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GALERKIN CHARACTERISTICS METHOD FOR CONVECTION-DIFFUSION PROBLEMS WITH MEMORY TERMS

JOZEF KAČUR AND MOHAMMED SHUKER MAHMOOD

Abstract. We use the modified method of characteristics for solving nonlinear convection diffusion problems with memory terms. The convergence of approximation scheme is proved under minimal regularity assumptions on the velocity field and on the solution. The results are supported by numerical experiments for contaminant transport with diffusion and non-equilibrium sorption isotherms.

Key Words. nonlinear diffusion, convection-adsorption, method of characteristics.

1. Introduction

We consider the following mathematical model for convection diffusion with memory term

$$\begin{aligned} &\partial_t b(x,u) + \operatorname{div}(\bar{F}(t,x,u) - k\nabla u) = f(t,x,u,s), \\ &s(t,x) = \int_0^t K(t,z)\psi(u(z,x))dz \end{aligned} \tag{1.1}$$

in $\Omega \times (0,T]$, $T < \infty$, $\Omega \subset \mathbb{R}^N$ is a bounded domain, $\partial\Omega \in C^{1,1}$, see [26]. If Ω is convex, then $\partial\Omega$ is assumed to be Lipschitz continuous. We consider a Dirichlet boundary condition

$$u(t,x) = 0 \quad \text{on } I \times \partial\Omega, \quad I = (0,T], \tag{1.2}$$

together with the initial condition

$$u(0,x) = u_0(x) \quad x \in \Omega. \tag{1.3}$$

We assume $0 < \varepsilon \le \partial_s b(x,s) \le M < \infty$, $k > 0$ and suppose that f is sublinear in u, s and $\psi(z)$ is sublinear in z. The convection term $\bar{F}$ is Lipschitz continuous in u.

The mathematical model (1.1)-(1.3) is motivated by contaminant transport in porous media intensively studied in the last years, see [4, 9, 10, 11, 19, 20, 21, 1]

$$\begin{aligned} &\partial_t(\theta C + \rho S) + \operatorname{div}(\bar{q}C - D\nabla C) = 0, \\ &\rho\partial_t S = d(\psi(C) - S), \end{aligned} \tag{1.4}$$

where C is the concentration of the contaminant, $\bar{q}$ is the velocity field (Darcy), D is the diffusion matrix, ρ is the bulk density, ψ is the sorption isotherm of the porous media with porosity θ. Here, S is the mass of contaminant adsorbed by the unit mass of porous medium. The coefficient d describes the rate of adsorption. If $d \to \infty$, then an equilibrium sorption process occurs with $S = \psi(C)$ and hence, $b(s) = \theta s + \rho\psi(s)$ generates the parabolic term in (1.1) with $f \equiv 0$. If $d << \infty$,

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the sorption process becomes non-equilibrium. Then, we can eliminate S from the ODE and obtain

$$b(x,z) \equiv \theta(x)z,$$
$$f(t,x,u,s) = d\left(-\psi(u(t,x)) + s_0\,\mathrm{e}^{-\frac{d}{\rho}t} + d\,s\right), \quad K(t,z) = \mathrm{e}^{-\frac{d}{\rho}(t-z)}$$

in our model (1.1). The most common isotherms are $\psi(z) = \frac{c_1 z}{1+c_2 z}$ $(c_1, c_2 > 0)$ (Langmuir isotherm) or $\psi(z) = cz^p$ ($0 < p < 1$ and $c > 0$) (Freundlich isotherm). In the case of the Freundlich isotherm, in the equilibrium mode we obtain the model

$$b(x,z) \equiv \theta(x)z + \rho z^p, \;\; f(t,x,u,s) \equiv 0,$$

which violates $\partial_z b(x,z) < M < \infty$. In such a case, our model can be considered as an approximation of the more general case including $\partial_z b(x,z) = \infty$ in some points z, see [17]. However, such a problem does not occur in the non-equilibrium model even if ψ is of Freundlich isotherm type (not Lipschitz continuous). Our model (1.1) includes locally both equilibrium (in the Freundlich isotherm type we have the approximation of the parabolic term) and non-equilibrium adsorption. Moreover, it is a convection dominated diffusion model. For simplicity, from now on we will drop the variables x in the terms b, $\bar{F}$, f.

The outline of this paper is as follows. In section 2, we define our numerical scheme. In section 3, we prove its convergence and adress related issues. Section 4 deals with the error estimate for our scheme. In section 5, we discuss the numerical implementation and present a variety of 1D and 2D examples.

2. Definition of the scheme

Our approximation scheme is as follows: Let $u_i \approx u(t_i, x)$, $t_i = i\tau$, $\tau = \frac{T}{n}, (n \in \mathbb{N})$. At time level $t = t_i$, we determine u_i successively for $i = 1, \dots, n$ from the linear elliptic problem of the form

$$b'(u_{i-1})\left(\frac{u_i - u_{i-1}\circ\varphi^i}{\tau}\right) - k\Delta u_i = f(t_i, u_{i-1}, s_i) - \mathrm{div}_x \bar{F}(t_i, u_{i-1}) \equiv H(t_i, u_{i-1}, s_i) \tag{2.5}$$

$$u_i = 0 \quad \text{on } \partial\Omega, \qquad s_i = \sum_{j=1}^{i-1} \alpha_{ij}\psi(u_j)\tau$$

where

$$\varphi^i = x - \tau\omega_h * \left(\frac{\bar{F}'_u(t_i, u_{i-1})}{b'(u_{i-1})}\right), \quad \alpha_{ij} = \frac{1}{\tau}\int_{t_{j-1}}^{t_j} K(t_i, z)dz \tag{2.6}$$

and $\omega_h * g$ is the convolution of the mollifier ω_h with $g \in L_\infty(\Omega)$. As a mollifier we can take $\omega_h(x) = \omega_1(\frac{x}{h})\frac{1}{h^N}$ where

$$\omega_1(x) := \begin{cases} \frac{1}{\kappa}\exp(\frac{|x|^2}{|x|^2-1}) & \text{for } |x| \le 1 \\ 0 & otherwise \end{cases}, \qquad \kappa = \int_{x\le 1} \exp(\frac{|x|^2}{|x|^2-1})\,.$$

The approximation scheme (2.5) represents the approximation of the two processes in the time interval $t \in (t_{i-1}, t_i)$ where the composition $u_{i-1}\circ\varphi^i$ represents the transport part of the concentration profile u_{i-1} along the approximated characteristics φ^i and the diffusion process is approximated by the implicit Euler scheme. We note that for the transport equation

$$\partial_t u + \bar{q}\cdot\nabla u = 0,$$

the exact characteristics $X(s,t_i,x)$ satisfies

$$\frac{dX(s,t_i,x)}{ds} = \bar{q}(s, X(s,t_i,x)), \quad s \in (t_{i-1}, t_i), \quad X(t_i,t_i,x) = x.$$

This ODE can be approximated by explicit Euler approximation

$$x - X(t_{i-1}, t_i, x) \approx \tau \bar{q}(t_i, x)$$

and thus $\varphi^i(x) = x - \tau\bar{q}(t_i,x)$ can be considered as an approximation of $X(t_{i-1}, t_i, x)$.

The concept of the method of the characteristics, see [7, 25, 27, 3, 2, 14, 8], is realizable, if the characteristics and also their approximations are not intersecting, i.e., φ^i is a one-to-one map. This can be guaranteed by requiring $\|\nabla\bar{q}\|_\infty \le M < \infty$ and for sufficiently small time step τ.

In our problem (1.1) the transport part of (1.1) is of the form

$$\partial_t b(u) + \mathrm{div}\bar{F}(t,u) = 0$$

which formally can be rewritten according to

$$\partial_t u + \frac{\bar{F}'_u(t,u)}{b'(u)} \cdot \nabla u = -\frac{\mathrm{div}_x \bar{F}(t,u)}{b'(u)}.$$

Note that the velocity field $\bar{q} = \frac{\bar{F}'_u(t,u)}{b'(u)}$ depends on the unknown u. Accordingly, it is difficult or impossible to guarantee $\|\nabla\bar{q}\|_\infty \le M < \infty$, which in return needs to require $\|\nabla u_i\|_\infty \le M < \infty$, $\forall$n $\quad i = 1, \dots, n$.

We follow [17, 18] and use the smoothed approximated characteristics φ^i, see (2.6). As we shall see below, the map φ^i will be one-to-one $\forall i = 1, \dots, n$, if we choose $h = \tau^\omega$ with $\omega \in (0,1)$.

It is worth to mention that in the scheme (2.5) $\psi(u)$ has been approximated by a piecewise constant function (in time)

$$\psi(u(t,x)) = \psi(u_i(x)).$$

This approximation can be improved using a piecewise linear continuous function

$$\psi(u(t)) = \frac{(t_i - t)}{\tau}\psi(u_{i-1}) + \frac{(t - t_{i-1})}{\tau}\psi(u_i), \quad t_{i-1} < t \le t_i.$$

An improvement in the approximation of the characteristics can be obtained by taking the solution u_i in (2.5) as a first approximation. Denoting it by $u_i^{\frac{1}{2}}$, we use

$$b'(u_{i-1}^{\frac{1}{2}}),\ \frac{1}{2}\left[\frac{\bar{F}'_u(t_i,u_{i-1})}{b'(u_{i-1})} + \frac{\bar{F}'_u(t,u_i^{\frac{1}{2}})}{b'(u_i^{\frac{1}{2}})}\right] \text{ instead of } b'(u_{i-1}), \quad \frac{\bar{F}'_u(t,x,u_{i-1})}{b'(u_{i-1})}$$

(this can be done also with respect to φ^i).

