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Numerical identification of parameters for a model of sedimentation processes

Aníbal Coronel[†], François James[‡] and Mauricio Sepúlveda[†]

[†] **GI²MA**, Departamento de Ingeniería Matemática, Universidad de Concepción, Casilla 160-C, Concepción, Chile

[‡] Mathématiques, Applications et Physique Mathématique d'Orléans, UMR CNRS 6628, UFR Sciences, Université d'Orléans, B.P. 6759, F-45067 Orléans Cedex 2, France.

E-mail: acoronel@ing-mat.udec.cl, james@labomath.univ-orleans.fr and mauricio@ing-mat.udec.cl

Abstract.

In this paper we present the identification of parameters in the flux and diffusion functions for a quasilinear strongly degenerate parabolic equation which models the physical phenomenon of flocculated sedimentation. We formulate the identification problem as a minimization of a suitable cost function and we derive its formal gradient by means of adjoint equation which is a backward linear degenerate parabolic equation with discontinuous coefficients. For the numerical approach, we start with the discrete Lagrangian formulation and assuming that the direct problem is discretized by the Engquist-Osher scheme obtain a discrete adjoint state associated to this scheme. The conjugate gradient method permits to find numerically the physical parameters. In particular, it allows to identify as well the critical concentration level at which solid flocs begin to touch each other and determines the change of parabolic to hyperbolic behavior in the model equation.

1. Introduction

Batch sedimentation is a classical procedure to separate flocculated suspension into a concentrated sediment of practical interest, and a clear fluid. It is used, for example in metallurgy, alimentation industry. The experimental setting consists of a vertical column, with a surface feeding at the top, and a discharge surface at the bottom. Under the influence of gravity, the suspension separates into a clear fluid, and a compressible sediment, which is collected at the bottom of the column. We refer to [13, 3, 4, 6] for more complete descriptions and details.

Under several constitutive and simplifying assumptions, it turns out that this mixture of two continuous media (fluid and solid flocs) can be described by a single model equation, namely a partial differential equation of mixed type, hyperbolic and parabolic. The unknown is the volumetric solid concentration ϕ , which is a function of the time t and the height in the column z .

Actually, the mixed type nature of the equation results from the different behaviour of the solid flocs on the one hand, the fluid on the other. The former indeed lies in a compression region, where the solid effective stress σ_e is not constant, while in the fluid zone, it can be taken equal to a constant. Therefore, in the solid zone (sediment), the equation will be of parabolic type, in the fluid zone, it will be hyperbolic.

More precisely, it can be assumed that σ_e is a nonlinear function of ϕ alone, with the following shape:

$$\sigma'_e(\phi) = \begin{cases} = 0 & \text{for } \phi \leq \phi_c \\ > 0 & \text{for } \phi > \phi_c \end{cases}$$

The concentration ϕ_c is the so-called *critical concentration*, above which the flocs get into contact with each other and form a network. The location of the interface $\phi = \phi_c$ is a specific problem in direct simulations.

Another constitutive relation can be obtained through Kynch's theory of kinematic sedimentation. It gives the velocity of the mixture as a function of the concentration ϕ ,

$$f(\phi, t) = q(\phi, t) + f_{bk}(\phi).$$

Here q is the volume average velocity of the mixture, $q = v_s\phi + v_f(1 - \phi)$ (v_s and v_f are the solid and fluid velocities), and f_{bk} the so-called batch flux density function. Kynch's theory gives a precise expression for this function.

We are interested here in the inverse problem which consists in identifying the constitutive laws f_{bk} and σ_e from experimental data. This kind of problem is in general impossible to solve in its full generality, that is considering f_{bk} and σ_e as general functions. Therefore we shall consider more precise constitutive assumptions, which give explicit expressions for both functions, depending on a finite number of parameters. Among these we emphasize the value of the critical concentration ϕ_c , which is of great practical importance, and very difficult to access from experimental data. We mention here that there are several experimental methods to obtain the involved parameters, see [11, 1] for an overview. They employ a set of data of local solid concentration and local permeability to the effective solid stress to obtain approximate correlation formulas and then by algebraic manipulation of this correlations determinate some empirical representation of f_{bk} and σ_e . In contrast to our approach, we need only experimental concentration data and we compute the optimal f_{bk} and σ_e .

There is a large list of authors who propose analytical and numerical methods for inverse problems in evolution partial differential equations. For example, parameter identification methods for parabolic PDEs can be found in [14, 15, 24, 29, 31] and references therein. Recently, Yamamoto and Zou reconstruct in [33] the radiative coefficient and the initial data for a linear parabolic equations using a piecewise linear finite element method for the discretization and a nonlinear gradient multigrid method for accelerating the reconstruction process. Several difficulties arise in the case specific we consider, since we want to reconstruct nonlinear coefficients, but such a strategy is likely useful to improve the results. Moreover, the hyperbolic degeneracy gives rise to

shocks in the concentration profiles. The existence and uniqueness for weak solutions to the direct problem rely on specific entropy conditions which has physical relevancy for the model and must be considered owing to the nonlinearity of the flux and degeneracy of the diffusion, see [3, 4, 9].

The existence of solutions for the inverse problem is a consequence of the continuous dependence of the entropy solutions with respect to the flux and the diffusion (see Theorem 2 below and [19, 21]). Its uniqueness cannot be ensured because of the hyperbolic behaviour, see [25, 26]. Therefore we shall rewrite the identification problem by adapting the technique developed by James and Sepúlveda, in [25, 26, 27], which is numerically tested as an efficient method to reconstruct the flux of a particular hyperbolic system. The idea is to write the inverse problem as an optimization problem for an appropriate cost function and then to apply the classical conjugate gradient method.

The continuous gradient stems from an adjoint state to the model consisting of a backward linear degenerate convection-diffusion equation with discontinuous coefficients and boundary conditions. As in the purely hyperbolic case, the adjoint equation is ill-posed in uniqueness. We obtain the discrete gradient by computing the exact gradient of the discrete formulation of the optimization problem. This has become a classical technique, instead of computing the discretization of the formal gradient, because identification problems are generally badly conditioned or ill-posed, see [17, 27]. All the computations are based upon the explicit (first and second order), semi-implicit and implicit Engquist-Osher (or generalized upwind scheme) for the numerical computation of the solution of the sedimentation model, see Bürger *et al* [9]. In each case, the adjoint scheme and the discrete gradient are provided.

The remainder of this paper is organized as follows. In section 2 we provide the formulation of the direct and inverse problems. In section 3 we analyze the question of the well posedness. In section 4 we present the formal calculus of the gradient. In section 5 we introduce the numerical schemes for the identification of the parameters and we present some numerical results.

2. Statement of the problem

2.1. The direct problem

Summarizing the results given in [2, 3, 4, 6] for the mathematical model of the sedimentation processes, we have the following IBVP

$$\frac{\partial \phi}{\partial t} + \frac{\partial}{\partial z} (q(t)\phi + f_{bk}(\phi)) = - \frac{\partial}{\partial z} \left(f_{bk}(\phi) \frac{\sigma'_e(\phi)}{\Delta \rho g \phi} \frac{\partial \phi}{\partial z} \right), \quad (z, t) \in Q_T, \quad (1)$$

$$\phi(z, 0) = \phi_0(z), \quad z \in [0, L], \quad (2)$$

$$\phi(L, t) = \phi_2(t), \quad t \in [0, T], \quad (3)$$

$$f_{bk}(\phi) \left(1 + \frac{\sigma'(\phi)}{\Delta \rho g \phi} \frac{\partial \phi}{\partial z} \right) \Big|_{z=0} = 0, \quad t \in [0, T], \quad (4)$$

where ϕ is the non-negative unknown function, $Q_T = [0, L] \times [0, T]$, $\Delta\rho$ and g are positive constants, q , f_{bk} , σ_e , ϕ_0 and ϕ_2 are given functions with the next supposed behavior

- q is a non-positive Lipschitz function, this is

$$q \in \text{Lip}([0, T]) \text{ and } q(t) \leq 0, \quad \forall t \in [0, T]. \quad (5)$$

- $f_{bk}(\phi)$ is a smooth function such that

$$f_{bk}(\phi) = \begin{cases} = 0 & \text{for } \phi \in \mathbb{R} -]0, \phi_{max}[, \\ < 0 & \text{for } \phi \in]0, \phi_{max}[. \end{cases} \quad 0 < \phi_{max} \leq 1 \quad (6)$$

- $\sigma_e(\phi)$ is a C^3 function, constant for $\phi < \phi_c$, with monotonic increasing for $\phi > \phi_c$ where $\phi_c \in]0, \phi_{max}[$ is a constant, and its first derivative, σ'_e , satisfies

$$\sigma'_e(\phi) = \begin{cases} = 0 & \text{for } \phi \leq \phi_c, \\ > 0 & \text{for } \phi > \phi_c. \end{cases} \quad (7)$$

- ϕ_0 and ϕ_2 are piecewise continuous functions such that

$$0 \leq \phi_0(z), \quad \phi_2(t) \leq \phi_{max}, \quad z \in [0, L], \quad t \in [0, T] \quad (8)$$

with ϕ_2 changing its monotonicity behavior a finite number of times.

In the setting of sedimentation theory $\phi(z, t)$ denotes the volumetric solid concentration at height z in time t , q the volume-averaged velocity of a suspension, f_{bk} the Kynch batch flux density function, ϕ_{max} is the maximum concentration value, σ_e the effective solid stress, L the height of thickener feeding level, T the total time for the process, $\Delta\rho$ the difference of solid and fluid mass densities, g the acceleration of gravity and ϕ_c is a critical concentration value or gel point, see [2, 13, 5, 6] for specific details.

