f_1 = F_0/a_0^2$, $a_1 = a_0/\sqrt{D}$. Using averaging method in r-direction with parameter a_r, we get $u(r) = u_v + mf_m(r) + ef_e(r)$, where $m = (u_0 - u_v)p_r/g_r$, $e = \frac{u_0-u_v}{g_r}$, $u_v = \frac{4Du_0k_r - F_0g_rR}{4Dk_r + a_0^2g_rR}$. For $D_1 = 1, F_0 = -10, a_0 = 2, a_r = 2, u_0 = 1, R = 5$ we have the following maximal errors: a) 1.278 for the parabolic spline, $a_r = 10^{-4}$, b) 0.0021 for the hyperbolic spline, see Figure 1.

7 1–D non-stationary model problem for a and u

The normed boundary-initial problem (2.1) not depending on r is given in the following form:

$$\begin{cases} m\gamma\beta\dfrac{\partial u}{\partial t} + \beta\dfrac{\partial a}{\partial t} = D_z\dfrac{\partial^2 u}{\partial z^2} + V_0\dfrac{\partial u}{\partial z}, \\ \frac{\partial a}{\partial t} = u - f(a), \ \ z\in[0,1], \ \ t>0, \end{cases} \tag{7.1}$$

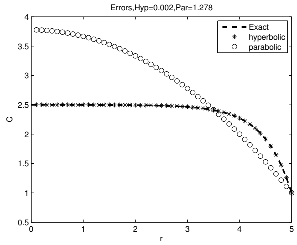

Figure 1. Solution of the model equations

where $u = u(z,t)$, $a = a(z,t)$, $f(a) = a/(1-ap)$, $u(1,t) = 1 - \tanh(0.2t)$, $u(z,0) = 0$ or $u(z,0) = 1$, $\frac{\partial u(0,t)}{\partial z} = \frac{\partial a(0,t)}{\partial z} = \frac{\partial a(L,t)}{\partial z} = 0$. Using MATLAB program routine "pdepe" we can obtain the concentrations $u(z,t), a(z,t)$.

8 Some numerical results

The results of calculations are obtained by MATLAB. We use the discrete grid values $t_n = n\frac{t_f}{N_t}$, $n = 0,\dots,N_t$, $z_i = i\frac{L}{N_z}$, $i = 0,\dots N_z$, $r_j = j\frac{R}{N_r}$, $j = 0,\dots N_r$, $N_z = 10$, $N_t = 50$, $N_r = 30$, $t_f = 5; 50$, $R = 0.15[m]$, $L = 1[m]$, and parameters $U_0 = 25g/l$, $\beta = 1; 3$, $\gamma = 1; 2$, $m = 0.4$, $D_r = 10^{-4}[\frac{m^2}{min}]$, $D_z = 5.10^{-4}[\frac{m^2}{min}]$, $V_0 = 0.1[\frac{m}{min}]$, $\alpha_1 = 0.2$, $\tilde{p} = 0; 0.1; 1; 5; 10, t_1 \in [0, t_f]$.

8.1 2–D problem

Computations are done for $u_1(r,z,0) = 0$, $\beta = 3$, $\gamma = 1$, $a_z = 10$, $t_f = 50$, $\tilde{p} = 0$, the final time is $\frac{t_f}{\beta\gamma} = 50/3[min]$. The results of calculations are shown in Figures 2–7.

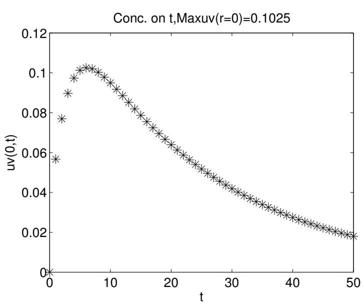

Figure 2. Averaging concentration u_v depending on t_1 for $r = 0$

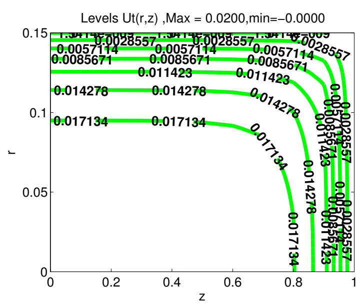

Figure 3. The levels of concentration $u(r,z,t_f)$ for $t_f = 50$

With different CAM solvers the following results are obtained: direct CAM orientation $a_r = 34.155$, backward CAM orientation $a_z = 11.53$, direct CAM orientation $a_r = 34.032$, backward CAM orientation $a_z = 11.5175$, direct CAM orientation $a_r = 34.0312$, backward CAM orientation $a_z = 11.5176$, direct

CAM orientation $a_r = 34.0312$. In all cases we have a quickly converging iteration process. The results of calculations are presented in Figures 8–11.