3. Convergence of the method

Let C denote a generic, positive constant. We shall assume

H$_1$) $b(x,s)$ is continuous in $x \in \bar{\Omega}$, $s \in R$ and Lipschitz continuous in s with $0 < \varepsilon < b'(x,s) \le M < \infty$.

H$_2$) $\bar{F}(t,x,s)$ is Lipschitz continuous in s and

$$|\bar{F}'_u(t,x,s)| \le C, |\mathrm{div}_x \bar{F}(t,x,s)| \le C(1+|s|)$$

H$_3$) $f(t,x,s,\eta)$ is continuous in its variables, sublinear in s and η such that

$$|f(t,x,s,\eta)| \le C(1+|s|+|\eta|)$$

H$_4$) $K(t,x,s): I\times\Omega\times R\to R$ is continuous, $\psi(s): R\to R$ is continuous and $|\psi(s)|\le C(1+|s|)$

H$_5$) $u_0\in L_\infty(\Omega)\cap W_2^2(\Omega)$.

Firstly, we prove that φ^i and its inverse are Lipschitz continuous.

Lemma 1. *Assume $\tau\le\tau_0$. Then uniformly in $i=1,...,n$ there holds*

$$\frac{1}{2}|x-y|<|\varphi^i(x)-\varphi^i(y)|\le 2|x-y|\quad \forall x,y\in\Omega.$$

Proof. Due to $\bar{q}_i=\frac{\bar{F}'_u(t_i,u_{i-1})}{b'(u_{i-1})}\in L_\infty(\Omega)$ we have $\|\bar{q}_i\|_\infty\le M$, $\forall\ i=1,\dots,n$. Then we deduce that $\|\omega_h*\bar{q}_i\|_\infty\le M$ and

$$\|\partial_x\omega_h*\bar{q}_i\|_\infty\le\frac{C}{h}\|\bar{q}_i\|_\infty\le\frac{CM}{h}.$$

Since $h=\tau^\omega$ with $\omega\in(0,1)$, it follows that

$$(1-\tau^{1-\omega}CM)|x-y|\le|\varphi^i(x)-\varphi^i(y)|\le(1+\tau^{1-\omega}CM)|x-y|\quad\forall x,y\in\Omega,$$

which allows to conclude. □

Now, the map φ^i is one-to-one from Ω to $\Omega_{\varphi^i}\subset\Omega^*$ where $\bar{\Omega}\subset\Omega^*$ (Ω^* is a small neighborhood of Ω provided $\tau\le\tau_0$) . We extend $u_{i-1}\in\mathring{W}_2^1(\Omega)$ to Ω^* denoting by $u_{i-1}\circ\varphi^i$ the value of the extended function at the point $\varphi^i(x)\in\Omega^*$. From Lemm 1 it follows

$$\|u_{i-1}\circ\varphi^i\|_0\le C\|u_{i-1}\|_0,\quad \|\nabla u_{i-1}\circ\varphi^i\|_0\le C\|\nabla u_{i-1}\|_0,$$

($\|.\|_0$ is $L_2(\Omega)$ norm).

Due to the regularity of our data ($\partial\Omega,u_0,$etc.) there exists a unique variational solution $u_i\in W_2^2(\Omega)\cap L_\infty(\Omega)$, see, e.g. [23], satisfying

$$\frac{1}{\tau}(b'(u_{i-1})(u_i-u_{i-1}\circ\varphi^i),v)+k(\nabla u_i,\nabla v)=H(t_i,u_{i-1},s_i,v)\tag{3.7}$$

$\forall v\in V\equiv\mathring{W}_2^1$, where $(u,v):=\int_\Omega uvdx$ and $\mathring{W}_2^1(\Omega)$, $W_2^2(\Omega)$ are standard Sobolov spaces. Since $u_i\in W_2^2$, (2.5) is satisfied for a.e. $x\in\Omega$. We prove some a priori estimates for $u_i, i=1,\dots,n$.

Lemma 2. *There holds $\|u_i\|_\infty\le C$, $i=1,\dots,n$, uniformly for n.*

Proof. Since $u_i\in W_2^2\cap L_\infty$, we substitute $v=u_i^{2p+1}(p=1,2,...)$ into (3.7) to obtain

$$\int_\Omega b'(u_{i-1})u_i^{2p+2}dx\le\int_\Omega b'(u_{i-1})\left[u_{i-1}\circ\varphi^i+\tau\frac{H_i}{b'(u_{i-1})}\right]u_i^{2p+1}dx,$$

where we have used

$$(2p+1)k\int_\Omega u_i^{2p}(\nabla u_i)^2dx\ge 0.$$

By Young's inequality

$$ab\le\frac{a^\alpha}{\alpha}+\frac{b^\beta}{\beta},\quad(\frac{1}{\alpha}+\frac{1}{\beta}=1),$$

we find that

$$\int_\Omega b'(u_{i-1})u_i^{2p+2}dx\le\frac{1}{2p+2}\int_\Omega b'(u_{i-1})\left(u_{i-1}\circ\varphi^i+\frac{H_i}{b'(u_{i-1})})\right)^{2p+2}dx$$
$$+\frac{2p+1}{2p+2}\int_\Omega b'(u_{i-1}){u_i}^{2p+2}dx.$$

To obtain $||u_i||_\infty$, we take the $(2p+2)$-th root and let $p \to \infty$. We get

$$\|u_i\|_\infty \leq \|u_{i-1} \circ \varphi^i\|_\infty + \tau \| \frac{H_i}{b'(u_{i-1})} \|_\infty \leq \|u_{i-1}\|_\infty + \tau C(1 + \|u_{i-1}\|_\infty)$$
$$= (1 + C\tau)\|u_{i-1}\|_\infty + C\tau.$$

From this recurrent inequality we deduce

$$\|u_i\|_\infty \leq C(1 + \|u_0\|_\infty).$$

□

Following [14], we can prove the following lemma.

Lemma 3. *There holds*

$$\left\| \frac{u_{i-1} - u_{i-1} \circ \varphi^i}{\tau} - \omega_h * \bar{q}_i \cdot \nabla u_i \right\|_0 \leq C\tau \|u_i\|_{W_2^2(\Omega)}, \quad \forall i = 1, ..., n, \tag{3.8}$$

uniformly in n.

Proof. It is sufficient to prove (3.8) for a smooth function u_{i-1} because of density results in $W_2^2(\Omega)$. In view of the mean value theorem we find

$$\tfrac{u_{i-1} - u_{i-1} \circ \varphi^i}{\tau} - \omega_h * \bar{q}_i \cdot \nabla u_{i-1} = \int_0^1 \big(\nabla u_{i-1}(x - s(\varphi^i(x) - x)\big)\, ds - \nabla u_{i-1})\omega_h * \bar{q}_i$$

$$= \omega_h * \bar{q}_i \int_0^1 \int_0^s \nabla^2 u_{i-1}(x - sz(\varphi^i(x) - x)) dz ds \omega_h * \bar{q}_i \tau.$$

From this and $\|\omega_h * \bar{q}_i\|_\infty \leq C$ we can easily deduce (3.8). □

We set $\delta u_i := \frac{u_i - u_{i-1}}{\tau}$.

Lemma 4. *The estimate*

$$\sum_{i=1}^n \|\delta u_i\|_0^2 \tau + \max_{1 \leq i \leq n} \|\nabla u_i\|_0^2 \leq C_1 + C_2 \tau^2 \sum_{i=1}^j \|u_i\|_{W_2^2}^2$$

holds uniformly for $i = 1, \ldots, n$.

Proof. We choose $v = (u_i - u_{i-1})$ in (3.7) and sum up for $i = 1, ..., j$. Using the splitting

$$u_i - u_{i-1} \circ \varphi^i = u_i - u_{i-1} + u_{i-1} - u_{i-1} \circ \varphi^i, \tag{3.9}$$

we obtain

$$\varepsilon \sum_{i=1}^j \|\delta u_i\|_0^2 \tau + \frac{k}{2} \|\nabla u_j\|_0^2 \leq \frac{k}{2} \|\nabla u_0\|_0^2 + \sum_{i=1}^j \left(\frac{u_{i-1} - u_{i-1} \circ \varphi^i}{\tau}, \delta u_i \right) \tau + \sum_{i=1}^j (H_i, \delta u_i)\tau$$
$$\equiv C + J_1 + J_2,$$

where we have used

$$b'(u_{i-1}) \geq \varepsilon, \quad (\nabla u_i, \nabla(u_i - u_{i-1})) \geq \frac{1}{2} \|\nabla u_i\|_0^2 - \frac{1}{2} \|\nabla u_{i-1}\|_0^2.$$

Observing $\|\omega * \bar{q}_i\|_\infty \leq C$, for any $\beta > 0$ we obtain

$$|J_1| \leq \beta \sum_{i=1}^j \|\delta u_i\|_0^2 \tau + C_\beta \sum_{i=1}^j \| \frac{u_{i-1} - u_{i-1} \circ \varphi^i}{\tau} \|_0^2 \tau \leq \beta \sum_{i=1}^j \|\delta u_i\|_0^2 \tau$$

$$+ C_\beta \sum_{i=1}^j \| \frac{u_{i-1} - u_{i-1} \circ \varphi^i}{\tau} \; - \omega_h * \bar{q}_i \nabla u_i \|_0^2 \tau + C_\beta \sum_{i=1}^j \|\nabla u_i\|_0^2 \tau.$$