The flux density function (or shortly flux) and the diffusion coefficient (or shortly diffusion) associated to equation (1) are defined by

$$f(\phi, t) = q(t)\phi + f_{bk}(\phi) \quad \text{and} \quad a(\phi) = -\frac{f_{bk}(\phi)\sigma'_e(\phi)}{\Delta\rho g\phi}, \quad (9)$$

respectively. Moreover we define the integrated diffusion coefficient A by

$$A(\phi) = \int_0^\phi a(s)ds. \quad (10)$$

Due to (6), (7) and (9), (1) is a second order parabolic partial differential equation for $\phi \in]\phi_c, \phi_{max}[$, a nonlinear hyperbolic conservation law for $\phi \in]0, \phi_c[$ and a linear advection equation for $\phi \in \mathbb{R} - [0, \phi_{max}]$. In brief, the IBVP is referenced as a quasilinear strongly degenerate parabolic equation. We remark that it is sufficient to consider the degeneracy on $[0, \phi_c] \cup \{\phi_{max}\}$ because for ϕ solution of the IBVP we have that $\phi \in [0, \phi_{max}]$ almost everywhere, see [4].

2.2. The inverse problem

Experimental results obtained in industrial and laboratory processes for flocculated sedimentation suggest to consider in the model (1)-(9), a dependence of finite number of parameters for the functions f_{bk} and σ_e , see [2, 13, 5] and [6]. The determination of this parameters implies to solve an “Identification Problem”, IP. We can formulate it, in general way, as follows

IP *Given an observation data $\phi^{obs}(z)$, at time T , and the functions $q(t)$, $\phi(z, 0)$, $\phi(L, t)$, explicitly, and $\phi(0, t)$, implicitly, satisfying (5), (2), (3) and (4) respectively, find the flux f and the diffusion a with f_{bk} and σ_e satisfying (6) and (7) such that the weak solution $\phi(z, T)$, in time T , of the IBVP (1)-(7) is as close as to $\phi^{obs}(z)$ in some suitable norm.*

We can write the IP, see [25, 26] and [27], as the optimization of a cost function J

$$\min_{f, a} J(\phi(\cdot, T)), \quad (11)$$

under the constraint for ϕ to satisfy weakly the IBVP (1)-(4), for some f and a . A natural example of cost function J is

$$J(\phi) = \frac{1}{2} \int_0^L |\phi(z, T) - \phi^{obs}(z)|^2 dz, \quad (12)$$

for other examples see [26].

We particularize the general situation by consider the parametric dependent analytic form of the flux and the diffusion. In this work, we seek f_{bk} by the usual formula of Richardson and Zaki [32], and σ_e by a constitutive law, [9], i.e.

$$f_{bk}(\phi) = u_\infty \phi \left(1 - \frac{\phi}{\phi_{max}}\right)^C, \quad (13)$$

$$\sigma_e(\phi) = \begin{cases} \text{Cte.} & \text{for } \phi \leq \phi_c, \\ \alpha ((\phi/\phi_c)^\beta - 1) & \text{for } \phi > \phi_c, \end{cases} \quad (14)$$

where u_∞ is the flow velocity of a singular particle in an unbounded medium and $C > 1, \alpha > 0, \beta > 1, \phi_c \in]0, \phi_{max}[$ are parameters (see [13, 23, 11] for another examples). Thus, in this particular case, if we denote by $\mathbf{e}$ the parameters to find, the problem (11) can be formulated in an equivalent way by

$$\min_{\mathbf{e}} J(\phi_{\mathbf{e}}(\cdot, T)),$$

where $\phi_{\mathbf{e}}$ is a weak solution of IBVP (1)-(4) with f_{bk} and σ_e given by (13)-(14), respectively.

The nonlinearity and degeneracy implies that solutions of the IBVP may become discontinuous in finite time. Thus, we need to interpret the IBVP in a weak way. In addition, it is well known that the IBVP is ill-posed in the classical weak sense because there is no uniqueness. In order to have a well-posed problem we must consider an additional condition or entropy condition, see [3, 4, 10].

3. Theoretical analysis of the IBVP and the IP

3.1. The direct problem

We adopt in this work the definition of weak entropy solution introduced by Bürger et al. in [10].

Definition 1 *Let $\phi \in L^\infty(Q_T) \cap BV(Q_T)$. Then ϕ is an entropy solution of the IBVP if the following four conditions are valid*

- (i) $\partial_z A(\phi) \in L^2(Q_T)$
- (ii) *For all $k \in \mathbb{R}$ and for all $\varphi \in C^\infty([0, 1] \times [0, T])$ such that $\varphi \geq 0$ and $\text{supp } \varphi \subset]0, 1[\times]0, T[$ the entropy inequality*

$$\begin{aligned} & \int \int_{Q_T} \left\{ |\phi - k| \partial_t \varphi + \text{sgn}(\phi - k) (f(\phi, t) - f(k, t) - \partial_z A(\phi)) \partial_z \varphi \right\} dz dt \\ & + \int_0^T \left\{ -\text{sgn}(\phi_2(t) - k) [f(\gamma_1 \phi, t) - f(k, t) - \gamma_1 \partial_z A(\phi)] \varphi(1, t) \right. \\ & \quad \left. + [\text{sgn}(\gamma_1 \phi - k) - \text{sgn}(\phi_2(t) - k)] [A(\gamma_1 \phi) - A(k)] \partial_z \varphi(1, t) \right\} dt \geq 0 \end{aligned}$$

is satisfied.

- (iii) *For almost all $t \in]0, T[$*

$$\gamma_0(f_{bk}(\phi) - \partial_z A(\phi)) = 0$$

- (iv) *For almost all $z \in [0, L]$*

$$\lim_{t \rightarrow 0} \phi(z, t) = \phi_0(z)$$

The notations γ_0 and γ_1 denote the traces in $BV(Q_T)$ at $x = 0$ and $x = 1$, respectively. For a precise definition see [4]. The item (i) is a technical regularity condition, (ii) is the entropy condition meanwhile that (iii) and (iv) are the weak formulation for the boundary condition (4) and the initial condition (2), respectively.

The definition 1 implies that the direct problem is well-posed, it was proved in [10], see also [4]. In that works, following the Kružkov [30] and Carrillo [16] ideas they establish several properties for the entropy solution of the direct problem. In particular they, provided the hypothesis (5)-(9), proved the following theorem

Theorem 1 *There is almost one entropy solution $\phi \in BV(Q_T)$ for the IBVP (1)-(4).*

3.2. Existence of solutions to the Inverse Problem

In this section we provide a sufficient condition for existence of at least one solution for our IP. The existence result is a consequence of the continuous dependence of the entropy solution with respect to the flux and diffusion. The non-uniqueness is a consequence of the degeneracy and the hyperbolic behavior.

The continuous dependence for a Cauchy Problem with spatially dependent flux was studied in [28, 21]. Their ideas, inspired by the works of Carrillo [16] and Cockburn and Gippenberg [19], can be extended to our IBVP with time dependent flux. First, we need the following lemma.

Lemma 1 *Assume that $A' > 0$, then for any $\varphi \geq 0$ in $C_0^\infty(Q_T)$ and $k \in \mathbb{R}$ we have*

$$\begin{aligned} \iint_{Q_T} \{|\phi - k| \partial_t \varphi + \operatorname{sgn}(\phi - k)(f(\phi, t) - f(k, t) - \partial_z A(\phi)) \partial_z \varphi\} dt dz \\ = \lim_{\epsilon \rightarrow 0} \iint_{Q_T} A'(\phi) (\partial_z \phi)^2 \operatorname{sgn}'_\epsilon(\phi - k) \varphi dt dz, \end{aligned} \quad (15)$$

where ϕ is an entropy solution of the IBVP and

$$\operatorname{sgn}_\epsilon(r) = \begin{cases} -1 & r < -\epsilon, \\ r/\epsilon & -\epsilon \leq r \leq \epsilon, \\ 1 & r > \epsilon. \end{cases}$$

Proof. Let $\psi_\epsilon(z) = -\operatorname{sgn}_\epsilon(A^{-1}(z) - k)$ and $A_{\psi_\epsilon}(\phi) = \int_k^\phi \psi_\epsilon(A(r)) dr$. Then, by a “weak chain rule” (see [16, 10]) we have

$$-\int_0^T \langle \partial_t \phi, -\operatorname{sgn}_\epsilon(\phi - k) \varphi \rangle dt = \iint_{Q_T} A_{\psi_\epsilon}(\phi) \partial_t \varphi dt dz, \quad (16)$$

where $\langle \cdot, \cdot \rangle$ denotes the usual pairing between $H^{-1}([0, L])$ and $H_0^1([0, L])$.

On the other hand, by definition 1, we follow that

$$\begin{aligned} -\int_0^T \langle \partial_t \phi, \operatorname{sgn}_\epsilon(\phi - k) \varphi \rangle dt + \\ \iint_{Q_T} [f(\phi, t) - f(k, t) - \partial_z A(\phi)] \partial_z (\operatorname{sgn}_\epsilon(\phi - k) \varphi) dt dz = 0. \end{aligned} \quad (17)$$

Combining (16) with (17) and passing to the limit when $\epsilon \rightarrow 0$, we obtain (15). $\square$

Theorem 2 *Let u and v be entropy solutions of the following IBVP's*

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial}{\partial z} (q_1(t)u + f_{bk_1}(u)) &= \frac{\partial^2 A(u)}{\partial z^2} \\ u(z, 0) &= u_0(z), \quad u(L, t) = u_L(t), \quad f_{bk_1}(\phi) - A(u) \frac{\partial u}{\partial z} \Big|_{z=0} = 0, \end{aligned}$$

and

$$\begin{aligned} \frac{\partial v}{\partial t} + \frac{\partial}{\partial z} (q_2(t)v + f_{bk_2}(v)) &= \frac{\partial^2 B(v)}{\partial z^2} \\ v(z, 0) &= v_0(z), \quad v(L, t) = v_L(t), \quad f_{bk_2}(v) - B(v) \frac{\partial v}{\partial z} \Big|_{z=0} = 0, \end{aligned}$$

respectively, where the assumptions (5)-(10) are fulfilled by each one of its coefficients, initial and boundary conditions. Then for almost all $t \in [0, T]$

$$\begin{aligned} \|u(\cdot, t) - v(\cdot, t)\|_{L^1([0, L])} &\leq \|u_0 - v_0\|_{L^1([0, L])} + tC\|q_1 - q_2\|_{Lip([0, T])} \\ &\quad + tC\|f_{bk_1} - f_{bk_2}\|_{Lip([0, u_{max}])} + \sqrt{t}C\|\sqrt{a} - \sqrt{b}\|_{L^\infty([\phi_c, \phi_{max}])} \end{aligned}$$

where $C > 0$ is a constant and $a(u) = A'(u)$, $b(v) = B'(v)$.

