

Research Article

Fixed-Point and STILS Method to Solve a Coupled System of Transport Equations

Daouda Sangare 

Laboratoire d'Analyse Numérique et d'Informatique (LANI), UFR SAT, Université Gaston Berger, Saint-Louis, Senegal

Correspondence should be addressed to Daouda Sangare; daouda.sangare@ugb.edu.sn

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In this paper, a coupled system of two transport equations is studied. The techniques are a fixed-point and Space-Time Integrated Least Square (STILS) method. The nonstationary advective transport equation is transformed to a “stationary” one by integrating space and time. Using a variational formulation and an adequate Poincaré inequality, we prove the existence and the uniqueness of the solution. The transport equation with a nonlinear feedback is solved using a fixed-point method.

1. Introduction

This work is motivated by the crystal dissolution and precipitation model in saturated porous medium [1]. In [1], the authors present a macroscopic model describing ions transport by fluid flow in a porous medium undergoing dissolution and precipitation reactions. Such models received much attention during the past years (e.g., [2–4]).

All these papers deal with the upscaled formulation of the phenomena. A rigorous justification, starting from a well-posed microscopic (pore-scale) model and applying a suitable upscaling, has been given for important classes of problems. For instance, [5] presents homogenization as a method for upscaling and contains an overview with particular emphasis on porous media flow including chemical reactions. In this respect, we also mention [6], where the reaction rates and isotherms are linear (see also [7] or [8]), where nonlinear cases as well as multivalued interface conditions are analyzed.

In [9], the authors study the pore-scale analogue of the model proposed in [1], which is built on Stokes flow in the pores, transport of dissolved ions by convection and diffusion, and dissolution-precipitation reactions on the surface of the porous skeleton. They use regularisation techniques and a fixed-point argument to obtain existence of a weak solution in general domains. The results obtained are a rigorous justification of the macroscopic model in [1].

In this paper, we give a mathematical analysis of the macroscopic model in [1] using the fixed-point theorem and the STILS method to solve the transport equations.

The least squares method is widely used to solve partial differential equations. We can refer to [10, 11] for application on elasticity and fluid mechanics problems. Some general mathematical results have been obtained for this method in the case of first-order time-dependent conservation laws. With the space-time objects below, the STILS method transforms a nonstationary problem into a “stationary” problem by integrating space and time. This “stationary” problem is of advective form. For instance, in [12], an equivalence between the advective formulation and that of anisotropic diffusion is established.

The STILS method is originated to [13, 14]. In [13, 14], a least squares method is used to solve a 2D stationary first-order conservation equation with regularity assumptions on the advection velocity. A comparison between the least squares solution and the renormalized solution in the sense of [15] for some equations is given in [16]. The STILS method leads to some numerical schemes which are much simpler than the usual ones (like the streamline diffusion method, the characteristic method, and the discontinuous finite element method with flux limiter). Some numerical examples are presented in [17–19].

In this paper, we make use of both the fixed-point theorem and the so called STILS method to solve nonlinear transport equations in the model described below.

This paper is organized as follows. Section 2 provides a brief presentation of the model proposed in [1]. Assumptions and preliminary results useful to the resolution are also presented. Section 3 is devoted to an existence and uniqueness theorem. The fixed-point theorem and the STILS method are both used to deal with the above mentioned model.

2. Model Equations and Problem Description

2.1. Model Equations. It is useful to recall the model equations suggested in [1] without going into the details. We assume having two species M_1 and M_2 , for example, ions, say M_1 being a cation and M_2 an anion. In addition, there may be a crystalline solid M_{12} present at the porous skeleton. M_1 and M_2 may precipitate at the surface of the porous skeleton to form M_{12} , and conversely, the crystalline solid may dissolve. The stoichiometry of the reaction is supposed to be as follows:

$$M_{12} \rightleftharpoons nM_1 + mM_2. \quad (1)$$

n and m denote positive numbers. Let $c_i, i = 1, 2$, be the molar concentration of M_i in the solution relative to the water volume, and let c_{12} be the molar concentration of M_{12} relative to the mass of the porous skeleton. The particle M_{12} is attached to the surface of the porous skeleton and thus is immobile. The conservation of the corresponding total masses leads to the partial differential equations