Similarly, we get

$$|J_2| \leq \beta \sum_{i=1}^{j} \|\delta u_i\|_0^2 \tau + C_\beta \sum_{i=1}^{j} \|H_i\|_0^2 \tau \leq \beta \sum_{i=1}^{j} \|\delta u_i\|_0^2 \tau + C_\beta \sum_{i=1}^{j} (1 + \|u_i\|_0^2)\tau.$$

Using these estimates, Lemma 3 and Gronwall's inequality we get the desired result. □

Lemma 5. *Uniformly in* n *there holds*

$$\sum_{i=1}^{n} \|u_i\|_{W_2^2}^2 \tau \leq C.$$

Proof. We multiply (2.5) by Δu_i, integrate over Ω and make use of the splitting (3.9). Then, we estimate

$$\int_\Omega |\Delta u_i|^2 dx \leq \beta \|\Delta u_i\|_0^2 + C_\beta \left(\|\delta u_i\|_0^2 + \left\| \frac{u_{i-1} - u_{i-1} \circ \varphi^i}{\tau} - \omega_h * \bar{q}_i \nabla u_{i-1} \right\|_0^2 \right)$$

$$+ C_\beta (\|\nabla u_{i-1}\|_0^2 + \|H_i\|_0^2).$$

Hence, for β small

$$\sum_{i=1}^{j} \|\Delta u_i\|_0^2 \tau \leq C_1 + C_2 \tau^2 \sum_{i=1}^{j} \| \, u_i\|_{W_2^2}^2 \tau$$

since $u_i|_{\partial\Omega} = 0$, $\|\Delta u_i\|_0$ is equivalent to $\|u_i\|_{W_2^2}$. Then, for $\tau \leq \tau_0$ we obtain the required estimate. □

By means of $\{u_i\}_{i=1}^n$ we construct Rothe's functions

$$\begin{aligned} &\bar{u}^n(t) := u_i \\ &u^n(t) := u_{i-1} + \delta u_i (t - t_{i-1}) \end{aligned} \qquad \text{for } t \in (t_{i-1}, t_i],\ i = 1, \dots, n \tag{3.10}$$

with $\bar{u}^n(0) = u_0$. The a priori estimates of Lemmas 4 and 5 can be rewritten according to

$$\int_I \|\partial_t u^n\|_0^2 dt \leq C, \quad \sup_{t \in I} (\|u^n(t)\| + \|\bar{u}^n(s)\|) \leq C, \tag{3.11}$$

where $\|.\|$ is the norm in $W_2^1(\Omega)$. As a result $\{u^n\}$ and $\{\bar{u}^n\}$ are compact in $L_2(I, L_2(\Omega))$, (see,e.g. [15]) and hence there exists $u \in C(I, L_2(\Omega))$ with $u \in L_\infty(I, W_2^1(\Omega))$ such that $u^{\bar{n}} \to u$ in $C(I, L_2(\Omega))$ for $n \to \infty$ and from

$$\int_I \|u^n - \bar{u}^n\|_0^2 dt \leq \frac{C}{n^2}, \tag{3.12}$$

where $\{\bar{n}\}$ is a subsequence of $\{n\}$, we obtain $\bar{u}^{\bar{n}} \to u$ a.e. in $I \times \Omega$, $\bar{u}^{\bar{n}}(t) \to u(t)$ in $W_2^1(\Omega)$. Then, we can easily prove that u is a variational solution of (1.1)-(1.3) satisfying

$$(\partial_t b(u(t)), v) + (\bar{F}(t, x, u) - k \nabla u, \nabla v) = (f(t, x, u(t), s(t)), v),$$

$$s(t, x) = \int_0^t K(t, z) \psi(u(z, x)) dz,$$

$\forall v \in \overset{\circ}{W}{}_2^1$, a.e. $t \in I$. This will be shown in the following theorem. We remark that the existence and uniqueness of the variational solution can be found in [21].

Theorem 1. *If the assumptions $(H_1)-(H_5)$ are satisfied, then*

$$u^n \to u \text{ in } C(I, L_2(\Omega)) \quad \text{and}$$
$$\bar{u}^n \to u \text{ in } L_p(I, W_2^1(\Omega)), \quad \forall p > 1$$

where u is a variational solution of (1.1)-(1.3), (see (3.11)) and u^n is from (2.5),(3.10).

Proof. We multiply (2.5) by $v \in \mathcal{D}(\Omega)$ ($C^\infty(\Omega)$ space) and integrate over $(0,t)\times\Omega$. We can rewrite it in the form

$$\int_0^t (b'(\bar{u}_\tau^n)\partial_t u^n, v)dt + \int_0^t (b'(\bar{u}_\tau^n)\omega_h * \bar{q}^n \cdot \nabla \bar{u}_\tau^n, v)dt$$

$$+\int_0^t (b'(\bar{u}_\tau^n)\bar{A}^n, v)dt + \int_0^t (k\nabla \bar{u}^n, \nabla v)dt = \int_0^t (\bar{f}^n(t,x,\bar{u}_\tau^n(t), \bar{s}^n(t)), v)dt$$

$$+\int_0^t (\operatorname{div}_x \bar{F}^n(t, \bar{u}_\tau^n(t))), v)dt, \forall v \in \mathcal{D}(\Omega), \tag{3.13}$$

where

$$\bar{A}^n(t) := \frac{u_{i-1} - u_{i-1}\circ\varphi^i}{\tau} - \omega_h * \bar{q}_i \cdot \nabla u_{i-1},$$

$\bar{F}^n(t, \bar{u}_\tau^n(t)) = \bar{F}(t_i, u_{i-1}), \bar{q}^n(t) = \bar{q}_i, t \in (t_{i-1}, t_i), i = 1, \ldots, n$ and $\bar{u}_\tau^n(t) = \bar{u}^n(t-\tau)$ with $\bar{u}_\tau^n(s) \equiv u_o$ for $s \in (-\tau, 0)$.

Due to the a priori estimate (3.12) and $\bar{u}^n \to u$ and $\bar{u}_\tau^n \to u$ a.e. in $I\times\Omega$, (a subsequence of $\{n\}$ we again denote by $\{n\}$) we have

$$\bar{q}^n = \frac{\bar{F}_u'^n(t,x,\bar{u}_\tau)}{b'(\bar{u}_\tau)} \quad \to \bar{q} = \frac{\bar{F}_u'(t,x,u)}{b'(u)} \text{ for a. e. in } I\times\Omega$$

and moreover, in $L_2(I\times\Omega)$, since $\bar{q}^n$ is uniformly bounded. Then, $\omega_h * \bar{q}^n \to \bar{q}$ in $L_2(I\times\Omega)$ for $n\to\infty$, since $h = \tau^\omega$. Then $b'(\bar{u}_\tau^n)\omega_h * \bar{q}^n \to \bar{F}_u'(t,x,u)$ in $L_2(I\times\Omega)$. Therefore and due to $\nabla\bar{u}^n \rightharpoonup \nabla u$ in $L_2(I\times\Omega) \equiv L_2(I, L_2)$ we obtain

$$\int_0^t (b'(\bar{u}_\tau^n)\omega_h * \bar{q}^n \cdot \nabla\bar{u}^n, v)dt \to \int_0^t (\bar{F}_u'(t,x,u)\cdot\nabla u, v)dt.$$

Due to Lemma 4 we have

$$\int_0^t (b'(\bar{u}_\tau^n)\bar{A}^n, v)dt \le M\int_0^t \|A^n(t)\|_0\|v\|_0 dt \le M\|v\|_0\sqrt{t}\left(\int_0^t \|A^n(t)\|_0^2 dt\right)^{1/2}$$

$$\le C\|v\|_0\left(\frac{1}{n^2}\int_I \|\bar{u}^n(t)\|_{W_2^2}^2 dt\right)^{1/2} \le \frac{C\|v\|_0}{n} \to 0 \quad \text{for } n\to\infty.$$

From (3.13) and $u^n \to u$ in $L_2(I\times\Omega)$ we deduce $\partial_t u^n \rightharpoonup \partial_t u$ in $L_2(I\times\Omega)$ and hence

$$\int_0^t (b'(\bar{u}_\tau^n)\partial_t u^n, v)dt \to \int_0^t (b'(u)\partial_t u, v)dt = \int_0^t (\partial_t b(x,u), v)dt \text{ for } n\to\infty.$$

Similarly, we get

$$\int_0^t (k\nabla\bar{u}^n, \nabla v)dt \to \int_0^t (k\nabla u, \nabla v)dt,$$

$$\int_0^t (\operatorname{div}_x \bar{F}^n(t, \bar{u}_\tau^n), v)dt \to \int_0^t (\operatorname{div}_x \bar{F}(t,x,u), v)dt.$$

Since $\bar{u}^n \to u$, $\bar{u}^n_\tau \to u$ for a.e. $(t,x) \in I \times \Omega$, we obtain

$$\bar{s}^n(t,x) = \sum_{j=1}^{i-1} \alpha_{ij}\psi(u_j)\tau + C_n = \int_0^{t_{i-1}} K(t,z)\psi(\bar{u}^n(z,x))dz + C_n$$

$$\to \int_0^t K(t,z)\psi(\bar{u}(z,x))dz \qquad \text{for any } t \in (t_{i-1}, t_i), i = 1, \dots, n$$

due to

$$C_n = |\int_{t_{i-1}}^t K(t,z)\psi(\bar{u}^n(z,x))dz| \to 0 \quad \text{as } n \to \infty.$$

Thus

$$\bar{s}^n(t,x) \to s(t,x) = \int_0^t K(t,z)\psi(u(x,z))dz$$

for $n \to \infty$ for a.e. $(t,x) \in I \times \Omega$. Therefore and due to $\|\bar{s}^n\|_\infty \le C$ we find

$$\int_0^t (\bar{f}^n(t,x,\bar{u}^n_\tau(t),\bar{s}^n),v)dt \to \int_0^t (f(t,x,u,s),v)dt.$$

From these facts and from (3.13) it follows that

$$\begin{aligned} &\int_0^t (\partial_t b(u),v)dt + \int_0^t (\bar{F}'_u(t,x,u).\nabla u + \operatorname{div}_x \bar{F}(t,x,u),v)dt \\ &+ \int_0^t (k\nabla u, \nabla v)dt = \int_0^t (f(t,u,s),v)dt \qquad \forall v \in \mathcal{D}(\Omega). \end{aligned} \tag{3.14}$$

Differentiating (3.14) with respect to t, using integration by parts and due to $\bar{u}^n \rightharpoonup u$ in $L_2(I, W_2^2(\Omega))$ we have $u(t) \in W_2^2$ for a.e. $t \in I$ in (3.14). Hence, u satisfies (1.1).