Proof. It is sufficient to prove this theorem when the equations are uniformly parabolic since the degenerate parabolic case is a consequence of the convergence of the vanishing viscosity method, see [4, 10]. The proof will be done by the generalized doubling of variables technique, see [16].

Let us introduce the test function $\varphi \in C_0^\infty(Q_T \times Q_T)$

$$\varphi(z, t, y, s) = \left\{ \int_{-\infty}^{t-\nu} \rho_\theta(s) ds - \int_{-\infty}^{t-\tau} \rho_\theta(s) ds \right\} \rho_\eta(z - y) \rho_\delta(t - s),$$

where $\nu, \tau \in]0, T[$ are Lebesgue points of $\|u(\cdot, t) - v(\cdot, t)\|_{L^1([0, L])}$, $\theta \in]0, \min\{\nu, T - \tau\}[$, $\eta, \delta > 0$ and $\rho_\epsilon(x) = (1/\epsilon)\rho(x/\epsilon)$ for $\epsilon > 0$ with $\rho \in C_0^\infty(\mathbb{R})$ such that ρ is a even function, $\rho(r) = 0$ for $|r| > 1$ and $\int \rho(r) dr = 1$.

We apply the lemma 1 twice. Firstly with φ as a test function in (z, t) , $\phi = u(z, t)$, $k = v(y, s)$ and integrate with respect to $(y, s) \in Q_T$. Then we apply the lemma with φ as a test function in (y, s) , $\phi = v(y, s)$ and $k = u(z, t)$ and integrate with respect to $(z, t) \in Q_T$. By summing up the results we obtain

$$\begin{aligned} & - \iiint\limits_{Q_T \times Q_T} \left\{ |u - v|(\partial_t \varphi + \partial_s \varphi) \right. \\ & \quad + \operatorname{sgn}(u - v)[(f(u, t) - f(v, t))\partial_z \varphi - (g(v, s) - g(u, s))\partial_y \varphi] \\ & \quad \left. - [\operatorname{sgn}(u - v)\partial_z A(u)\partial_z \varphi + \operatorname{sgn}(v - u)\partial_y B(v)\partial_y \varphi] \right\} dz dt dy ds \\ & = - \lim_{\epsilon \rightarrow 0} \iiint\limits_{Q_T \times Q_T} \left\{ A'(u)(\partial_z u)^2 + B'(v)(\partial_y v)^2 \right\} \operatorname{sgn}'_\epsilon(v - u) \varphi dz dt dy ds \\ & \leq - \lim_{\epsilon \rightarrow 0} \iiint\limits_{Q_T \times Q_T} 2\sqrt{A'(u)}\sqrt{B'(v)}\partial_z u \partial_y v \operatorname{sgn}'_\epsilon(v - u) \varphi dz dt dy ds = S_1 \end{aligned}$$

Now, by triangle inequality we get

$$I_1 + I_2 + I_3 \leq - \iiint\limits_{Q_T \times Q_T} |u - v|(\partial_t \varphi + \partial_s \varphi) dz dt dy ds \leq S_1 + S_2 + S_3$$

where

$$\begin{aligned} I_1 &= - \iiint\limits_{Q_T \times Q_T} |u(y, t) - v(y, t)|(\partial_t \varphi + \partial_s \varphi) dz dt dy ds \\ I_2 &= - \iiint\limits_{Q_T \times Q_T} |v(y, t) - v(y, s)|(\partial_t \varphi + \partial_s \varphi) dz dt dy ds \\ I_3 &= - \iiint\limits_{Q_T \times Q_T} |u(z, t) - u(y, t)|(\partial_t \varphi + \partial_s \varphi) dz dt dy ds \\ S_2 &= \iiint\limits_{Q_T \times Q_T} \operatorname{sgn}(u - v)[(f(u, t) - f(v, t))\partial_z \varphi - (g(v, s) - g(u, s))\partial_y \varphi] dz dt dy ds \\ S_3 &= - \iiint\limits_{Q_T \times Q_T} [\operatorname{sgn}(u - v)\partial_z A(u)\partial_z \varphi + \operatorname{sgn}(v - u)\partial_y B(v)\partial_y \varphi] dz dt dy ds. \end{aligned}$$

Taking into account that $\partial_t \varphi + \partial_s \varphi = [\rho_\theta(t - \nu) - \rho_\theta(t - \tau)]\rho_\eta(z - y)\rho_\delta(t - s)$ and

$\partial_z \varphi + \partial_y \varphi = 0$, we obtain that

$$\lim_{\theta \rightarrow 0} I_1 = \|u(\cdot, \tau) - v(\cdot, \tau)\|_{L^1([0, L])} - \|u(\cdot, \nu) - v(\cdot, \nu)\|_{L^1([0, L])},$$

$$\lim_{\theta \rightarrow 0} I_2 = 0,$$

$$\lim_{\theta \rightarrow 0} I_3 \geq -2\eta \sup_{t \in (\nu, \tau)} |u(\cdot, t)|_{BV([0, L])},$$

$$\lim_{\theta, \eta, \delta \rightarrow 0} S_2 \leq (\|q_1 - q_2\|_{Lip} + \|f_{bk1} - f_{bk2}\|_{Lip}) \sup_{t \in (\nu, \tau)} |u(\cdot, t)|_{BV([0, L])}$$

and

$$\lim_{\theta \rightarrow 0} S_1 + S_3 \leq (\tau - \nu) \sup_{t \in (\nu, \tau)} |u(\cdot, t)|_{BV([0, L])} \frac{2}{\eta} \|\sqrt{B'} - \sqrt{A'}\|_{L^\infty([\phi_c, \phi_{max}])}^2.$$

This estimates yields the result. $\square$

Corollary 1 *Let $\mathcal{M} = Lip([0, T]) \times Lip([0, u_{max}]) \times L^\infty([\phi_c, \phi_{max}])$. The mapping $\tilde{J} : (q, f_{bk}, a) \mapsto J(\phi_{q, f_{bk}, a})$ defined from $\mathcal{M}$ to $\mathbb{R}_+$ is continuous. Then, if $(q, f_{bk}, a) \in \mathcal{F}$, where $\mathcal{F}$ is a compact subset of $\mathcal{M}$, there exist at least one solution for the IP.*

Because the square root is not a Lipschitz function it is interesting to note that if we consider the mapping $\hat{J} : (q, f_{bk}, \sqrt{a}) \mapsto J(\phi_{q, f_{bk}, a})$ from $\mathcal{M}$ to $\mathbb{R}_+$ is Lipschitz continuous, obtaining a strong result of continuity of the cost function respect to “ $\sqrt{a}$ ” than “ a ”.

It is known that IP is ill-posed in uniqueness if we consider for instance the identification of the parameters of the flux an only shock observation, when $A = 0$ (see [17] for more details). We hope to solve in practice this problem of uniqueness following the same idea of [17]: considering several experimental observations with rarefaction waves and limited number of real parameters to identify.

4. Lagrangian formulation and formal calculus

We define a Lagrangian for the problem (11) by setting

$$\mathcal{L}(\phi, \psi; f, a) = J(\phi) - E(\phi, \psi; f, a),$$

where ψ is a smooth test function, ϕ is the state variable and

$$\begin{aligned} E(\phi, \psi; f, a) = & - \int_{Q_T} \left(\phi \frac{\partial \psi}{\partial t} + f(\phi) \frac{\partial \psi}{\partial z} + A(\phi) \frac{\partial^2 \psi}{\partial z^2} \right) \\ & + \int_{z=L} \left(\psi f(\phi_2) - \psi \frac{\partial A}{\partial z}(\phi_2) + A(\phi_2) \frac{\partial \psi}{\partial z} \right) \\ & - \int_{z=0} \left(\psi q(t) \phi + A(\phi) \frac{\partial \psi}{\partial z} \right) + \int_{t=T} \psi \phi - \int_{t=0} \psi \phi_0. \end{aligned}$$

When we formally take the derivative of $\mathcal{L}$ in the direction $\delta \phi$ we obtain

$$\begin{aligned} \left\langle \frac{\partial \mathcal{L}}{\partial \phi}, \delta \phi \right\rangle = & \int_{Q_T} \delta \phi \left(\frac{\partial \psi}{\partial t} + f'(\phi) \frac{\partial \psi}{\partial z} + a(\phi) \frac{\partial^2 \psi}{\partial z^2} \right) \\ & + \int_{z=0} \delta \phi \left(\psi q(t) + a(\phi) \frac{\partial \psi}{\partial z} \right) + \int_{t=T} \delta \phi (\phi - \phi^{obs} - \psi), \end{aligned}$$

where we used the fact that ϕ_0, ϕ_2 and ϕ^{obs} are fixed. Now, we are interested in canceling $\partial\mathcal{L}/\partial\phi$, then ψ should be solution of

$$\frac{\partial\psi}{\partial t} + (q(t) + f'_{bk}(\phi)) \frac{\partial\psi}{\partial z} = -a(\phi) \frac{\partial^2\psi}{\partial z^2}, \quad (z, t) \in Q_T, \quad (18)$$

$$\psi(z, T) = \phi(z, T) - \phi^{obs}(z), \quad z \in [0, L], \quad (19)$$

$$\psi q(t) - a(\phi) \frac{\partial\psi}{\partial z} \Big|_{z=0} = 0, \quad t \in [0, T]. \quad (20)$$

This problem is a backward boundary value problem for a linear parabolic degenerate equation with discontinuous coefficients. The end condition (19) depends on the cost function, in this case it corresponds to J . In more general case we have the relation $\int_{t=T} \delta\phi\psi = \langle \partial J / \partial\phi, \delta\phi \rangle$, for all $\delta\phi$ smooth. No boundary condition is needed at $z = L$, for the case of batch sedimentation $q = \phi_2 = 0$, since the characteristics are entering the domain for the direct problem.