$$\frac{\partial}{\partial t}(\theta c_1) + n\rho \frac{\partial}{\partial t} c_{12} - \operatorname{div}(\theta D \nabla c_1 - q^* c_1) = 0, \quad (2)$$

$$\frac{\partial}{\partial t}(\theta c_2) + m\rho \frac{\partial}{\partial t} c_{12} - \operatorname{div}(\theta D \nabla c_2 - q^* c_2) = 0, \quad (3)$$

where the water content θ is supposed to be constant and not affected by the reaction (1), ρ is the bulk density, D is the diffusion/dispersion tensor, and q^* is the specific discharge vector. If we define

$$c = mc_1 - nc_2, \quad (4)$$

then equations (2) and (3) imply that the quantity c verifies

$$\frac{\partial}{\partial t} c - \operatorname{div}\left(D \nabla c - \frac{q^*}{\theta} c\right) = 0. \quad (5)$$

Another equation for c_{12} results from a description of the precipitation and dissolution processes. Following the detailed discussion in [1], we have

$$\frac{\rho}{\theta} \frac{\partial}{\partial t} c_{12} - k^*(r_p - r_d) = 0, \quad (6)$$

where r_d and $r_p = k_p r(c_1, c_2)$ are, respectively, the dissolution and precipitation rates and k^* the reaction velocity. r is a non-linear smooth nonnegative function depending on c_1 and c_2 . A typical example is leading to

$$r(x, y) = x^n y^m. \quad (7)$$

Summarizing the discussion done in about precipitation-dissolution reaction, we have for the crystalline solid the equation

$$\frac{\rho}{\theta} \frac{\partial}{\partial t} c_{12} \in k^*(k_p r(c_1, c_2) - k_d H(c_{12})) \quad (8)$$

or equivalently

$$\frac{\rho}{\theta} \frac{\partial}{\partial t} c_{12} = k^*(k_p r(c_1, c_2) - k_d w), \quad (9)$$

where

$$w \in H(c_{12}), \quad (10)$$

which means $0 \leq w \leq 1$ for $c_{12} = 0$ and $w = 1$ for $c_{12} > 0$. H is the set-valued Heaviside function defined by

$$H(u) = \begin{cases} 1 & \text{for } u > 0, \\ [0, 1] & \text{for } u = 0, \\ 0 & \text{for } u < 0. \end{cases} \quad (11)$$

We make now some assumptions which lead to the model we study in this paper. Equation (4) gives

$$c_2 = \frac{1}{n}(mc_1 - c). \quad (12)$$

Then, in this model, we consider equations (2), (5), and (9).

If the dispersive transport is negligible compared to the advective transport, it is reasonable to tend D to zero. This assumption cancels the corresponding terms in (2) and (5). We assume also that $c_{12} > 0$ anywhere; it means $w = 1$ in (9). The velocity of the solute transport $q = q^*/\theta$ in (2) is the gradient of the hydraulic potential. Setting

$$\begin{aligned} c_{12} &:= \frac{n\rho}{\theta} c_{12}, \\ \alpha &:= k^* k_p, \\ \beta &:= \frac{k_d}{k_p}, \end{aligned} \quad (13)$$

the model equations have the following form:

$$\frac{\partial}{\partial t} c_1 + \frac{\partial}{\partial t} c_{12} + q \cdot \nabla c_1 = 0, \quad (14)$$

$$\frac{\partial}{\partial t} c + q \cdot \nabla c = 0, \quad (15)$$

$$\frac{\partial}{\partial t} c_{12} = \alpha \left(r \left(c_1, \frac{1}{n}(mc_1 - c) \right) - \beta \right). \quad (16)$$

In this paper, we study the coupled system (14)–(16) in addition to the appropriate boundary conditions.

2.2. Problem Description

2.2.1. Notations. Let $\Omega \subset \mathbb{R}^d$, $d = 1, 2, 3$, be a domain with a Lipschitz boundary $\partial\Omega$ satisfying the cone property.