Now, we prove $\bar{u}^n \to u$ in $L_2(I, W_2^1)$. We can extend (3.13) for $v \in \mathring{W}_2^1(\Omega)$ and also for $v \in L_2(I, \mathring{W}_2^1)$. Then, we put $v = u - \bar{u}^n$. Since $\bar{u}^n \to u$ in $L_2(I, L_2)$, we obtain that all the terms in (3.13) except the elliptic one converge to 0 for $n \to \infty$. The elliptic term can be estimated from below according to

$$\int_0^t (k\nabla \bar{u}^n, \nabla(u - \bar{u}^n)dt = \int_0^t (k\nabla \bar{u} - \bar{u}^n, \nabla(u - \bar{u}^n)dt$$

$$- \int_0^t (k\nabla u, \nabla(u - \bar{u}^n)dt \ge C\int_0^t (\|(u - \bar{u}^n)\|^2 dt - D_n.$$

Since $\bar{u}^n \rightharpoonup u$ in $L_2(I, W_2^1)$, there holds

$$D_n := \int_0^t (k\nabla u, \nabla(u - \bar{u}^n))dt \to 0.$$

Finally, from (3.13) we obtain the required result

$$C\int_0^t \|u - \bar{u}^n\|^2 dt \to 0 \text{ for } \quad n \to \infty, \forall t \in (0,T).$$

From this result and $\bar{u}^n(t) \to u(t)$ in $L_2(\Omega)$ we obtain $\bar{u}^n(t) \to u(t)$ in $W_2^1(\Omega)$. Since $\|\bar{u}^n(t)\| \le C, \forall t \in I$, we get $\bar{u}^n \to u$ in $L_p(I, W_2^1(\Omega)), \forall p > 1$. The uniqueness of the variational solution u, see [21] implies that the original sequence $\{\bar{u}^n\}$ is convergent. Thus the proof is complete. □

Remarks:

1- The result in Theorem 1 is also valid for the non-homogeneous Dirichlet boundary condition where

$$u(x,t) = \psi(x) \text{ on } \qquad \partial\Omega$$

under the assumption that ψ can be extended to $u_\psi \in W_2^1(\Omega)$ such that the trace

u_ψ on $\partial\Omega$ equals ψ. Then we look for $w := u - u_\psi \in \overset{\circ}{W}{}_2^1(\Omega)$, where in (1.1) we substitute $u \Longleftrightarrow w + u_\psi$.

2- The result obtained in Theorem 1 can be extended also to Newton type boundary condition.

$$-k\partial_\nu u = h(u - \psi).$$

However, for a mixed type boundary condition (Dirichlet and Neumann) the regularity $u_i \in W_2^2(\Omega)$ for the corresponding elliptic problem in (2.5) cannot be guaranteed . In that case of a less regular solution, the convergence can be proven using the technique in [17, 18].

4. Error estimate

The approximation scheme (2.5) requires the solution of linear elliptic problems. In the error analysis we have technical difficulties to control the term,

$$\frac{1}{\tau}\left[b'(u_{i-1})(u_i - u_{i-1} \circ \varphi^i)\right]$$

in our approximation scheme. It seems that the approximation

$$\frac{1}{\tau}\left[b(u_i) - b(u_{i-1} \circ \phi_i)\right]$$

of the parabolic term (including convection) is more appropriate for the error analysis. But on the other hand, it would require solution of the nonlinear elliptic problems and consquently an application of some Newton-type iterations which we have not considered in convergence analysis. To obtain stronger error estimates results, we shall consider only linear parabolic term where $b(s) = s$. Moreover, we shall assume that

H$_6$) $\partial_s \bar{F}(t,x,s), f(t,x,s,z)$ are Lipschitz continuous in t, s, z (uniformly for $x \in \Omega$); $\psi(s)$ is Lipschitz continuous and $K(t,s)$ is Lipschitz continuous in t.

H$_7$) We assume that the variational solution u of (1.1)-(1.2) is Lipschitz continuous in x, uniformly for $t \in I$, i.e. $\nabla u \in L_\infty(Q_T)$. In addition, we assume that $\partial_t^2 u \in L_2(I, L_2(\Omega))$.

Since $b(s) = s$, the characteristics mapping $\varphi^i(x)$ is given in the form

$$\varphi^i(x) = x - \tau\omega_h * \bar{F}'_u(t_i, u_{i-1}). \tag{4.15}$$

We set $\bar{u}^i = \frac{1}{\tau}\int_{t_{i-1}}^{t_i} u(t)dt$ and $e_i = \bar{u}^i - u_i$, where u_i is from (3.7) and u is the variational solution. Integrating (1.1) over (t_{i-1}, t_i) and rearranging the parabolic term, we get

$$(\bar{u}^i - \bar{u}^{i-1}, v) + (\bar{F}'_u(t_i, \bar{u}^{i-1}) \cdot \nabla\bar{u}^i, v)\tau + k(\nabla\bar{u}^i, \nabla v)\tau = \int_{t_{i-1}}^{t_i} (H(t,u,s), v)dt$$

$$+(\bar{u}^i - u(t_i) - (u^{i-1} - u(t_{i-1}), v) + \int_{t_{i-1}}^{t_i} \left(\left[\bar{F}'_u(t,u) - \bar{F}'_u(t_i, \bar{u}^{i-1})\right]\nabla u, v\right)dt \tag{4.16}$$

$\forall v \in V$. We now subtract (3.7) from (4.16), choose $v = e_i$ and sum up for $i = 1, ..., j$. Using the splitting

$$u_i - u_{i-1} \circ \varphi^i = u_i - u_{i-1} + u_{i-1} - u_{i-1} \circ \varphi^i$$

we can rewrite it in the form

$$\frac{1}{2}\|e_j\|_0^2 + k\sum_{i=1}^{j}\|\nabla e_i\|_0^2\tau = -\sum_{i=1}^{j}(\tau\bar{F}'_u(t_i, \bar{u}^{i-1})\nabla\bar{u}^{i-1} - (u_{i-1} - u_{i-1} \circ \varphi^i), e_i)$$

$$+\sum_{i=1}^{j}(L_i,e_i)+\sum_{i=1}^{j}(\int_{t_{i-1}}^{t_i}(H(t,u(t),s(t))-H(t_i,u_{i-1},s_{i-1}))dt,e_i)+J_0 \tag{4.17}$$

where $L_i=\bar{u}^i-u(t_i)-(u^{i-1}-u(t_{i-1}))$ and

$$J_0=\sum_{i=1}^{j}\int_{t_{i-1}}^{t_i}\left(\left[\bar{F}'_u(t,u)-\bar{F}'_u(t_i,\bar{u}^{i-1})\right]\nabla u,e_i\right)dt.$$

The corresponding terms are denoted by $J_1+J_2=J_3+J_4+J_5+J_0$. To estimate $|J_3|$ we use the formula

$$u_{i-1}-u_{i-1}\circ\varphi^i=\tau\int_0^1\nabla u_{i-1}(x+s(\varphi^i(x)-x))ds\cdot\omega_h*\bar{F}'_u(t_i,u_{i-1})$$

and write

$$\begin{aligned}-J_3=&\ \tau\sum_{i=1}^{j}(\left[\bar{F}'_u(t_i,\bar{u}^{i-1})-\bar{F}'_u(t_i,u_{i-1})\right]\nabla\bar{u}^{i-1},e_i)\\&+\tau\sum_{i=1}^{j}\int_\Omega\bar{F}'_u(t_i,u_{i-1})(\nabla\bar{u}^{i-1}-\nabla u_{i-1})e_i(x)dx\\&+\tau\sum_{i-1}^{j}\int_\Omega\int_0^1\bar{F}'_u(t_i,u_{i-1})\left[\nabla u_{i-1}(x)-\nabla u_{i-1}(x-s(\varphi^i(x)-x))\right]dse_i(x)dx\\&+\tau\sum_{i=1}^{j}\int_\Omega\left[\bar{F}'_u(t_i,u_{i-1})-\omega_h*\bar{F}'_u(t_i,u_{i-1})\right]\int_0^1\nabla u_i(x+s(\varphi^i(x)-x))dse_i(x)dx\\&=J_{3,1}+J_{3,2}+J_{3,3}+J_{3,4}.\end{aligned}$$