Let $\phi_{f,a}$ be solution of the IBVP. If $\phi_{f,a}$ is smooth, then we have $E(\phi_{f,a}, \psi; f, a) = 0$ for each ψ smooth. In this way, $\mathcal{L}(\phi_{f,a}, \psi; f, a) = J(\phi_{f,a}) = \tilde{J}(f, a)$. Thus

$$\begin{aligned} \nabla \tilde{J}(f, a) &= \left(\left\langle \frac{\partial\mathcal{L}}{\partial\phi_{f,a}}, \phi_{f,a} \right\rangle + \frac{\partial\mathcal{L}}{\partial f}, \left\langle \frac{\partial\mathcal{L}}{\partial\phi_{f,a}}, \phi_{f,a} \right\rangle + \frac{\partial\mathcal{L}}{\partial a} \right) \\ &= \left\langle \frac{\partial\mathcal{L}}{\partial\phi_{f,a}}, \phi_{f,a} \right\rangle (1, 1) + \left(\frac{\partial\mathcal{L}}{\partial f}, \frac{\partial\mathcal{L}}{\partial a} \right). \end{aligned}$$

In this equality, for ψ solution of (18)-(20) the first term in the right-hand side is zero, so that we obtain

$$\begin{aligned} \langle \nabla \tilde{J}, (\delta f, \delta a) \rangle &= \langle \nabla \mathcal{L}, (\delta f, \delta a) \rangle = - \langle \nabla E, (\delta f, \delta a) \rangle \\ &= \int_{Q_T} \left(\delta f(\phi_{f,a}) \frac{\partial\psi}{\partial z}, a(\phi_{f,a}) \frac{\partial^2\psi}{\partial z^2} \right) \\ &\quad + \int_{z=L} \left(\delta f(\phi_2) \psi, a(\phi_2) \frac{\partial\psi}{\partial z} \right) - \int_{z=0} \left(0, a(\phi_1) \frac{\partial\psi}{\partial z} \right) \end{aligned} \quad (21)$$

5. Numerical schemes and discrete study

We divide the interval $(0, L)$ into M subintervals of length $\Delta z = L/M$ and the interval $(0, T)$ into N subintervals of length $\Delta t = T/N$. For $n = 0, \dots, N$ and $j = 0, \dots, M$ we will denote by ϕ_j^n the value of numerical solution at $(j\Delta z, n\Delta t)$ and by $\phi_j^0, \phi_2^n, \phi_j^{obs}$ the corresponding approximation of $\phi_0, \phi_2, \phi^{obs}$, respectively.

At discrete level the minimization corresponds to the following problem

$$\min_{\mathbf{e}} J_{\Delta}(\phi_j^n(\mathbf{e}))$$

where J_{Δ} is the discrete form of cost function. In the case of (12) is given by

$$J_{\Delta}(\phi_j^n(\mathbf{e})) = \frac{1}{2} \sum_{j=0}^M \Delta z |\phi_j^N - \phi_j^{obs}|^2.$$

In this way we define the discrete Lagrangian associated by

$$\mathcal{L}(\phi_j^n, \psi_j^n; \mathbf{e}) = \frac{1}{\Delta z} J_\Delta(\phi_j^n) - E_\Delta(\phi_j^n, \psi_j^n; \mathbf{e}),$$

where $E_\Delta(\phi_j^n, \psi_j^n; \mathbf{e})$ denotes a discrete weak formulation, it will be obtained by summation by parts of the numerical scheme by means we calculated the numerical solution of IBVP and ψ_j^n will be chosen as solution of a discrete adjoint problem.

5.1. First and second order explicit EO scheme

In [9] the IBVP was well discretized by means of the first and second order Engquist-Osher scheme. The first order EO scheme is

$$\begin{aligned} \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + q(n\Delta t) \frac{\phi_{j+1}^n - \phi_j^n}{\Delta z} + \frac{f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n) - f_{bk}^{EO}(\phi_{j-1}^n, \phi_j^n)}{\Delta z} \\ = \frac{A(\phi_{j+1}^n) - 2A(\phi_j^n) + A(\phi_{j-1}^n)}{(\Delta z)^2}, \quad j = 1, \dots, M-1, \end{aligned} \quad (22)$$

where

$$\begin{aligned} f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n) &= f_{bk}^+(\phi_j^n) + f_{bk}^-(\phi_{j+1}^n) \\ &= \left[f_{bk}(0) + \int_0^{\phi_j^n} \max(f'_{bk}(s), 0) ds \right] + \left[\int_0^{\phi_{j+1}^n} \min(f'_{bk}(s), 0) ds \right]. \end{aligned}$$

The second order EO scheme is defined by

$$\begin{aligned} \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + q(n\Delta t) \frac{\phi_{j+1}^L - \phi_j^R}{\Delta z} + \frac{f_{bk}^{EO}(\phi_j^R, \phi_{j+1}^L) - f_{bk}^{EO}(\phi_{j-1}^R, \phi_j^L)}{\Delta z} \\ = \frac{A(\phi_{j+1}^n) - 2A(\phi_j^n) + A(\phi_{j-1}^n)}{(\Delta z)^2}, \quad j = 1, \dots, M-1, \end{aligned} \quad (23)$$

where

$$\phi_j^L = \phi_j^n - \frac{\Delta z}{2} s_j^n \quad \text{and} \quad \phi_j^R = \phi_j^n + \frac{\Delta z}{2} s_j^n.$$

Here $s_1^n = s_{M-1}^n = 0$ and for $j = 2, \dots, M-2$ we have

$$s_j^n = \text{mm}\left(\theta \frac{\phi_j^n - \phi_{j-1}^n}{\Delta z}, \frac{\phi_{j+1}^n - \phi_{j-1}^n}{2\Delta z}, \theta \frac{\phi_{j+1}^n - \phi_j^n}{\Delta z}\right), \quad \theta \in [0, 2],$$

with mm the minmod function

$$\text{mm}(a, b, c) = \begin{cases} \min(a, b, c), & \text{if } a, b, c > 0, \\ \max(a, b, c), & \text{if } a, b, c < 0, \\ 0, & \text{otherwise.} \end{cases}$$

In both cases, first and second order, ϕ_M^n is obtained by $\phi_M^n = \phi_2(n\Delta t)$ and ϕ_0^n by the following formula

$$\frac{\phi_0^{n+1} - \phi_0^n}{\Delta t} + q(n\Delta t) \frac{\phi_1^n - \phi_0^n}{\Delta z} + \frac{f_{bk}^{EO}(\phi_0^n, \phi_1^n)}{\Delta z} = \frac{A(\phi_1^n) - A(\phi_0^n)}{(\Delta z)^2}.$$

Denoting by $\lambda = \Delta t / \Delta z$ and $\nu = \Delta t / (\Delta z)^2$ the discrete weak formulation for (22) is given by

$$\begin{aligned}
 E_\Delta(\phi_j^n, \psi_j^n, \mathbf{e}) &= \sum_{n,j} \left\{ \phi_j^{n+1} - \phi_j^n + \lambda q(n\Delta t)(\phi_{j+1}^n - \phi_j^n) + \lambda \left(f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n, \mathbf{e}) \right. \right. \\
 &\quad \left. \left. - f_{bk}^{EO}(\phi_{j-1}^n, \phi_j^n, \mathbf{e}) \right) - \nu (A(\phi_{j+1}^n, \mathbf{e}) - 2A(\phi_j^n, \mathbf{e}) + A(\phi_{j-1}^n, \mathbf{e})) \right\} \psi_j^{n+1} \\
 &= \sum_{n,j} \left\{ \phi_j^n \left[\psi_j^n - \psi_j^{n+1} + \lambda q(n\Delta t)(\psi_{j-1}^{n+1} - \psi_j^{n+1}) \right] \right. \\
 &\quad \left. + \lambda f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n)(\psi_j^{n+1} - \psi_{j+1}^{n+1}) - \nu A(\phi_j^n)(\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1}) \right\} \\
 &\quad + \sum_{j=0}^{M-1} \left\{ \phi_j^N \psi_j^N - \phi_j^0 \psi_j^0 \right\} \\
 &\quad + \sum_{n=0}^{N-1} \left\{ \lambda \left[q(n\Delta t) \phi_M^n \psi_{M-1}^{n+1} - q(n\Delta t) \phi_0^n \psi_{-1}^{n+1} + f_{bk}^{EO}(\phi_{M-1}^n, \phi_M^n) \psi_M^{n+1} \right] \right. \\
 &\quad \left. - \nu \left[A(\phi_M^n) \psi_{M-1}^{n+1} - A(\phi_{M-1}^n) \psi_M^{n+1} - A(\phi_0^n)(\psi_{-1}^{n+1} - \psi_0^{n+1}) \right] \right\},
 \end{aligned}$$

where we approximated the boundary condition at $z = 0$ by

$$f_{bk}(\phi) \left(1 + \frac{\sigma'(\phi)}{\Delta \rho g \phi} \frac{\partial \phi}{\partial z} \right) \Big|_{z=0} \approx f_{bk}^{EO}(\phi_{-1}^n, \phi_0^n) - \frac{A(\phi_0^n) - A(\phi_{-1}^n)}{\Delta z} = 0.$$

Taking the derivative of E_Δ with respect to ϕ_j^n we obtain

$$\begin{aligned}
 \frac{\partial E_\Delta}{\partial \phi_j^n} &= \psi_j^n - \psi_j^{n+1} + \lambda q(n\Delta t)(\psi_{j-1}^{n+1} - \psi_j^{n+1}) \\
 &\quad + \lambda \left\{ \min(f'_{bk}(\phi_j^n), 0) \psi_{j-1}^{n+1} + |f'_{bk}(\phi_j^n)| \psi_j^{n+1} - \max(f'_{bk}(\phi_j^n), 0) \psi_{j+1}^{n+1} \right\} \\
 &\quad - \nu a(\phi_j^n)(\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1}) + \psi_j^N \delta_{n,N} \\
 &\quad - \left[\lambda q(n\Delta t) \psi_{-1}^{n+1} - \nu a(\phi_0^n)(\psi_{-1}^{n+1} - \psi_0^{n+1}) \right] \delta_{j,0} \\
 &\quad + \left[\lambda \max(f'_{bk}(\phi_{M-1}^n), 0) + \nu a(\phi_{M-1}^n) \right] \psi_M^{n+1} \delta_{j,M-1}.
 \end{aligned}$$