If $T > 0$ is given, set $\Omega_T = \Omega \times]0, T[$. Let

$$\begin{aligned} \Gamma^- &= \{x \in \partial\Omega, q(x) \cdot n(x) < 0\}, \\ \Gamma^+ &= \{x \in \partial\Omega, q(x) \cdot n(x) > 0\}, \end{aligned} \tag{17}$$

where $n(x)$ is the outer normal to $\partial\Omega$ at x . Let

$$\begin{aligned} \Gamma_T^- &= \Gamma^- \times [0, T] \cup \Omega \times \{0\}, \\ a &= (q, 1)^t, \\ \nabla_t &= \left(\nabla, \frac{\partial}{\partial t} \right)^t. \end{aligned} \tag{18}$$

Let $H^m(\Omega)$ be the classical Hilbert space of order m , and

$$H_0^1(\Omega) = \{\varphi \in H^1(\Omega); \varphi = 0 \text{ on } \partial\Omega\}. \tag{19}$$

We also define the following Hilbert space V :

$$V = \{\phi \in L^2(\Omega_T); (a \cdot \nabla_t \phi) \in L^2(\Omega_T)\}, \tag{20}$$

equipped with the graph norm:

$$\|v\|_V^2 = \|v\|_{L^2(\Omega_T)}^2 + \|a \cdot \nabla_t v\|_{L^2(\Omega_T)}^2, \quad \forall v \in V. \tag{21}$$

Let

$$H(a, \Omega_T; \Gamma^-) = \{\phi \in V \text{ such that } \phi = 0 \text{ on } \Gamma^- \times]0, T[\}. \tag{22}$$

The problem consists in finding

$$c, c_1 : \Omega_T \longrightarrow \mathbb{R}, \tag{23}$$

satisfying the following partial differential equation system

$$\left\{ \begin{array}{l} (P1) \left\{ \begin{array}{l} \frac{\partial c}{\partial t} + q \cdot \nabla c = 0 \text{ in } \Omega_T, \\ c = g \text{ on } \Gamma_T^-, \\ c(x, 0) = c_0(x) \text{ in } \Omega, \end{array} \right. \\ (P2) \left\{ \begin{array}{l} \frac{\partial c_1}{\partial t} + q \cdot \nabla c_1 = \left(r \left(c_1, \frac{1}{n} (m c_1 - c) \right) - \beta \right) \text{ in } \Omega_T, \\ c_1 = g_1 \text{ on } \Gamma_T^-, \\ c_1(x, 0) = c_{10}(x) \text{ in } \Omega. \end{array} \right. \end{array} \right. \tag{24}$$

Equations (14) and (16) give system (P2). In systems (P1) and (P2), initial conditions and inflow boundary conditions are given for c and c_1 . The technique is to solve

first (P1) and after (P2). With the solutions c and c_1 and equation (16), we obtain c_{12} .

2.2.2. Preliminary Results. The STILS method will be used to solve the problem (P1) like in [12, 20]. The method leads to a variational formulation problem, and we use the classical Lax-Milgram theorem to find the solution. So we give the following lemma to prove the bilinear map coercivity.

Lemma 1 (curved Poincaré inequality). *There exists a constant $k = 2T$ such that*

$$\|u\|_{L^2(\Omega_T)} \leq k \|a \cdot \nabla_t u\|_{L^2(\Omega_T)}, \quad \forall u \in H(a, \Omega_T; \Gamma^-). \tag{25}$$

The proof is in [20].

Let $H(X, x, t)$ be a polynomial with respect to X with bounded coefficients h_i defined in Ω_T .

$$H(X, x, t) = \sum_{i=0}^n h_i(x, t) X^i. \tag{26}$$

Let $a_i, i = 0, \dots, n$ be defined by

$$a_i = \sup_{\Omega_T} |h_i(x, t)|. \tag{27}$$

(P2) is also a transport problem with a nonlinear feedback. We use both STILS method and fixed-point theorem to solve the problem. So we need $(c_1^k)_{k \in \mathbb{N}}$ to be bounded in $L^\infty(\Omega_T)$; hence, we give the following lemma.