Using the assumptions H$_6$) and H$_7$) we estimate

$$|J_{3,1}|\le C_1\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt+C_2\tau,$$

where $\sum_{i=1}^{j}\|e_i\|_0^2\tau=\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt$. By Young's inequality we have

$$|J_{3,2}|\le C_\varepsilon\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt+\varepsilon\int_0^t\|\nabla\bar{e}^n(t)\|_0^2dt.$$

We express $J_{3,3}$ in the form

$$J_{3,3}=$$

$$\tau^2\sum_{i=1}^{j}\int_\Omega\int_0^1\int_0^1\bar{F}'_u(t_i,u_{i-1})\nabla^2u_{i-1}(x+sz(\varphi^i(x)-x))\omega_h*\bar{F}'_u(t_i,u_{i-1})e_i(x)dsdzdx,$$

(∇^2u_{i-1} being the Hessian of u_{i-1}). Hence, we obtain the estimate

$$|J_{3,3}|\le\varepsilon\sum_{i=1}^{j}\|e_i\|_0^2\tau+C_\varepsilon\tau\sum_{i=1}^{j}\|u_i\|^2_{W_2^2(\Omega)}\tau\le\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt+\tau C_1,$$

and finally, estimating $J_{3,4}$ we use

$$\|\bar{F}'_u(t_i,u_{i-1})-\omega_h*\bar{F}'_u(t_i,u_{i-1})\|_\infty\le C\tau^{1/2}\|\bar{F}'_u(t_i,u_{i-1})\|_{C^{0,1/2}}$$

where $C^{0,\beta}$ is the space of β-Hölder continuous functions on $\bar{\Omega}$ with the norm $\|\cdot\|_{C^{0,\beta}}$, see [22]. Using assumption H_6), the boundedness of $\|\bar{F}'_u(t_i,u_{i-1})\|_\infty$ and the continuous imbedding $W_2^2(\Omega)\hookrightarrow C^{0,1/2}$, for $N\le 3$ we obtain

$$\|\bar{F}'_u(t_i,u_{i-1})\|_{C^{0,1/2}}\le C(1+\|u_{i-1}\|_{W_2^2(\Omega)}).$$

Then, we estimate

$$|J_{3,4}| \le C_1 \int_0^{t_j} \|\bar{e}^n(t)\|^2 dt + C_2 \tau \sum_{i=1}^{j} \|u_i\|^2_{W_2^2} \tau \le C_1 \int_0^{t_j} \|\bar{e}^n(t)\|^2 dt + C_2 \tau.$$

Summarizing the above estimates yields

$$|J_3| \le \varepsilon \int_0^{t_j} \|\nabla \bar{e}^n(t)\|_0^2 dt + C_\varepsilon \int_0^j \|\bar{e}^n(t)\|_0^2 dt + C_2 \tau. \tag{4.18}$$

To estimate J_4 we write

$$L_i \equiv \int_{t_{i-1}}^{t_i} (\partial_t u - \overline{\partial_t^\tau u}) dt$$

where $\overline{\partial_t^\tau u} = \frac{1}{\tau} \int_{t-\tau}^t \partial_t u dz$, making use of $\partial_t^2 u \in L_2(I, L_2)$ (see H_7)) we find

$$|J_4| \le \varepsilon \int_0^{t_j} \|\bar{e}^n(t)\|_0^2 dt + C_\varepsilon \frac{1}{\tau} \sum_{i=1}^{j} \| \int_{t_{i-1}}^{t_i} (\partial_t u - \overline{\partial_t^\tau u}) dt \|_0^2$$

$$\le \varepsilon \int_0^{t_j} \|\bar{e}^n(t)\|_0^2 dt + C_\varepsilon \frac{1}{\tau} \int_0^{t_j} \|\partial_t u - \overline{\partial_t^\tau u}\|_0^2 dt \le \varepsilon \int_0^{t_j} \|\bar{e}^n(t)\|_0^2 dt +$$

$$C_\varepsilon \tau \int_0^{t_j} \|\partial_t^2 u\|_0^2 dt \le \varepsilon \int_0^{t_j} \|\bar{e}^n(t)\|_0^2 dt + C_\varepsilon \tau. \tag{4.19}$$

By virtue of the assumption H_6) the term J_5 can be estimated as follows

$$|J_5| \le \varepsilon \int_0^{t_j} \|\bar{e}^n(t)\|_0^2 dt + C_\varepsilon \sum_{i=1}^{j} \int_{t_{i-1}}^{t_i} \|(H(t, u(t), s(t)) - H(t_i, u_i, s_{i-1}))\|_0^2 dt$$

$$\equiv \varepsilon \int_0^{t_j} \|\bar{e}^n(t)\|_0^2 dt + J_6. \tag{4.20}$$

We estimate $J_6 \le 2C_\varepsilon (J_{6,1} + J_{6,2})$ according to the splitting

$$H(t, u(t), s(t)) - H(t_i, u_{i-1}, s_{i-1}) = H(t, u(t), s(t)) - H(t_i, \bar{u}^{i-1}, s(t_{i-1}))$$
$$+ H(t_i, \bar{u}^{i-1}, s(t_{i-1})) - H(t_i, u_{i-1}, s_{i-1}).$$

Then using the Lipschitz continuity of H in its variables we deduce

$$J_{6,1} = \sum_{i=1}^{j} \int_{t_{i-1}}^{t_i} \|(H(t, u(t), s(t)) - H(t_i, \bar{u}^{i-1}, s(t_{i-1}))\|_0^2 dt$$

$$\le C \sum_{i=1}^{j} \left(\tau^2 + \int_{t_{i-1}}^{t_i} \|u(t) - \bar{u}^{i-1}\|_0^2 + \int_{t_{i-1}}^{t_i} \|s(t) - s(t_{i-1})\|_0^2 dt \right) \le C\tau, \tag{4.21}$$

where for $t \in (t_{i-1}, t_i)$ we have

$$\|s(t) - s(t_{i-1})\| \le \left\| \int_{t_{i-1}}^{t} K(t,s) \psi(u(s)) ds \right\|_0 +$$

$$+ \left\| \int_0^{t_{i-1}} |K(t,s) - K(t_{i-1}, s)| \psi(u(s)) ds \right\| \le C\tau.$$

Finally, we estimate

$$J_{6,2} = \sum_{i=1}^{j} \int_{t_{i-1}}^{t_i} \|(H(t_i, \bar{u}^{i-1}, s(t_{i-1})) - H(t_i, u_{i-1}, s_{i-1}))\|_0^2 dt$$

$$\leq C\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt + C\sum_{i=1}^{j}\int_{t_{i-1}}^{t_i}\|s(t_{i-1})-s_{i-1}\|_0^2dt. \tag{4.22}$$

We can use the inequality

$$|s(t_{i-1})-s_{i-1}| \leq \sum_{l=1}^{i-1}\int_{t_{l-1}}^{t_l} K(t_{i-1},s)\left(|u-\bar{u}^{l-1}|+|\bar{u}^{l-1}-u_{l-1}|\right)ds$$

to estimate

$$\sum_{i=1}^{j}\tau\|s(t_{i-1})-s_{i-1}\|_0^2 \leq C\tau + C\sum_{i=1}^{j}\tau\sum_{l=1}^{i-1}\tau\|\bar{e}_l^n\|_0^2 \leq C\tau + C\int_0^{t_j}\int_0^s\|\bar{e}^n(z)\|_0^2dzds.$$

Therefore and due to (4.22) we obtain

$$J_{6,2} \leq C\tau + C_2\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt. \tag{4.23}$$

Finally, due to H6), H7) we estimate

$$|J_0| \leq \varepsilon\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt + C_\varepsilon\sum_{j=1}^{n}\int_{t_{i-1}}^{t_i}\|u-\bar{u}^{i-1}\|^2dt \leq$$

$$\varepsilon\int_0^{t_j}\|\bar{e}^n(t)\|_0^2dt + C_\varepsilon\tau,$$

since

$$\|u(t)-\bar{u}^{j-1}\|_0 \leq \int_{t_{j-2}}^{t_{j+1}}\|\partial_t u\|_0dt$$

and $\partial_t u \in L_2(I, L_2(\Omega))$. Using this and the estimates (4.18)-(4.23) in (4.16), we deduce the final error estimate because of Gronwall's argument. We thus obtain the following result.

Theorem 2. *Let the assumptions of Theorem 1 be satisfied and let $b(s) = s$. If $H_6) - H_7)$ hold, then*

$$\|e_j\|_0^2 + \sum_{i=1}^{j}\|\nabla e_i\|_0^2\tau \leq \frac{C}{n}.$$

Consequently, it holds

$$\|u(t_i)-u_i\|_0^2 \leq \frac{C}{n} \quad \forall i = 1,..n, \int_0^t\|u(t)-\bar{u}_n(t)\|^2dt \leq \frac{C}{n}.$$

5. Numerical implementation

Our scheme remedied three problems in the model (1.1)-(1.3), the nonlinearity of $b(u)$, the non-equilibrium isotherm (the memory term is taken into account) which have been treated in section 2. The third problem is the convection dominance which is treated using the method of characteristics where the crucial point is to evaluate the inner product

$$(u_{i-1}\circ\varphi^i, \phi_j) = \int_{E_j} u_{i-1}\circ\varphi^i(x)\phi_j(x)dx \tag{5.24}$$

where ϕ_j is a basis function, $j = 1, ...P$ and

$$u_{i-1}(x) = \sum_j U_{i-1}^j\phi_j(x).$$

U^j_{i-1} represents the value of the function $u_{i-1}(x)$ at the point x_j. For the sake of simplicity we consider a uniform partition of Ω into the elements $\{Ej\}_{j=1}^{P}$. The errors in the evaluation of this inner product is the source of the numerical instabilities. To evaluate (5.24) we follow the concept of Bermejo [2, 3] (initiated by Morton et.al., see [25]). This concept of evaluation is unconditionally stable and efficient, see [2, 3]. We sketch its basic numerical implementation.