If we consider that $(\partial \mathcal{L}_\Delta) / (\partial \phi_j^n)$ should be zero we have the follow adjoint scheme to (22)

$$\begin{aligned}
 \frac{\psi_j^n - \psi_j^{n+1}}{\Delta t} + q(n\Delta t) \frac{\psi_{j-1}^{n+1} - \psi_j^{n+1}}{\Delta z} + \frac{FA_1}{\Delta z} &= \frac{a(\phi_j^n)(\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1})}{(\Delta z)^2}, \\
 \psi_j^N &= \frac{\partial J_\Delta}{\partial \phi_j^N},
 \end{aligned}$$

$$q(n\Delta t) \psi_{-1}^{n+1} - a(\phi_0^n) \frac{\psi_{-1}^{n+1} - \psi_0^{n+1}}{\Delta z} = 0,$$

$$\left[\lambda \max(f'_{bk}(\phi_{M-1}^n), 0) + \nu a(\phi_{M-1}^n) \right] \psi_M^{n+1} = 0,$$

where

$$FA_1 = \min(f'_{bk}(\phi_j^n), 0) \psi_{j-1}^{n+1} + |f'_{bk}(\phi_j^n)| \psi_j^{n+1} - \max(f'_{bk}(\phi_j^n), 0) \psi_{j+1}^{n+1}. \quad (24)$$

Thus, we obtain the discrete gradient

$$\begin{aligned}
 \nabla \hat{J}_\Delta(\mathbf{e}) &= -\nabla_{\mathbf{e}} E_\Delta \Delta z \\
 &= -\sum_{n,j} \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n)(\psi_j^{n+1} - \psi_{j+1}^{n+1}) \\
 &\quad - \lambda \nabla_{\mathbf{e}} A(\phi_j^n)(\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1}) - \sum_{n=0}^{N-1} \left\{ \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_{M-1}^n, \phi_M^n) \psi_M^{n+1} \right. \\
 &\quad \left. - \lambda \left[\nabla_{\mathbf{e}} A(\phi_M^n) \psi_{M-1}^{n+1} - \nabla_{\mathbf{e}} A(\phi_{M-1}^n) \psi_M^{n+1} - \nabla_{\mathbf{e}} A(\phi_0^n)(\psi_{-1}^{n+1} - \psi_0^{n+1}) \right] \right\}.
 \end{aligned}$$

If we use (23) instead of (22) we get the adjoint scheme

$$\begin{aligned}
 \frac{\psi_j^n - \psi_j^{n+1}}{\Delta t} + \frac{q(n\Delta t)Fq}{\Delta z} + \frac{FA_2}{\Delta z} &= \frac{a(\phi_j^n)(\psi_{j-1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1})}{\Delta z^2} \\
 \psi_j^N &= \frac{\partial J_\Delta}{\partial \phi_j^N} \\
 q(n\Delta t) \frac{\partial \phi_0^L}{\partial \phi_0^n} \psi_{-1}^{n+1} - a(\phi_0^n) \frac{\psi_{-1}^{n+1} - \psi_0^{n+1}}{\Delta z} &= 0 \\
 \lambda \max(f'_{bk}(\phi_{M-1}^R), 0) \frac{\partial \phi_{M-1}^R}{\partial \phi_0^n} \psi_{M-1}^{n+1} + \nu a(\phi_{M-1}^n) \psi_M^{n+1} &= 0,
 \end{aligned}$$

where

$$\begin{aligned}
 FA_2 &= \min(f'_{bk}(\phi_{j-1}^L), 0) \frac{\partial \phi_{j-1}^L}{\partial \phi_j^n} (\psi_{j-2}^{n+1} - \psi_{j-1}^{n+1}) \\
 &\quad + \left\{ \max(f'_{bk}(\phi_{j-1}^R), 0) \frac{\partial \phi_{j-1}^R}{\partial \phi_j^n} + \min(f'_{bk}(\phi_j^L), 0) \frac{\partial \phi_j^L}{\partial \phi_j^n} \right\} (\psi_{j-1}^{n+1} - \psi_j^{n+1}) \\
 &\quad + \left\{ \max(f'_{bk}(\phi_j^R), 0) \frac{\partial \phi_j^R}{\partial \phi_j^n} + \min(f'_{bk}(\phi_{j+1}^L), 0) \frac{\partial \phi_{j+1}^L}{\partial \phi_j^n} \right\} (\psi_j^{n+1} - \psi_{j+1}^{n+1}) \\
 &\quad + \max(f'_{bk}(\phi_{j+1}^R), 0) \frac{\partial \phi_{j+1}^R}{\partial \phi_j^n} (\psi_{j+1}^{n+1} - \psi_{j+2}^{n+1}), \\
 Fq &= \left(\frac{\partial \phi_{j-1}^L}{\partial \phi_j^n} - \frac{\partial \phi_{j-1}^R}{\partial \phi_j^n} \right) (\psi_{j-2}^{n+1} - \psi_{j-1}^{n+1}) + \left(\frac{\partial \phi_j^L}{\partial \phi_j^n} - \frac{\partial \phi_j^R}{\partial \phi_j^n} \right) (\psi_{j-1}^{n+1} - \psi_j^{n+1}) \\
 &\quad + \left(\frac{\partial \phi_{j+1}^L}{\partial \phi_j^n} - \frac{\partial \phi_{j+1}^R}{\partial \phi_j^n} \right) (\psi_j^{n+1} - \psi_{j+1}^{n+1}).
 \end{aligned}$$

In this case the gradient is given by

$$\begin{aligned}
 \nabla \hat{J}_\Delta(\mathbf{e}) &= -\sum_{n,j} \left\{ \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_j^R, \phi_{j+1}^L)(\psi_j^{n+1} - \psi_{j+1}^{n+1}) \right. \\
 &\quad \left. - \lambda \nabla_{\mathbf{e}} A(\phi_j^n)(\psi_{j+1}^{n+1} - 2\psi_j^{n+1} + \psi_{j+1}^{n+1}) \right\} - \sum_{n=0}^{N-1} \left\{ \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_{M-1}^R, \phi_M^L) \psi_{M-1}^{n+1} \right. \\
 &\quad \left. - \lambda \left[\nabla_{\mathbf{e}} A(\phi_M^n) \psi_{M-1}^{n+1} - \nabla_{\mathbf{e}} A(\phi_{M-1}^n) \psi_M^{n+1} - \nabla_{\mathbf{e}} A(\phi_0^n)(\psi_0^{n+1} - \psi_{-1}^{n+1}) \right] \right\}.
 \end{aligned}$$

If the following CFL condition

$$\lambda \max_{t \in [0, T]} |q(t)| + \lambda \max_{\phi \in [0, \phi_{max}]} |f'_{bk}(\phi)| + 2\nu \max_{\phi \in [\phi_c, \phi_{max}]} |a(\phi)| \leq 1,$$

is satisfied, then the first and second order schemes are stable. For another CFL condition see [9].

5.2. Implicit and semi-implicit schemes

The direct problem can be discretized by semi-implicitly scheme

$$\begin{aligned} \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + q(n\Delta t) \frac{\phi_{j+1}^n - \phi_j^n}{\Delta z} + \frac{f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n) - f_{bk}^{EO}(\phi_{j-1}^n, \phi_j^n)}{\Delta z} \\ = \frac{A(\phi_{j+1}^{n+1}) - 2A(\phi_j^{n+1}) + A(\phi_{j-1}^{n+1})}{(\Delta z)^2}, \quad j = 1, \dots, M-1 \end{aligned} \quad (25)$$

or by the implicit scheme

$$\begin{aligned} \frac{\phi_j^{n+1} - \phi_j^n}{\Delta t} + q((n+1)\Delta t) \frac{\phi_{j+1}^{n+1} - \phi_j^{n+1}}{\Delta z} + \frac{f_{bk}^{EO}(\phi_j^{n+1}, \phi_{j+1}^{n+1}) - f_{bk}^{EO}(\phi_{j-1}^{n+1}, \phi_j^{n+1})}{\Delta z} \\ = \frac{A(\phi_{j+1}^{n+1}) - 2A(\phi_j^{n+1}) + A(\phi_{j-1}^{n+1})}{(\Delta z)^2}, \quad j = 1, \dots, M-1 \end{aligned} \quad (26)$$

In both cases the boundary condition at $z = L$ is discretized by $\phi_M^{n+1} = \phi_2((n+1)\Delta t)$ while the boundary condition at $z = 0$ is calculated by the interior scheme with the following approximation

$$\left(f_{bk}(u) - \frac{\partial A(u)}{\partial z} \right) \Big|_{z=0} \approx f_{bk}^{EO}(\phi_{-1}^{n+1}, \phi_0^{n+1}) - \frac{A(\phi_0^{n+1}) - A(\phi_{-1}^{n+1})}{\Delta z} = 0.$$

Applying the same strategy as the previous section for to calculate the gradient, we have the adjoint state

$$\begin{aligned} \frac{\psi_j^n - \psi_j^{n+1}}{\Delta t} + q(n\Delta t) \frac{\psi_{j-1}^n - \psi_j^n}{\Delta t} + \frac{FA_1}{\Delta z} &= a(\phi_j^n) \frac{\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n}{(\Delta z)^2} \\ (1 + 2\nu a(\phi_j^N)) \psi_j^N &= \frac{\partial J_\Delta}{\partial \phi_j^N} \\ q(n\Delta t) \psi_{-1}^{n+1} - a(\phi_0^n) \frac{\psi_{-1}^n - \psi_0^n}{\Delta z} &= 0 \\ \lambda \max\{f'_{bk}(\phi_{M-1}^n), 0\} \psi_M^{n+1} + \nu a(\phi_{M-1}^n) \psi_M^n &= 0 \end{aligned}$$

for (25) and

$$\begin{aligned} \frac{\psi_j^n - \psi_j^{n+1}}{\Delta t} + q(n\Delta t) \frac{\psi_{j-1}^n - \psi_j^n}{\Delta t} + \frac{FAI}{\Delta z} &= a(\phi_j^n) \frac{\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n}{(\Delta z)^2} \\ \psi_j^N &= \frac{\partial J_\Delta}{\partial \phi_j^{N-1}} \\ q(n\Delta t) \psi_{-1}^n - a(\phi_0^n) \frac{\psi_{-1}^n - \psi_0^n}{\Delta z} &= 0 \\ \{\lambda \max\{f'_{bk}(\phi_{M-1}^n), 0\} + \nu a(\phi_{M-1}^n)\} \psi_M^n &= 0 \end{aligned}$$

for (26), where FA_1 is given by (24) and

$$FAI = \min(f'_{bk}(\phi_j^n), 0)\psi_{j-1}^n + |f'_{bk}(\phi_j^n)|\psi_j^n - \max(f'_{bk}(\phi_j^n), 0)\psi_{j+1}^n.$$