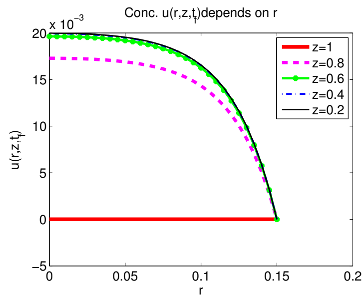

Figure 4. Concentration $u(r, z, t_f)$ profile depending on r for $t_f = 50$

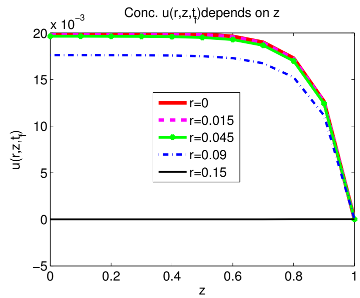

Figure 5. Concentration $u(r, z, t_f)$ profile depending on z for $t_f = 50$

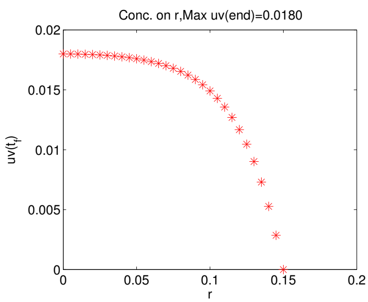

Figure 6. Averaging concentration $u_v(r, t_f)$ depending on r for $t_f = 50$

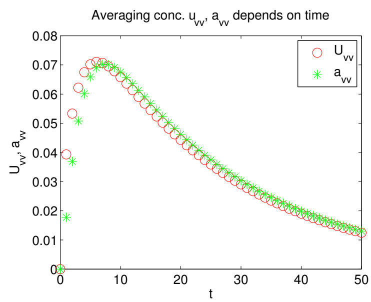

Figure 7. Averaging concentration $u_{vv}(t_1)$ and $a_{vv}(t_1)$ depending on t_1

The maximal values of $u(r, z, t_f) = 0.0198, u_{vv}(t_1) = 0.0706, a_{vv}(t_1) = 0.0698$ and $u_{vv}(t_f) = 0.013$ are equal for both CAM orientation.

The maximal dimensional value of concentration at the final time $0.50[\frac{g}{l}]$ agrees well with the experiment value $0.54[\frac{g}{l}]$. Experimental data have been obtained studying the filtration process through hemp shives using the adsorption column "Adsorption CE 583" at laboratory of Faculty of Engineering, RTA.

Matrix A has the following eigenvalues: $\lambda_1 = -3.61, \lambda_2 = -0.042$. We can see, that at the outlet of the domain $0.5L \leq z \leq L$ the concentration u is small and:

1. the averaging concentration of u_v for $r = 0$ is decreasing in the time with maximal value at $t_1 = 5$ (Figure 2),
2. the concentration u for $t_1 = 50$ is maximal for $r = 0$ and it increases in z-direction (Figures 3–6),
3. the averaging concentrations of u_{vv} and a_{vv} are equal for both CAM orientation and depend on time, $a_{vv} > u_{vv}$ only for $t_1 > 10$,
4. the averaging concentration for CAM in r-direction of $u_v(z, t_f)$ is maximal at $z = 0$ and decreases in z-direction (Figure 11).