Lemma 2. *Let T be a positive real number and $u^0 \in D(\Omega_T)$ a positive function such that*

$$T < \frac{\sup_{\Omega_T} (u^0)}{\sum_{i=0}^n a_i \left(\sup_{\Omega_T} u^0 \right)^i}. \tag{28}$$

Let $(u^k)_{k \in \mathbb{N}}$ be the sequence of functions defined by

$$\begin{cases} a \cdot \nabla_t u^k = H(u^{k-1}, x, t) \text{ in } \Omega_T, \\ u^k = 0 \text{ on } \Gamma_T^-. \end{cases} \tag{29}$$

Then, we have

$$\forall k \in \mathbb{N}, \sup_{\Omega_T} |u^k| \leq \sup_{\Omega_T} (u^0). \tag{30}$$

Proof. Assume that there exists $k \in \mathbb{N}^*$ such that

$$\sup_{\Omega_T} (|u^j|) \leq \sup_{\Omega_T} (u^0), \quad \forall j = 0, \dots, k-1. \tag{31}$$

We know that the velocity field q is bounded in its time component and has a constant dot product (equal to 1, too) with the vector $(0, \dots, 0, 1)$. This ensures (see Proposition 7

in [12]) that Ω_T is filled by the characteristics in the following ways:

There exists an $S > 0$ such that for almost each point (x, t) of Ω_T , there exists an integral curve

$$\zeta : [0, S] \longrightarrow \Omega_T \text{ such that } \frac{\partial \zeta}{\partial s} = a(\zeta) \quad (32)$$

that connect (x, t) to the space-time inflow boundary:

$$\begin{aligned} \zeta(0) &= (x_0, t_0) \in \Gamma_T^-, \\ \zeta(t) &= (x, t), \quad \forall t \in [0, S]. \end{aligned} \quad (33)$$

On this integral curve (characteristic), system (29) gives

$$u^k(x(t), t) = \int_{t_0}^t H(u^{k-1}, x(s), s) ds. \quad (34)$$

Hence,

$$|u^k(x(t), t)| \leq T \sum_{i=0}^n a_i \left(\sup_{\Omega_T} (u^0) \right)^i \leq \sup_{\Omega_T} (u^0), \quad (35)$$

thanks to (28). Moreover, since Ω_T is filled by characteristics, we have

$$\sup_{\Omega_T} (|u^k|) \leq \sup_{\Omega_T} (u^0). \quad (36)$$

Finally, we conclude that for any $n \in \mathbb{N}$, $\sup_{\Omega_T} (|u^n|) \leq \sup_{\Omega_T} (u^0)$. This ends the proof of the lemma. \square

3. Existence and Uniqueness Theorem

Theorem 3. *Let $(g, g_1) \in L^\infty(\Gamma_T^-) \times L^\infty(\Gamma_T^-)$ and $(c_0, c_{10}) \in L^\infty(\Omega) \times L^\infty(\Omega)$. System (24) has an unique solution $(c, c_1) \in V^2$.*

Proof. The proof will be done in two steps.

Step one. In the system (P1), we assume that the divergence of the velocity q is zero; then, we can use the result in [12] or in [21, 22] cited in [12] to prove the existence of the boundary trace on Γ_T of a function in V .

So, using the extension $d \in V$ of g in system (P1), this later is equivalent to searching w in $H(a, \Omega_T; \Gamma^-)$ such that

$$(PMC) \begin{cases} a \cdot \nabla_t w - F = 0 \text{ in } \Omega_T, \\ w = 0 \text{ on } \Gamma_T^-, \\ w(x, 0) = c_0(x) - d(x, 0) \text{ in } \Omega, \end{cases} \quad (37)$$

with $F = -(\partial d / \partial t) - (1/\theta)q \cdot \nabla d$. Now, like in [12], we define the following convex quadratic form J :

$$J(w) = \int_{\Omega_T} (a \cdot \nabla_t w - F)^2 dx dt. \quad (38)$$

The Gateau derivative of J is

$$DJ(w)\varphi = \int_{\Omega_T} (a \cdot \nabla_t w - F)a \cdot \nabla_t \varphi dx dt. \quad (39)$$

Hence, w is the solution of (37) if and only if w satisfies

$$\int_{\Omega_T} (a \cdot \nabla_t w)(a \cdot \nabla_t \varphi) dx dt = \int_{\Omega_T} F(a \cdot \nabla_t \varphi) dx dt, \quad \forall \varphi \in H(a, \Omega_T; \Gamma^-). \quad (40)$$

Using the Lax-Milgram theorem, we have the solution of the variational problem (40). Lemma 1 is used to prove the bilinear application coercivity.