The gradient in the case of semi-implicit is given by

$$\begin{aligned} \nabla \hat{J}_\Delta(\mathbf{e}) &= -\nabla_{\mathbf{e}} E_\Delta \Delta z \\ &= -\sum_{n,j} \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n)(\psi_j^{n+1} - \psi_{j+1}^{n+1}) - \lambda \nabla_{\mathbf{e}} A(\phi_j^n)(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n) \\ &\quad - \sum_{n=0}^{N-1} \left\{ \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_{M-1}^n, \phi_M^n) \psi_M^{n+1} \right. \\ &\quad \left. - \lambda \left[\nabla_{\mathbf{e}} A(\phi_M^n) \psi_{M-1}^n - \nabla_{\mathbf{e}} A(\phi_{M-1}^n) \psi_M^n - \nabla_{\mathbf{e}} A(\phi_0^n)(\psi_{-1}^n - \psi_0^n) \right] \right\}, \end{aligned}$$

whereas in the implicit ones is

$$\begin{aligned} \nabla \hat{J}_\Delta(\mathbf{e}) &= -\nabla_{\mathbf{e}} E_\Delta \Delta z \\ &= -\sum_{n,j} \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_j^n, \phi_{j+1}^n)(\psi_j^n - \psi_{j+1}^n) - \lambda \nabla_{\mathbf{e}} A(\phi_j^n)(\psi_{j-1}^n - 2\psi_j^n + \psi_{j+1}^n) \\ &\quad - \sum_{n=0}^{N-1} \left\{ \Delta t \nabla_{\mathbf{e}} f_{bk}^{EO}(\phi_{M-1}^n, \phi_M^n) \psi_M^n \right. \\ &\quad \left. - \lambda \left[\nabla_{\mathbf{e}} A(\phi_M^n) \psi_{M-1}^n - \nabla_{\mathbf{e}} A(\phi_{M-1}^n) \psi_M^n - \nabla_{\mathbf{e}} A(\phi_0^n)(\psi_{-1}^n - \psi_0^n) \right] \right\}, \end{aligned}$$

The CFL condition for the semi-implicit scheme is given by

$$\lambda \left(\max_{t \in [0, T]} |q(t)| + \max_{\phi \in [0, \phi_{max}]} |f'_{bk}(\phi)| \right) \leq 1.$$

Meanwhile, the implicit scheme is “CFL free”, see [9].

The unconditional stability of the implicit scheme is useful for the reason that it allows the choose of a coarse grid without losing the convergence to the entropy solution. Therefore, the implicit scheme is a good alternative to simulate numerically the physical problem with a few (reasonable) steps of time to overcome the cumbersome number of steps of time in the explicit and semi-implicit schemes.

5.3. Numerical tests

5.3.1. Identification from analytic data. Let us consider f_{bk} and σ_e like (13) and (14) with the value of the parameters given by the Table 1. Then the function $\phi_1(z, t) = z^2 + (t/30000)^2$ is solution of the following IBVP

$$\begin{aligned} \frac{\partial \phi}{\partial t} + \frac{\partial}{\partial z}(f_{bk}(\phi)) &= \frac{\partial^2 A(\phi)}{\partial^2 z} + g_1(z, t) & (z, t) \in Q_T \\ \phi(z, 0) &= 0.05 & z \in [0, 1] \\ \phi(1, t) &= \phi_1(1, t) & t \in [0, T] \\ f_{bk}(\phi) - \frac{\partial A(\phi)}{\partial z} \Big|_{z=0} &= b_1(t) & t \in [0, T] \end{aligned}$$

Table 1. Parameters for direct simulation [20].

C	α	β	ϕ_c
15.6	5.0	6.0	0.1

Table 2. Identified parameters with the second order EO explicit scheme.

ϕ^{obs}	J	C	α	β	ϕ_c
ϕ_1	8.245e-6	16.09203	5.50039	6.50071	0.10053
$1.01\phi_1$	4.553e-6	16.08856	5.50039	6.50069	0.10280

where the source term g_1 is defined by

$$g_1(z, t) = \frac{\partial \phi_1}{\partial t} + \frac{\partial}{\partial z}(f_{bk}(\phi_1)) - \frac{\partial^2 A(\phi_1)}{\partial^2 z}$$

and the boundary condition b_1 is given by

$$b_1(t) = f_{bk}(\phi_1(0, t)) - \frac{\partial A(\phi_1(0, t))}{\partial z}.$$

The identified parameters given at Table 2 are obtained with the second order explicit EO scheme ($\theta = 1.0$) and the observed data $\phi_1(z, 12000)$ and the noised form $1.01\phi_1(z, 12000)$. The grid parameters are $M = 200$ and $CFL = 0.98$. The initial guess corresponds to $C = 16.1$, $\alpha = 5.5$, $\beta = 6.5$ and $\phi_c = 0.2$. See Figures 1 and 2.

5.3.2. Identification from simulated data. We present here a validation of the above Lagrangian method as well as a comparison between the four numerical schemes developed. Since we did not have access to real experimental data, the idea consists in using as an observation the result of a direct simulation. We used the standard simulation given by Concha [20], which is very close to experimental data results. All tests are developed for batch sedimentation velocity $q = 0$, with an initially homogeneous suspension of concentration, namely $\phi_0 = 0.05$. The column is assumed to be closed, that is $\phi_2 = 0$. The physical constants considered are $u_\infty = -1.7200 \times 10^{-4}$, $\phi_{max} = 0.7$, $\Delta\rho = 1500$ and $g = 9.81$. We summarize in Table 1 the parameters used for this simulation, which we want to recover in the inverse problem.

Three tests are performed, the first one is concerned only with the flux identification, that is parameter C . The second test identifies the diffusion together with the flux, that is parameters C , α and β , the critical concentration ϕ_c being fixed. Finally, we perform the complete identification on the four parameters. We start with the following values: $\mathbf{e} = (16.5, 5.0, 6.0, 0.1)$, $\mathbf{e} = (16.5, 5.5, 6.5, 0.1)$ and $\mathbf{e} = (16.5, 5.5, 6.5, 0.2)$ for the test 1, test 2 and test 3 respectively. Other several initial points were considered with very similar and close results. The identification problem is solved at $T = 12144$ seconds in the three cases, and a simulation at $T = 30000$ seconds with the identified parameters is proposed.

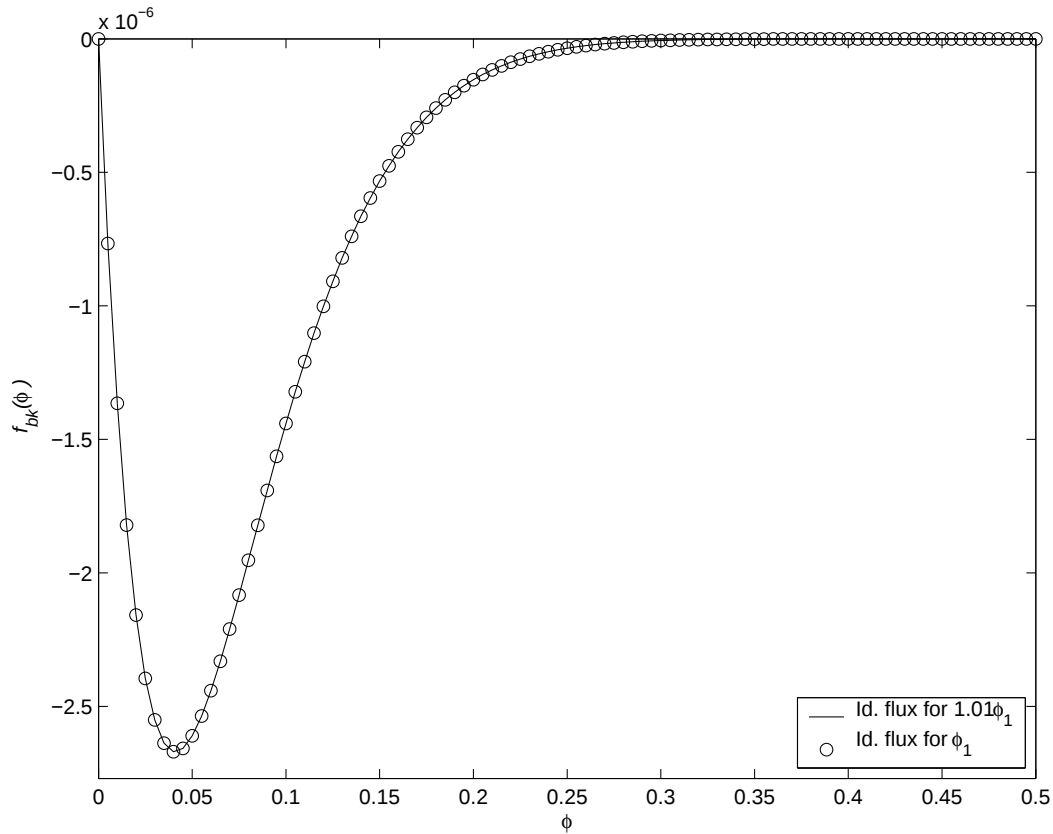


Figure 1. The identified flux for the observations ϕ_1 and $1.01\phi_1$, with the second order EO scheme at $T = 12000$ with $\Delta x = 0.005$, $CFL = 0.98$ and $\theta = 1$.

For each test, we compare the four numerical schemes presented above, namely the first order scheme **EO1**, the second order scheme **EO2**, the semi-implicit scheme **EOS** and the fully implicit scheme **EOI**. For the explicit and semi-implicit schemes we employ the $CFL = 0.5$ and in the case of explicit second order scheme we consider $\theta = 1$. For the implicit scheme we take $\Delta t = \Delta x$. Four different meshes were used, with $M = 10, 50, 100, 200$ steps.