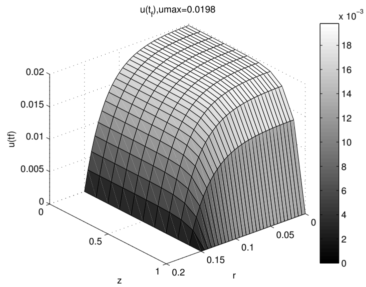

Figure 8. Concentration $u(r,z,t_f)$ for $t_f = 50$

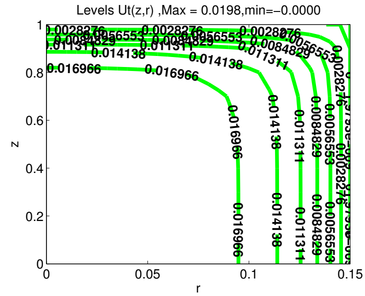

Figure 9. Averaging concentration $u_v(r,z,t_f)$ depending on r for $t_f = 50$

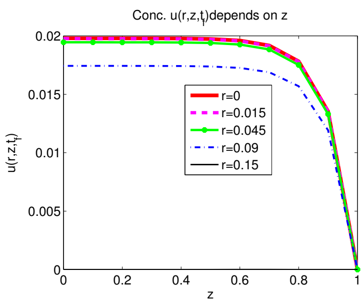

Figure 10. Averaging concentration $u_v(r,z,t_f)$ depending on z for $t_f = 50$

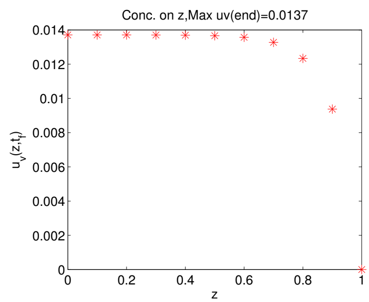

Figure 11. Averaging concentration $u_v(z,t_f)$ depending on z for $t_f = 50$

The maximal values of $u_v(r,t_f), u_v(0,t), u(r,z,t_f), u_{vv}(t),\ a_{vv}(t),\ u_{vv}(t_f)$ for different $\tilde{p}$ are presented in Table 1.

Table 1. The maximal values of $u_v(r,t_f)$, $u_v(0,t)$, $u(r,z,t_f)$, $u_{vv}(t)$, $a_{vv}(t)$ and $u_{vv}(t_f)$ depending on $\tilde{p}$

$\tilde{p}$	$u_v(r,t_f)$	$u_v(0,t)$	$u(r,z,t_f)$	$u_{vv}(t)$	$a_{vv}(t)$	$u_{vv}(t_f)$
0	.0180	.1025	.0198	.0706	.0698	.013
0.1	.0179	.1029	.0199	.0714	.0700	.013
1.0	.0172	.1067	.0191	.0740	.0683	.012
5.0	.0144	.1249	.0160	.0865	.0603	.010
10	.0118	.1474	.0131	.1022	.0505	.008
1.0^*	.0214	.0863	.0237	.0598	.0561	.015
1.0_*	.0012	.2400	.0013	.1604	.1405	.0008

We can see, that with increasing $\tilde{p}$ the filtration process goes faster (see $u_v(r,t_f)$, $u_{vv}(t)$,$a_{vv}(t)$,$u_{vv}(t_f)$), but the maximum value of concentration is increasing (see $u_v(0,t)$, $u_{vv}(t)$). For $\tilde{p} = 5$ in Figure 12 we can see that the averaging concentration $u_{vv} > a_{vv}$ for all $t_1 \in [0,t_f]$.

In the Table 1 by $\tilde{p} = 1.0^*$ are the maximal values for $\beta = 3, \gamma = 2$ ($\lambda_1 = -2.29, \lambda_2 = -0.033$). We can see that the filtration process goes more

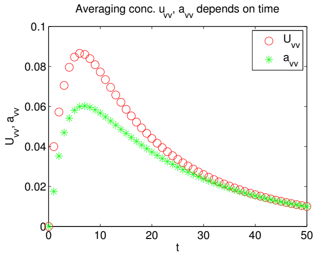

Figure 12. Averaging concentration $u_{vv}(t_1)$ and $a_{vv}(t_1)$ depending on t_1

slowly. For $\tilde{p} = 1.0_*$ and $\beta = 1, \gamma = 1$ ($\lambda_1 = -3.84, \lambda_2 = -0.119$) the filtration process goes more quickly.