The idea that the integral involving the product of two piecewise bilinear polynomials on different grids is equivalent to cubic spline interpolation at the knots of the displaced grid along the characteristic curves (when using C° finite elements with linear basis function). In other words, for all points $\varphi^i_j = \varphi^i(x_j)$, $\varphi^i_j = (\varphi^i_{1p}, \varphi^i_{2q})$ represents the displacement along the characteristic of the point x_j, where p and q denote the coordinate index of the center point in the regular displaced element such that $j = (p-1) * J + q$ and $1 \leq j \leq P(= I * J)$. Then the integral (5.24) which is denoted by $\mathcal{S}$ as shown by Bermejo [25], is a value of a bicubic spline at the point φ^i_j which is as in [25]. Then

$$\mathcal{S}(\varphi^i_{1p}, \varphi^i_{2q}) = \textstyle\sum_{s=1}^{J}\sum_{r=1}^{I} u^{(rs)}_{(i-1)} K_r(\varphi^i_{1p}) K_s(\varphi^i_{2q}) \tag{5.25}$$
$$= (u_{i-1} \circ \varphi^i, \phi_j(x)) \qquad j = 1, ...P,$$

where p, q determine j and $K_r(\varphi^i_{1p})$, $K_s(\varphi^i_{2q})$ are piecewise cubic polynomials in φ^i_{1hp} and φ^i_{2hq} respectively, u_{i-1} is the solution at the time t_{i-1}, see [2]. To characterize this bicubic spline we move back the coordinates $\varphi^i_j = (\varphi^i_{1p}, \varphi^i_{2q})$ to the fixed grid point $x_j = (x_{1p}, x_{2q})$. Then we have

$$\mathcal{S}(x_j) = A[U_{i-1}]_j, \qquad j = 1, 2, ..., P. \tag{5.26}$$

where the subscript denotes the j-th component of $A[U_{i-1}]$, where A is the $P \times P$ matrix, $A = A(a_{lj})$, $a_{lj} = \int_{E_j} \phi_l(x)\phi_j(x)$. We express the spline $\mathcal{S}(x_j)$ in terms of the bicubic B-spline

$$\mathcal{S}(x) = \sum_{j=1}^{P} \mu^{(i)}_j B_j(x). \tag{5.27}$$

where $B_j = B_{1j} \otimes B_{2j}$ is the Cartesian product of the natural cubic splines B_{1j} and B_{2j} corresponding to x_1 and x_2 respectively, see [6]. The coefficients $\mu^{(i)}_j$ can be determined from (5.27), (5.26) choosing $x = x_j, (j = 1, ..., P)$ and solving the linear system (5.26). Substituting the coordinates φ^i_j in (5.27) we arrive at

$$\mathcal{S}(\varphi^i_j) = \sum_{j=1}^{P} \mu^{(i)}_j B_j(\varphi^i_j)$$

which represents the approximation of $(u_{i-1} \circ \varphi^i, \phi_j)$.

Now, concerning the evaluation of the $\partial_t S$ in (1.4) for the non-equilibrium case, we use exact integration for the ordinary differential equation in (1.4) (for the adsorption isotherm) which is of the form

$$S(t) = S_0 \, \mathrm{e}^{-at} + \int_0^t \mathrm{e}^{-a(t-s)} \, \psi(C(s))ds.$$

Solution	Number of iterations (k)	Time	Time step	Space step
1	3	t=2	Δt=1/10	Δx=1/10
2	3	t=2	Δt=1/20	Δx=1/20
3	3	t=2	Δt=1/50	Δx=1/50
1	5	t=6	Δt=1/10	Δx=1/10
2	5	t=6	Δt=1/20	Δx=1/20
3	5	t=6	Δt=1/50	Δx=1/50

TABLE 1. Discretization and iteration parameters for example 1

Then

$$\partial_t S = d\left[\psi(C(t)) - \left(S_0\, \mathrm{e}^{-at} + \int_0^t \mathrm{e}^{-a(t-s)}\, \psi(C(s))ds\right)\right]$$

Approximating the integral in the expression above by choosing $\psi(C(t,x))$ as a piecewise constant function, we have

$$s_{i+1} = \mathrm{e}^{-a\tau}\, s_i + \alpha_{i+1,i}\psi(C_i(x)) \quad \text{for } i = 1, \dots, n \tag{5.28}$$

where $\alpha_{i+1,j} = \mathrm{e}^{-a\tau}\, \alpha_{i,j}$, since $\alpha_{i,j} = \int_{t_{j-1}}^{t_j} \mathrm{e}^{-a(t_i-s)}\, ds$. As a result we do not need to store the values of C_j $(j = 1, \dots, i-1)$ for the evaluation of S_i. In our numerical experiments, we approximate the memory term more precisely using linear approximation of $\psi(C(t,x))$ instead of piecewise constant approximation.

Comparison of numerical with exact solutions

To demonstrate the effectiveness of our numerical scheme, we will compare the numerical solution with an analytical one. We shall consider the model problem

$$\begin{aligned} &\partial_t(u + u^{1/2}) + \partial_x u - D\partial_x^2 u = 0, \\ &u(0,t) = u_0\Psi(t), \quad u(x,0) = 0,\ x > 0 \end{aligned} \tag{5.29}$$

where Ψ is a smooth increasing function with $\Psi(0) = 0$ and $\Psi(t) \to 1$ for $t \to \infty$. We shall specify it later. Notice that (5.29) is a special case of (1.4), where adsorption in equilibrium mode is considered only.
The exact solution , $u(x,t) = f(x - vt)$, is the travelling wave which is given by, see [18]

$$f(\xi) = \begin{cases} u_0(1 - \exp\left(\frac{1}{2D}\frac{1}{1+\sqrt{u_0}}\xi\right))^2, & \xi < 0 \\ 0 \quad , & \xi > 0 \end{cases} \tag{5.30}$$

Here $v = \frac{\sqrt{u_0}}{1+\sqrt{u_0}}$ and $\Psi(t) = \frac{1}{u_0} f(-vt)$. $f(\xi) \to u_0$ for $\xi \to -\infty$, which can be easily justified.

In our numerical experiments, we choose $u_0 = 2$, i.e., $v = \frac{1}{2}$, $\Psi(t) = (1 - \exp\left(-\frac{t}{8D}\right))^2$. Since D is small, $\Psi(t)$ is very close to 1 for $t > \delta > 0$ with small δ.

Example 1: We use the data $u_0 = 2.0, D = 0.01$, with the discretization and iteration parameters listed in Table 1. In Figure 1 we present the exact and numerical solution with the corresponding discretization parameters. In this case, the Courant number equals 1.

Example 2: We consider the more regular case with stronger diffusion. We choose $u_0 = 2, D = 0.1$, with the discretization and iteration parameters

Solution	Number of iterations k	Time	Time step	Space step
1	3	t=2	Δt=1/10	Δx=1/10
2	3	t=2	Δt=1/5	Δx=1/10
3	3	t=2	Δt=1/2	Δx=1/10
1	3	t=6	Δt=1/10	Δx=1/10
2	3	t=6	Δt=1/5	Δx=1/10
3	3	t=6	Δt=1/2	Δx=1/10

TABLE 2. Discretization and iteration parameters for example 2

in the Table 2. Less iteration steps occur due to the higher regularity of the solution. The comparison with the exact solution is depicted in Figure 2 for $t = 2$ and $t = 6$. The real velocity (retarded) of contaminant transport equals $\frac{1}{2}$, while the water velocity of the model (5.29) equals 1. The approximate solution 2 corresponds to the discretization parameters with the Courant number larger than 1.

Numerical experiments in 1D and 2D

We present 1D and 2D numerical experiments supporting our concept of approximation. However, this concept can also be used in the three dimensional case. We consider

$$\begin{aligned} &\theta\partial_t u + \rho\partial_t S + \bar{q}\cdot\nabla u - D\Delta u = 0 \quad \text{in } x \in (0,L), t > 0, \\ &\partial_t S = d(u^p - S) \end{aligned} \tag{5.31}$$

with constants $\theta, \rho, \bar{q}, p, D$, along with the Dirichlet boundary conditions

$$u(t,0) = u(t,L) = 0.$$

We consider $S(0,x) \equiv 0$. The initial profile is given in pulse form:

$$u(0,x) = \begin{cases} 1, & 0.1 \le x \le 0.5 \\ 0, & otherwise \end{cases}$$

According to the procedure described in section 1 and (5.28) we eliminate the kinetic equation in (5.31).

In the following examples we choose the number of iterations $k = 3$. The concentration profile $u(t,x)$ at $t = 1, 2$ and 6 is depicted in Figures below for the following choices of $\theta, \rho, \bar{q}, p, D$:

Example 3: We shall take the following data $\theta = 0.5, \rho = 1.5, \bar{q} = 3, D = 0.05$, $d = 10$. This example was run with the following discretization: $\Delta x = 1/10, \Delta t = 1/200$. This example is used to investigate the influence of p on the solution. The solution plotted in Figures 3-6.