In Figures 3-4 and table 3 we show numerical results for the first test. The Figures 5-6 and table 4 shows the results of the second test and the results for the third test are given in Figures 7-8 and table 5.

All schemes give satisfactory results, and it should be emphasized that the value of the critical concentration ϕ_c is correctly recovered. The explicit scheme is of course the simplest to implement, but turns out to be worst one in terms of computational time. Indeed the stability restriction requires such a high number of time steps that the benefit of the computational simplicity is lost (here $\Delta t \approx \Delta x^2$). In the semi-explicit and fully implicit schemes, Gauss-Seidel and Newton methods are needed to solve linear and nonlinear systems, but this is compensated by the less restrictive CFL condition. For the semi-explicit the restriction becomes the same as in the hyperbolic case, that is $\Delta t \approx \Delta x$, and finally the implicit scheme is CFL free.

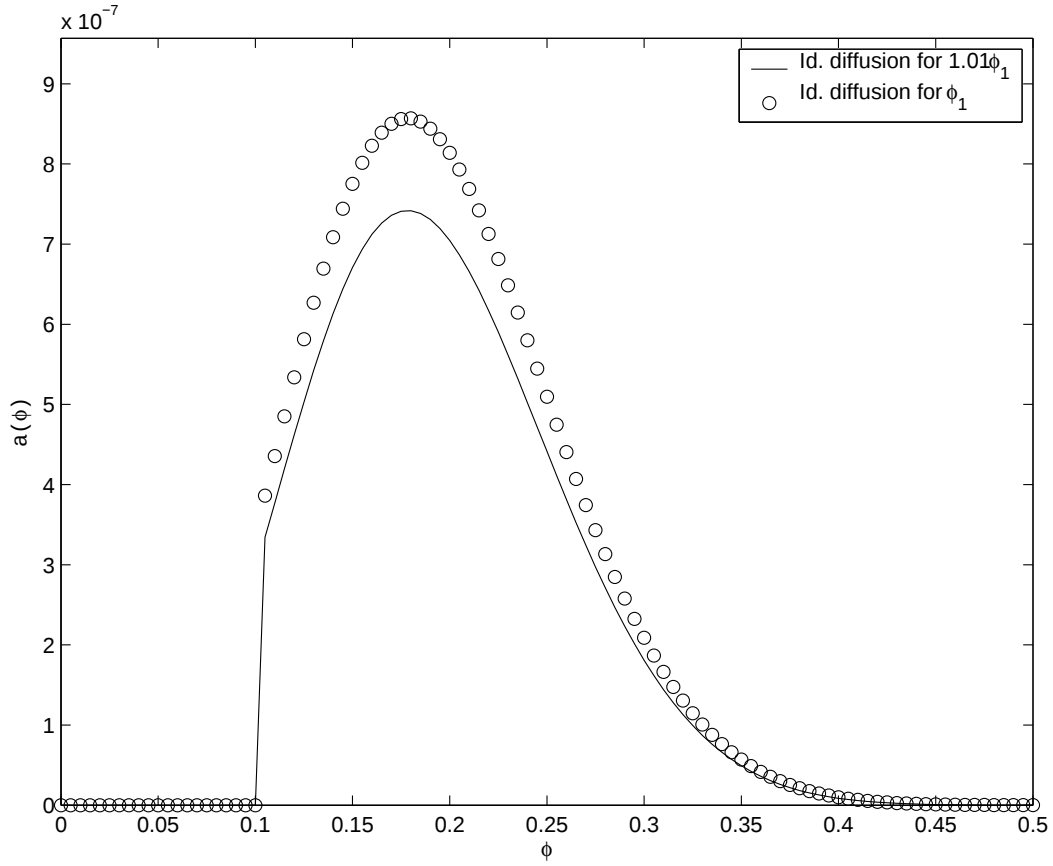


Figure 2. The identified diffusion for observations ϕ_1 and $1.01\phi_1$, with the second order EO scheme at $T = 12000$ with $\Delta x = 0.005$, $CFL = 0.98$ and $\theta = 1$.

Table 3. Identification of the flux: values of the parameter C .

M	EO1	EO2	EOS	EOI
10	15.34225	15.78555	17.21670	14.00079
50	15.62241	15.95830	15.50107	15.25519
100	15.60076	15.77236	15.70925	15.39562
200	15.58900	15.66536	15.64600	15.47951

Acknowledgments

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Table 4. Identification of the flux and diffusion except the critical concentration ϕ_c .

M	Scheme	C	α	β
10	EO1	15.28574	5.48153	6.46587
	EO2	15.73031	5.48855	6.47817
	EOS	17.02054	5.53600	6.38967
	EOI	13.92483	5.47128	6.46003
50	EO1	15.59482	5.37159	6.07586
	EO2	15.90027	5.43575	6.25493
	EOS	15.72207	5.47796	6.46396
	EOI	15.16180	5.45272	6.43251
100	EO1	15.54214	5.30271	6.12221
	EO2	15.69580	5.42393	6.34055
	EOS	15.57037	5.44297	6.40494
	EOI	15.31271	5.37628	6.30522
200	EO1	15.59575	5.13254	5.86232
	EO2	15.66016	5.30389	6.02822
	EOS	15.58839	5.27715	6.13142
	EOI	15.48579	5.12949	5.88291

Table 5. Identification of the flux and diffusion.

M	Scheme	C	α	β	ϕ_c
10	EO1	15.55524	5.50000	6.50000	0.20000
	EO2	15.97224	5.50000	6.50000	0.20000
	EOS	17.67741	5.49970	6.49966	0.32618
	EOI	14.29822	5.50000	6.50000	0.20000
50	EO1	15.82567	5.50008	6.50008	0.10650
	EO2	16.04526	5.50008	6.50008	0.10196
	EOS	16.05873	5.50019	6.50023	0.10593
	EOI	15.83821	5.50004	6.50003	0.11159
100	EO1	16.06191	5.50020	6.50023	0.10849
	EO2	16.07651	5.50023	6.50026	0.10225
	EOS	16.08611	5.50028	6.50039	0.10886
	EOI	16.09204	5.50019	6.50021	0.11058
200	EO1	16.08896	5.50026	6.50035	0.10551
	EO2	16.10939	5.50028	6.50037	0.10183
	EOS	16.09543	5.50031	6.50047	0.10635
	EOI	16.09969	5.50026	6.50034	0.10711

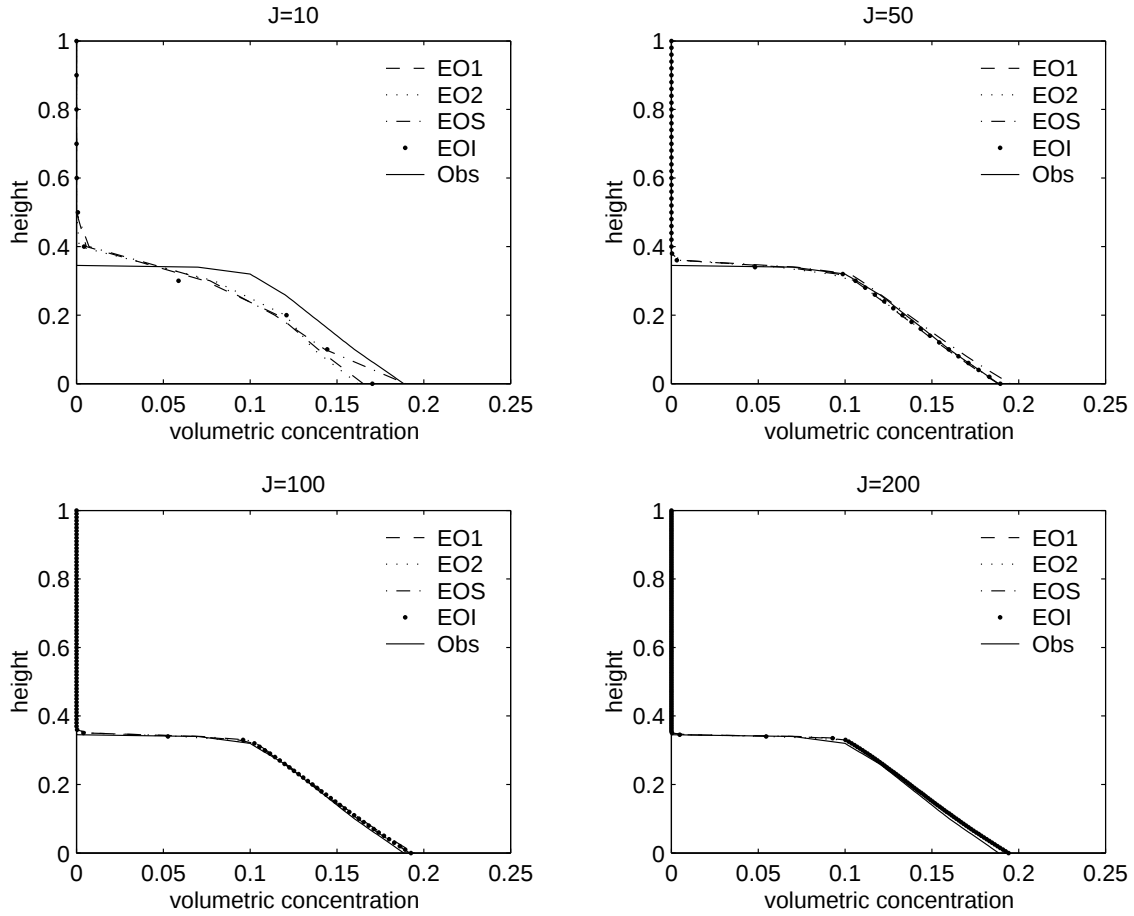


Figure 3. Numerical and observed concentration curves at $T = 12144$ for test 1.