Table 2. The values of $u_v(0, t_f)$, $u_{vv}(t_f), a_{vv}(t_f)$ and $Ma-$ maximal value of $a_{vv}(t)$ depending on $\tilde{p}$

$\tilde{p}$	$u_v(0,t_f)$	$u_{vv}(t_f)$	$a_{vv}(t_f)$	Ma
0	.0496	.0453	.0473	.2975
0.1	.0484	.0445	.0462	.2944
1.0	.0410	.0375	.0376	.2647
5.0	.0230	.0210	.0197	.1507
10	.0155	.0141	.0128	.0882
1.0^*	.0490	.0448	.0314	.0896
1.0_*	4.1e-4	3.7e-4	$4.2e-4$	.0875

For the initial condition by $t = 0, u_1 = 1$ we have the following results (see Table 2):

1. the filtration process for initial full container of pollutants concentration goes slower compared with continues in time flow at the inlet (Table 1),
2. $u_{vv}(t_f) < a_{vv}(t_f)$ for $\tilde{p} \leq 1.0$,
3. similarly to Table 1 the nonlinear sorption process is faster,
4. for $\beta = 1, \tilde{p} = 1.0_*$ we have the fast process with the maximal value of $a = 0.875$.

8.2 1–D problem

For $u(z, 0) = u_0 = 0$ and $u(z, 0) = u_0 = 1$ the results of numerical calculations of the problem (7.1) are represented in Table 3. We can see, that the filtration process for $u_0 = 1$ (full container at t=0) is slower compared to $u_0 = 0$. In linear case ($\tilde{p} = 0$) and for $\tilde{p} = 0.1; 1$ we have $a > u$, but for other $\tilde{p}$ we have $a < u$.

In the Figures 13–16 we see detalized results of calculation for $u_0 = 0$.

In the Figures 13, 14 the linear sorption process is represented, where $u(z, t), a(z, t)$ depend on z for fixed time moments: at the initial time $t = 0$ the pollutants concentration at inlet $z = 1$ is $u(1, 0) = 1$, but $u(z, 0) = 0$ for $z < 1$.

Table 3. The values of $u(0,t_f)$, $a(0,t_f)$ and Ma-maximal value of $a(z,t)$ depending on p

$p, u_0 = 0$	$u(0,t_f)$	$a(0,t_f)$	Ma	$p, u_0 = 1$	$u(0,t_f)$	$a(0,t_f)$	Ma
0	.1280	.1363	.6102	0	.1619	.1774	.6099
0.1	.1214	.1286	.5930	0.1	.1466	.1590	.5914
1.0	.0654	.0676	.4287	1.0	.0656	.0681	.4223
5.0	.0209	.0206	.1636	5.0	.0209	.0204	.1614
10	.0125	.0119	.0911	10	.0125	.0119	.0896
1.0^*	.1955	.1663	.4284	1.0^*	.2194	.1885	.4174
1.0_*	$1e-6$	$1e-6$	.4308	1.0_*	$1e-6$	$1e-6$	.4286

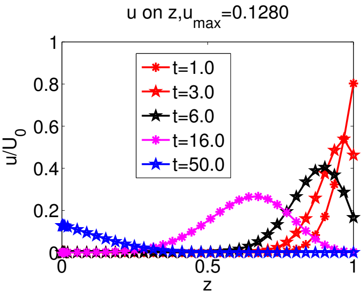

Figure 13. Concentration $u(z,t)$ depending on z for $t = 1; 3; 6; 16; 50, u_0 = 0, \tilde{p} = 0$

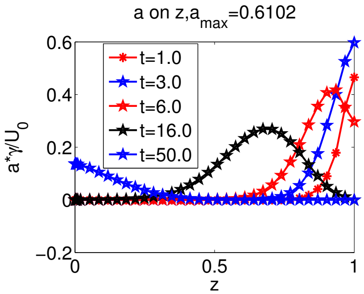

Figure 14. Concentration $a(z,t)$ depending on z for $t = 1; 3; 6; 16; 50, u_0 = 0, \tilde{p} = 0$

For $t > 0$ the concentration of pollutants is defined according the law at inlet of cylinder $u(1,t) = 1 - \tanh(0.2t)$, we consider the flow from the inlet $z = 1$ inside cylinder $z < 1$ and filters with sorbent, where the maximal concentration is $a_{max} = 0.6102$ at $t = 3$. The pollutants concentration is decreasing for $z > 0$ and at the final time moment $t = 50$ the concentration in the outlet $z = 0$ is $u = 0.128$.