Step two. This last step is devoted to the problem (P2). We set

$$G(c_1) = -\alpha \left(r \left(c_1, \frac{1}{n}(mc_1 - c) \right) - \beta \right), \quad (41)$$

which is a polynomial function with respect to c_1 with coefficients depending on c . Then, (P3) becomes

$$\begin{cases} a \cdot \nabla_t c_1 == G(c_1) \text{ in } \Omega_T, \\ c_1 = g_1 \text{ in } \Gamma_T^-, \\ c_1(x, 0) = c_{10}(x) \text{ in } \Omega. \end{cases} \quad (42)$$

This is a transport equation with a nonlinear feedback $G(c_1)$ due to the chemical reactions (dissolution-precipitation). To solve it, we first split (42) into the following systems:

$$(PT1) \begin{cases} a \cdot \nabla_t \bar{c} == G(\bar{c} + \tilde{c}) \text{ in } \Omega_T, \\ \bar{c} = 0 \text{ on } \Gamma_T^-, \\ \bar{c}(x, 0) = 0 \text{ in } \Omega. \end{cases} \quad (43)$$

$$(PT2) \begin{cases} a \cdot \nabla_t \tilde{c} == 0 \text{ in } \Omega_T, \\ \tilde{c} = g_1 \text{ on } \Gamma_T^-, \\ \tilde{c}(x, 0) = c_{10}(x) \text{ in } \Omega. \end{cases} \quad (44)$$

In order to solve the nonlinear system (43), we use the fixed-point theory. For $T > 0$ and $c^0 \in D(\Omega_T)$ satisfying (28), let $(c^k)_{k \in \mathbb{N}}$ be the sequence of functions defined by

$$(PT1_k) \begin{cases} a \cdot \nabla_t c^k = G(c^{k-1} + \tilde{c}) \text{ in } \Omega_T, \\ c^k = 0 \text{ on } \Gamma_T^-, \\ c^k(x, 0) = 0 \text{ in } \Omega. \end{cases} \quad (45)$$

Using Lemma 2, we prove that $(c^k)_{k \in \mathbb{N}}$ is bounded in $L^\infty(\Omega_T)$.

Put $c_1^k = c^k + \tilde{c}$ solution of

$$\begin{cases} a \cdot \nabla_t c_1^k = G(c_1^{k-1}) \text{ in } \Omega_T, \\ c_1^k = g_1 \text{ on } \Gamma_T^-, \\ c_1^k(x, 0) = c_{10}(x) \text{ in } \Omega. \end{cases} \quad (46)$$

Let us show that $(c_1^k)_{k \in \mathbb{N}}$ is a Cauchy sequence in V and that its limit c_1 is the solution of (42).

Let p and q be integers such that

$$a \cdot \nabla_t c_1^p = G(c_1^{p-1}), \quad (47)$$

$$a \cdot \nabla_t c_1^q = G(c_1^{q-1}). \quad (48)$$

Equations (47) and (48) give

$$a \cdot \nabla_t (c_1^p - c_1^q) = G(c_1^{p-1}) - G(c_1^{q-1}). \quad (49)$$

By a variational formulation, (49) give

$$\begin{aligned} & \int_{\Omega_T} a \cdot \nabla_t (c_1^p - c_1^q) (a \cdot \nabla_t w) dxdt \\ &= \int_{\Omega_T} [G(c_1^{p-1}) - G(c_1^{q-1})] (a \cdot \nabla_t w) dxdt, \quad \forall w \in V. \end{aligned} \quad (50)$$

We choose $w = c_1^p - c_1^q$ then

$$\begin{aligned} & \int_{\Omega_T} a \cdot \nabla_t (c_1^p - c_1^q) (a \cdot \nabla_t (c_1^p - c_1^q)) dxdt \\ &= \int_{\Omega_T} [G(c_1^{p-1}) - G(c_1^{q-1})] (a \cdot \nabla_t (c_1^p - c_1^q)) dxdt. \end{aligned} \quad (51)$$