Example 4: In this example numerical experiments are reported in two dimensions model with nonequilibrium adsorption $d = 10$. Other parameters are the same as in example 3 except $\theta = 1$. For simplicity we consider the initial condition

$$u(0,x,y) = \begin{cases} 1, & 0.1 \le x \le 0.5, 1 \le y \le 3 \\ 0, & otherwise \end{cases}$$

and the boundary conditions are

$$u(0,y,t) = u(L,y,t) = 0, u(x,0,t) = u(x,L,t) = 0$$

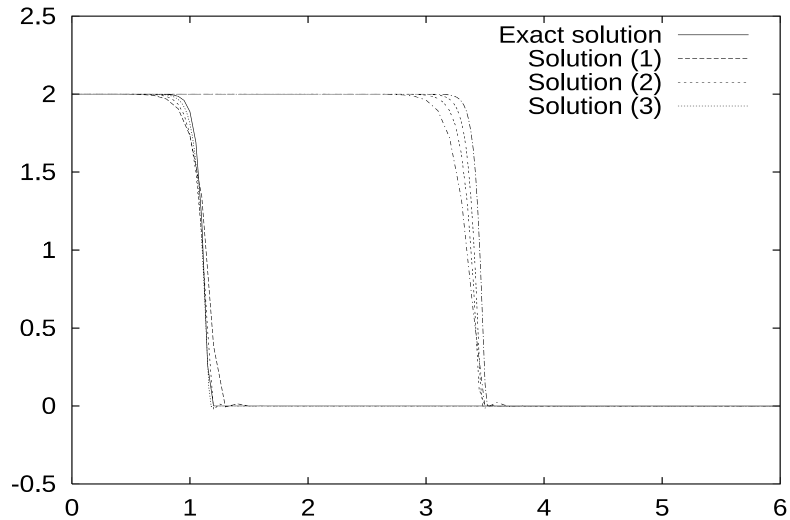

FIGURE 1. Comparison exact and numerical solutions for $t = 2, t = 6, D = 0.01$.

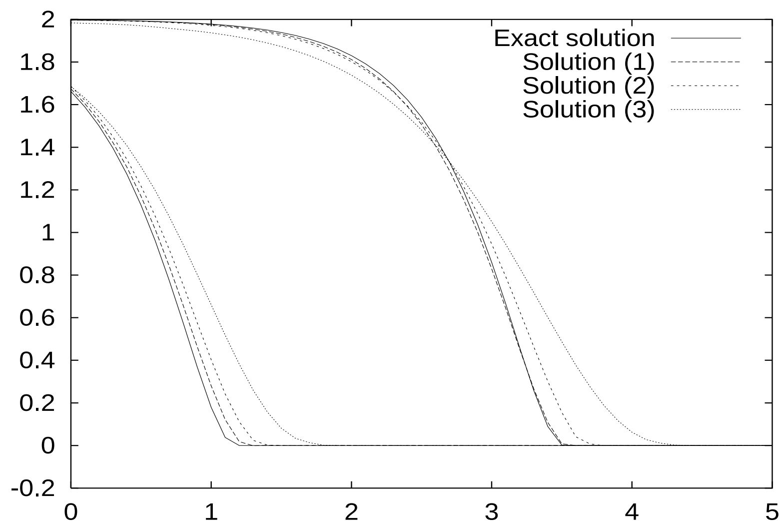

FIGURE 2. Comparison exact and numerical solutions for $t = 2, t = 6, D = 0.1$.

The concentration profiles have been drawn for $p = 0.4$. The discretization parameters are: $\Delta x = \Delta y = 1/10$, $\Delta t = 1/200$. The solutions are depicted in Figures 6-9.

References

[1] J. Barrett and P. Knabner: An improved error bound for a Lagrange-Galerkin method for contaminant transport with non-lipschitian adsorption kinetics. SIAM J. Numer. Annal. 5 (1998), pp. 1862-1883.

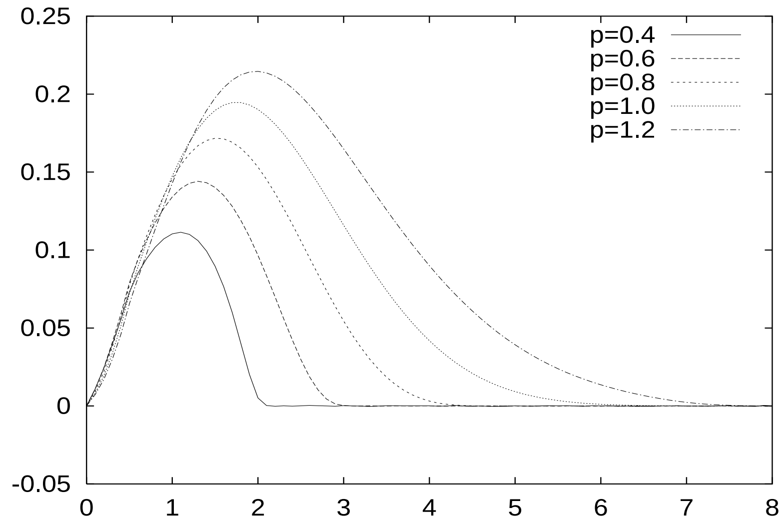

FIGURE 3. Concentration in nonequilibrium adsorption case at t=1

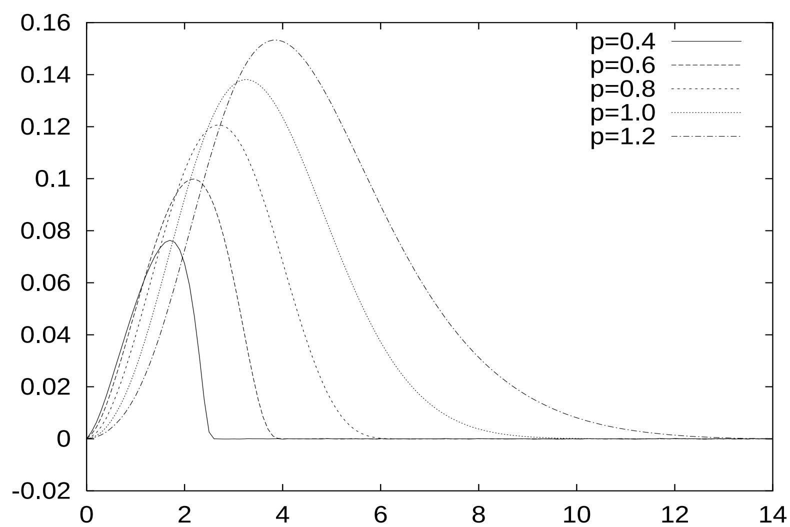

FIGURE 4. Concentration in nonequilibrium adsorption case at t=2

[2] R. Bermejo: *A Galerkin-Characteristics algorithm for transport-diffusion equation.* SIAM J. Numer. Annal. 32 (1995), pp. 425-455.
[3] R. Bermejo: *Analysis of an algorithm for the Galerkin-Characteristics method.* Numer. Math 60 (1991), pp. 163-194.
[4] C. N. Dawson, C. J. Van Duijn and R. E. Grundy: *Large time asymptotics in contaminant transport in porous media.* SIAM J. Appl. Math. Vol. 56, N4, (1996), pp. 965-993.
[5] C. N. Dawson: *Analysis of an upwind-mixed finite element method for nonlinear contaminant transport equation.* SIAM J. Numer. Annal. 5 (1998), pp. 1709-1725.
[6] C. DE Boor: *A practical guide to splines.* Springer-Verlag,N Yorks, Berlin, Heidelberg (1978)

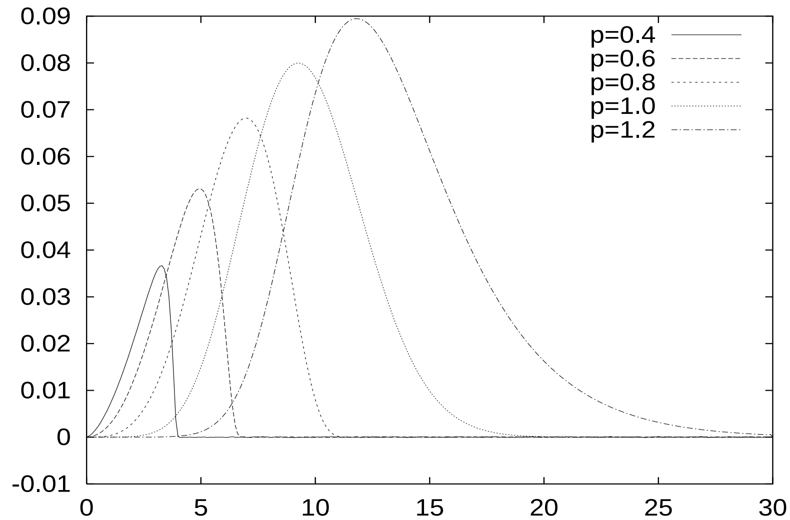

FIGURE 5. Concentration in nonequilibrium adsorption case at t=6

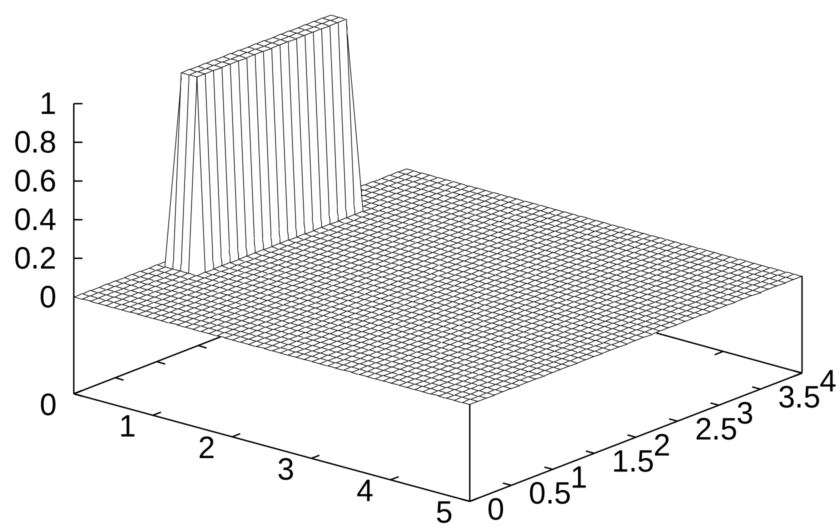

FIGURE 6. Initial condition

[7] J. Douglas, T. F. Russell: *Numerical methods for convection dominated diffusion problems based on combining the method of the characteristics with finite elements or finite differences.* SIAM J. Numer. Annal. 19 (1982), pp. 871-885.