In the Figures 15–16 the corresponding nonlinear sorption process is represented with $\tilde{p} = 10$, where $u(z,t), a(z,t)$ depends on t for fixed $z = 0$ (outlet), $z = 0.5$, $z = 1$ (inlet): at the inlet pollutants concentration decreases in time as $u(1,t) = 1 - \tanh(0.2t)$, but inside of the cylinder $z = 0.5$ and at outlet corresponding to $t = 8$, $t = 15$ the strong maximal value (peak) of u is formed, it is decreasing in time and at the final time moment $t = 50$ in the outlet $z = 0$ is $u = 0.0125$. This is 10 times smaller value comparing with $\tilde{p} = 0$, and the filtration process is faster. A similar behaviour is obtained for sorbent with maximal value at inlet $a_{max} = 0.0911$ ($a_{max} = 0.6102$ in the linear case).

In the Figures 17–18 we can see results of calculation for $u(z,t)$ depending on t for fixed $z = 0$ (outlet), $z = 0.5$, $z = 1$ (inlet) and $u_0 = 1, \tilde{p} = 1; 10$. Comparing Figure 17 ($\tilde{p} = 1, u_0 = 1$) with Figure 15 ($\tilde{p} = 10, u_0 = 0$) we see that the maxima for $\tilde{p} = 1$ are smaller (no peaks) and $u(0,50) = 0.0656 > 0.0125$ (for $\tilde{p} = 10$). Comparing the Figure 17 with Figure 18 ($\tilde{p} = 10, u_0 = 1$) we can see that the maxima are greater and in the final time $u(1,50) = 0.0125$ are equal to values in Figure 15.

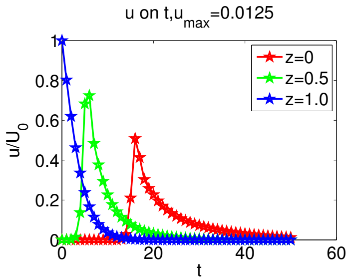

Figure 15. Concentration $u(z,t)$ depending on t for $u_0 = 0, \tilde{p} = 10, z = 0; 0.5; 1$

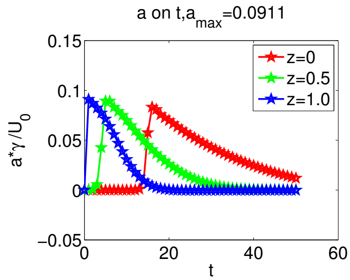

Figure 16. Concentration $a(z,t)$ depending on t for $u_0 = 0, \tilde{p} = 10, z = 0; 0.5; 1$

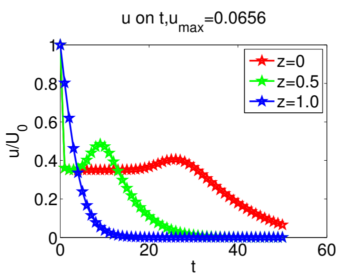

Figure 17. Concentration $u(z,t)$ depending on t for $u_0 = 1, \tilde{p} = 1, z = 0; 0.5; 1$

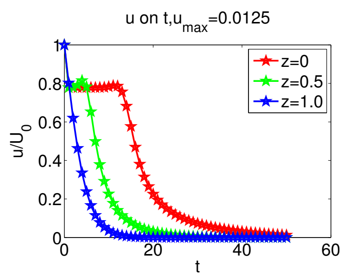

Figure 18. Concentration $u(z,t)$ depending on t for $u_0 = 1, \tilde{p} = 10, z = 0; 0.5; 1$

9 Conclusions

The approximation of corresponding initial boundary value problem of the system of PDEs is based on the conservative averaging method (CAM), where the new hyperbolic type splines are used. For these splines the best parameter for minimal error is calculated using the direct and backward orientation for CAM. Numerical experiments confirmed the correctness of the best parameter calculation using a convergent iteration process. The problem of the system of 3D PDEs with constant coefficients is approximated by the initial value problem of a system of the first order ODEs. The 1-D differential and discrete problems are solved analytically. The maximal calculated dimensional value of liquid concentration at the final time was compared with experimentally obtained concentration. It was observed that both the results are in good agreement. Such a mathematical model allows us to obtain analytical solution with a simple engineering algorithm for mass transfer equations for modelling the filtration process. The mathematical model can be used under consideration filtration process modelling to determine the impurity concentration in the solution of filtration depending on the time.

Acknowledgements

This work was partially supported by the grant 623/2014 of the Latvian Council of Science and the European Regional Funding for project SAM 1.1.1.1./A/16/004.

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