Hence,

$$\|a \cdot \nabla_t (c_1^p - c_1^q)\|_{L^2(\Omega_T)}^2 = \int_{\Omega_T} [G(c_1^{p-1}) - G(c_1^{q-1})] (a \cdot \nabla_t (c_1^p - c_1^q)) dxdt. \quad (52)$$

Since the function G is regular enough, we have

$$G(c_1^{p-1}) - G(c_1^{q-1}) = G'(s) (c_1^{p-1} - c_1^{q-1}). \quad (53)$$

So using the Cauchy-Schwarz inequality in the right hand side of (52), we get

$$\|a \cdot \nabla_t (c_1^p - c_1^q)\|_{L^2(\Omega_T)}^2 \leq \max_{0 \leq s \leq \gamma} |G'(s)| \|a \cdot \nabla_t (c_1^p - c_1^q)\|_{L^2(\Omega_T)} \|c_1^{p-1} - c_1^{q-1}\|_{L^2(\Omega_T)}. \quad (54)$$

Hence,

$$\|a \cdot \nabla_t (c_1^p - c_1^q)\|_{L^2(\Omega_T)} \leq \max_{0 \leq s \leq \gamma} |G'(s)| \|c_1^{p-1} - c_1^{q-1}\|_{L^2(\Omega_T)}. \quad (55)$$

Let $\tau = \max_{0 \leq s \leq \gamma} |G'(s)|$; we have

$$\|a \cdot \nabla_t (c_1^p - c_1^q)\|_{L^2(\Omega_T)} \leq \tau \|c_1^{p-1} - c_1^{q-1}\|_{L^2(\Omega_T)}. \quad (56)$$

Using the curved Poincaré inequality of Lemma 1, we get

$$\|c_1^p - c_1^q\|_V \leq 2\tau T \|c_1^{p-1} - c_1^{q-1}\|_V. \quad (57)$$

So, if $T < 1/2\tau$, the sequence $(c_1^k)_{k \in \mathbb{N}}$ is a Cauchy sequence in V which is a Hilbert space then converges to $c_1 \in V$.

Let us now prove that the limit c_1 of $(c_1^k)_{k \in \mathbb{N}}$ is the solution of (42). For this purpose, we write

$$\begin{aligned} a \cdot \nabla_t c_1 - G(c_1) &= a \cdot \nabla_t c_1 - a \cdot \nabla_t c_1^k + a \cdot \nabla_t c_1^k - G(c_1^{k-1}) \\ &\quad + G(c_1^{k-1}) - G(c_1), \quad \forall k \in \mathbb{N}. \end{aligned} \quad (58)$$

Since $a \cdot \nabla_t c_1 - a \cdot \nabla_t c_1^k$ tends to zero in $L^2(\Omega_T)$ and $a \cdot \nabla_t c_1^k - G(c_1^{k-1}) = 0$, it remains to be proved that $G(c_1^{k-1}) - G(c_1)$ tends to zero. We have

$$G(c_1^{k-1}) - G(c_1) = G'(s) (c_1^{k-1} - c_1). \quad (59)$$

We know that G' is bounded and (c_1^{k-1}) tends to c_1 in V so $G(c_1^{k-1}) - G(c_1)$ tends to zero. Then, c_1 is the solution of the first equation of (42). The boundary and initial conditions are obtained by the continuity of the trace mapping. \square

4. Conclusion

The existence and uniqueness solutions of a coupled transport equations have been proved by a fixed-point and STILS method. Free divergence of the transport velocity is considered in this work, but the method used can be extended to no free divergence case. The techniques used in this paper can be applied in other coupled nonstationary systems. The spatial operator in N dimension, for example, can be replaced by an operator in $N + 1$ dimension, where the $N + 1$ component is the time derivative. The obtained result can be improved adding a concrete example like solving a salt-wedge intrusion model or a coupled system arising in epidemiology. All those things and the numerical simulation will be done in the future work.

Data Availability

There are no data supporting this study.

Conflicts of Interest

The author declares that there are no conflicts of interest regarding the publication of this work.

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