[8] J. Douglas, C.-S. Huang, F. Pereira: *The modified method of characteristics with adjusted advection,* Numer. Math. 83, 3, 353-369, (1999).

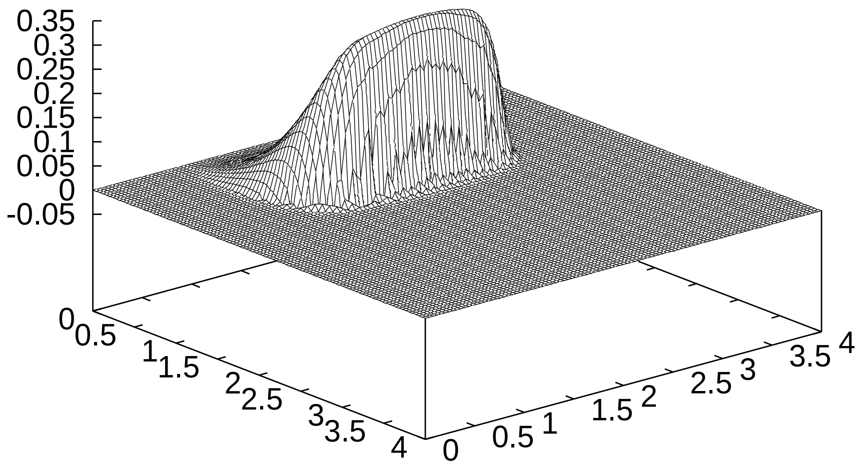

FIGURE 7. Concentration in nonequilibrium case $p = 0.4$ at $t = 1$

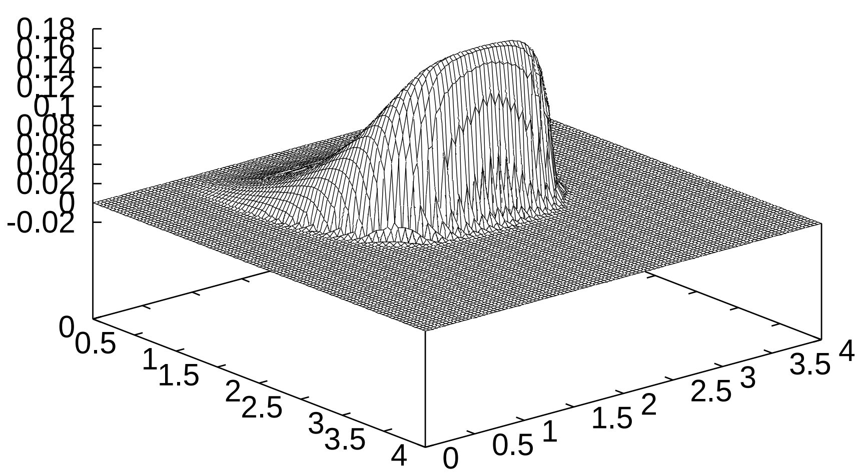

FIGURE 8. Concentration in nonequilibrium case $p = 0.4$ at $t = 2$

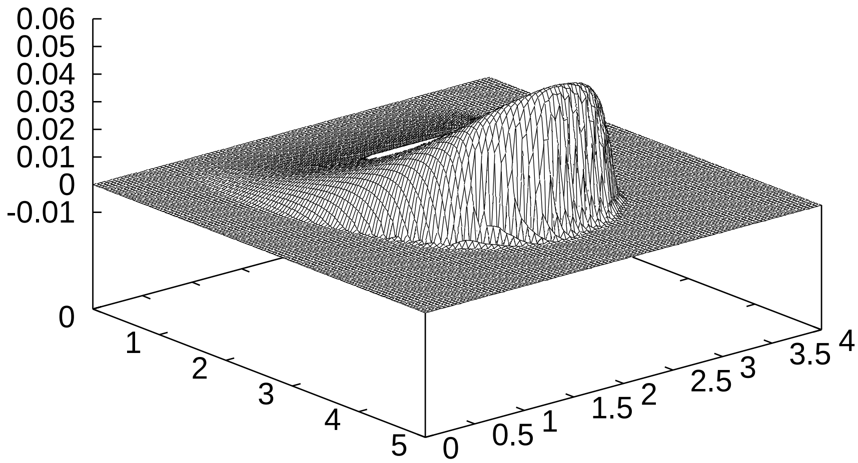

FIGURE 9. Concentration in nonequilibrium case $p = 0.4$ at $t = 6$

[9] C. J. Van Duijn, P. Knabner: *Solute transport in porous media with equilibrium and non-equilibrium multiple-site adsorption: Traveling waves.* J. Reine Angewandte Math., 415, (1991), pp. 1-49.

[10] C. J. Van Duijn, P. Knabner: *Transport in porous media 8* (1992), pp. 167-226.

[11] R.E. Grundy, C.J. Van Duijn, C. N. Dawson: *Asymptotic profiles with finite mass in one-dimensional contaminant transport through porous media: The fast reaction case.* Q. J Mech. appl. Math., Vol. 12, pp. 69-106 (1994).

[12] W. Jäger, J. Kačur: *Solution of porous medium systems by linear approximation scheme.* Num.Math. 60, pp. 407-427 (1991).

[13] W. Jäger, J. Kačur: *Solution of doubly nonlinear and degenerate parabolic problems by relaxation schemes.* M^2AN Mathematical modeling and numerical analysis Vol. 29, N5, pp. 605-627 (1995).

[14] J. W. Jerome: *Convection-dominated nonlinear systems: Analysis of the Douglas-Russell transport-diffusion algorithm based on approximate characteristics and invariant regions.* SIAM J. Numer. Anal., Vol. 25, N4, (1988), pp. 815-836.

[15] J. Kačur: *Method of Rothe in evolution equations.* Teubner-Texte zur Mathematic, 80, Leipzig (1985).

[16] J. Kačur: *Solution to strongly nonlinear parabolic problems by a linear approximation scheme.* Mathematics Preprint No. IV-M1-96, Comenius University Faculty of Mathematics and Physics, (1996), pp. 1-26, appear in IMA J. Num.

[17] J. Kačur: *Solution of degenerate convection-diffusion problems by the method of characteristics,* SIAM J. Numer. Ana. 2001, Vol.39,NO. 3, pp858-879.

[18] J. Kačur J. and M. Sh. Mahmood, Solution of Solute transport in unsaturated porous media by the by the method of characteristics, Numer Methods partial differential Eq, 19, 732-761, (2003).

[19] P. Knabner: *Mathematische Modelle für Transport und Sorption gelöster Stoffe in porösen Medien.* Meth. Verf. Math. Phys.,36 (1991)

[20] P. Knabner: *Finite-Element-Approximation of Solute Transport in Porous Media with General Adsorption Processes.* "Flow and Transport in Porous Media" Ed. Xiao Shutie, Summer school, Beijing, 8-26 August 1988, World Scientific (1992), pp. 223-292.
[21] P. Knabner, F. Otto: *Solute transport in porous media with equilibrium and non-equilibrium multiple-site dosorption: Uniqueness of the solution,* Nonlinear Analysis, TMA 42/3 (2000), 381-403.
[22] A. Kufner, O. John, S. Fučík: *Function spaces.* Noordhoff, Leiden, 1977.
[23] O. A. Ladyzhenskaja, N. N. Uralceva: *Linear and quasilinear elliptic equations.* Academic Press, 1968
[24] M. Sh. Mahmood : *Galerkin characteristics algorithm for contaminant transport in porous media with equilibrium and nonequilibrium adsorptions.* PhD. thesis 2000, Department of Numerical Analysis, Faculty of Mathematics and Physics, Comenius University Comenius University.
[25] K. W. Morton, A. Priestley, and Süli: *Stability of the Lagrange-Galerkin method with non-exact integration.* RAIRO model. Math. Anal.Numer. 4 (1988) pp. 225-250.
[26] J. Nečas: *Les méthodes directes en théorie des élliptiques.* Academia, Prague (1967).
[27] O. Pironneau: *On the transport-diffusion algorithm and its applications to the Naiver-Stokes equations.* Numer. Math., 38 (1982), pp. 309-332.
[28] F. Otto: L^1*-contraction principle and uniqueness for quasilinear elliptic-parabolic equations,* C. R. Acad. Sci. Paris T 321, Ser. I, (1995), pp. 105-110.

Department of Numerical Analysis, Faculty of Mathematics and Physics, Comenius University, 842 15 Bratislava, Slovakia
E-mail: kacur@fmph.uniba.sk

Department of Applied Mathematics, Mechanical Engineering Faculty, University of Žilina, 010 26 Žilina, Slovakia
E-mail: mahmoodm@fstroj.uniza.sk