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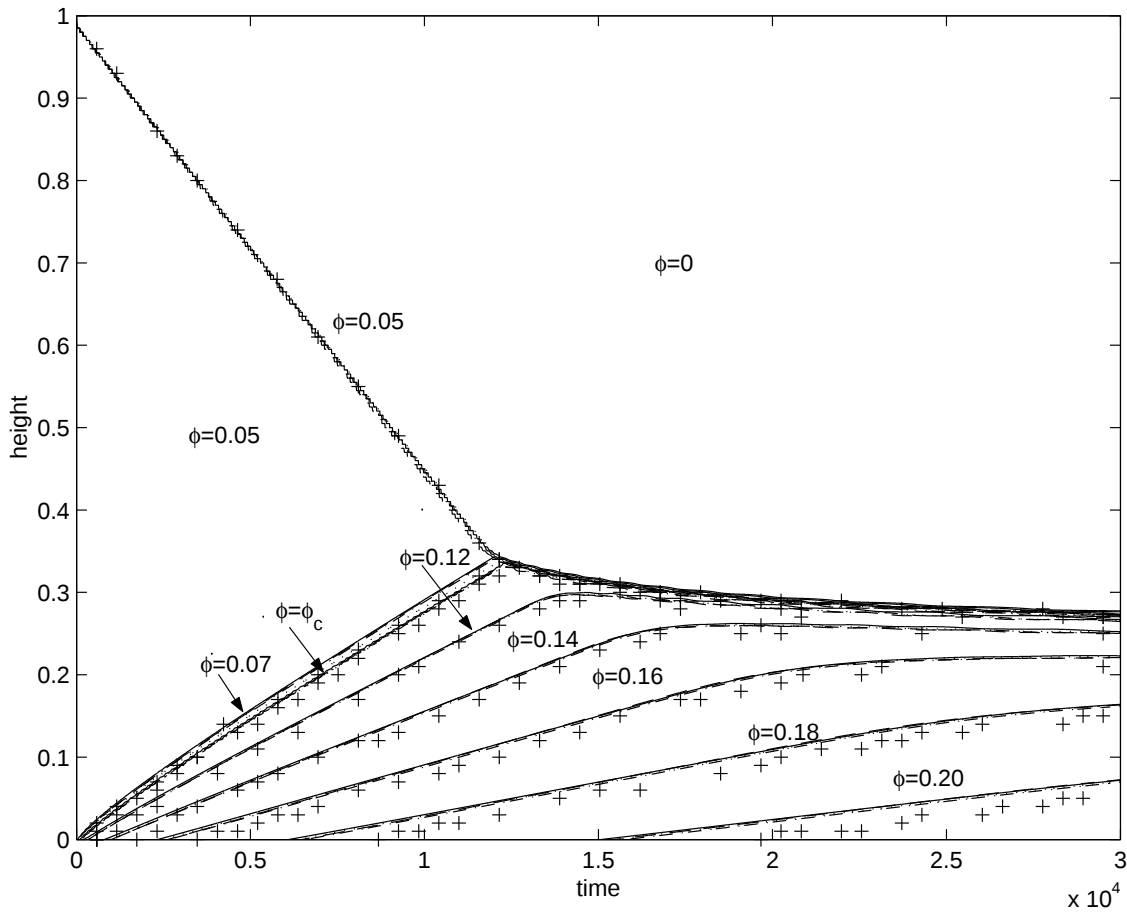


Figure 4. Isoconcentrations curves for test 1 with $M = 200$, $T = 30000$. We denote by . - . the results for EO1, by ... for EO2, by - for EOS, by -- for EOI and by +++ for the observation data.

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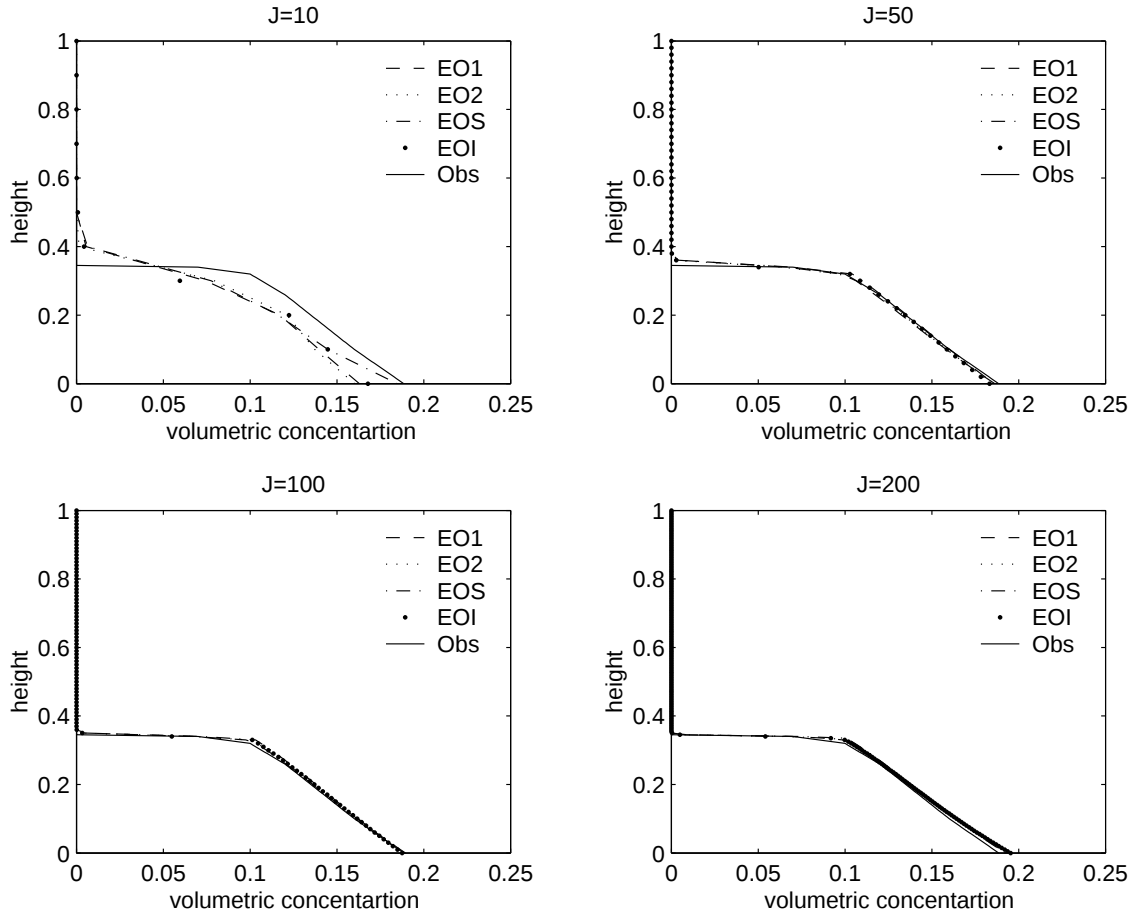


Figure 5. Numerical and observed concentration curves at $T = 12144$ for test 2.

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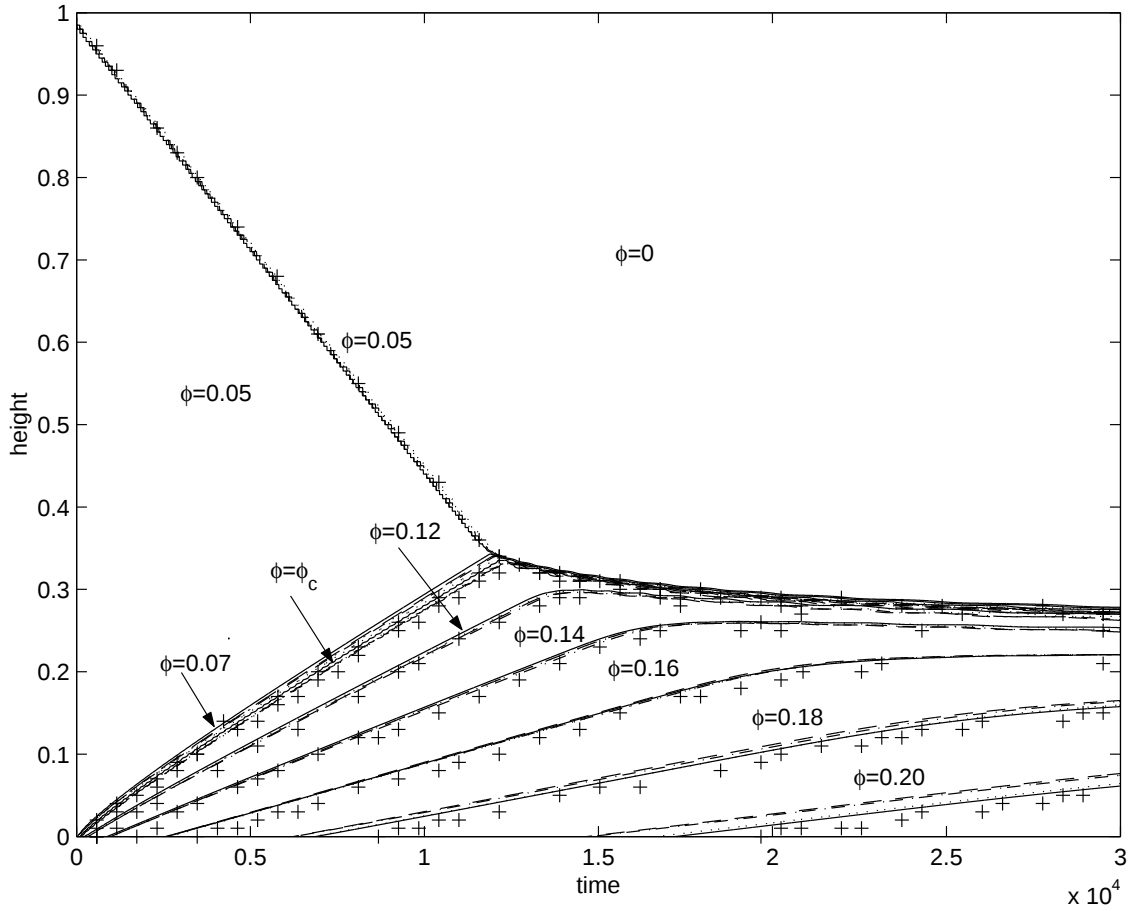


Figure 6. Isoconcentrations curves for test 2 with $M = 200$, $T = 30000$. We denote by .-. the results for EO1, by ... for EO2, by - for EOS, by -- for EOI and by +++ for the observation data.

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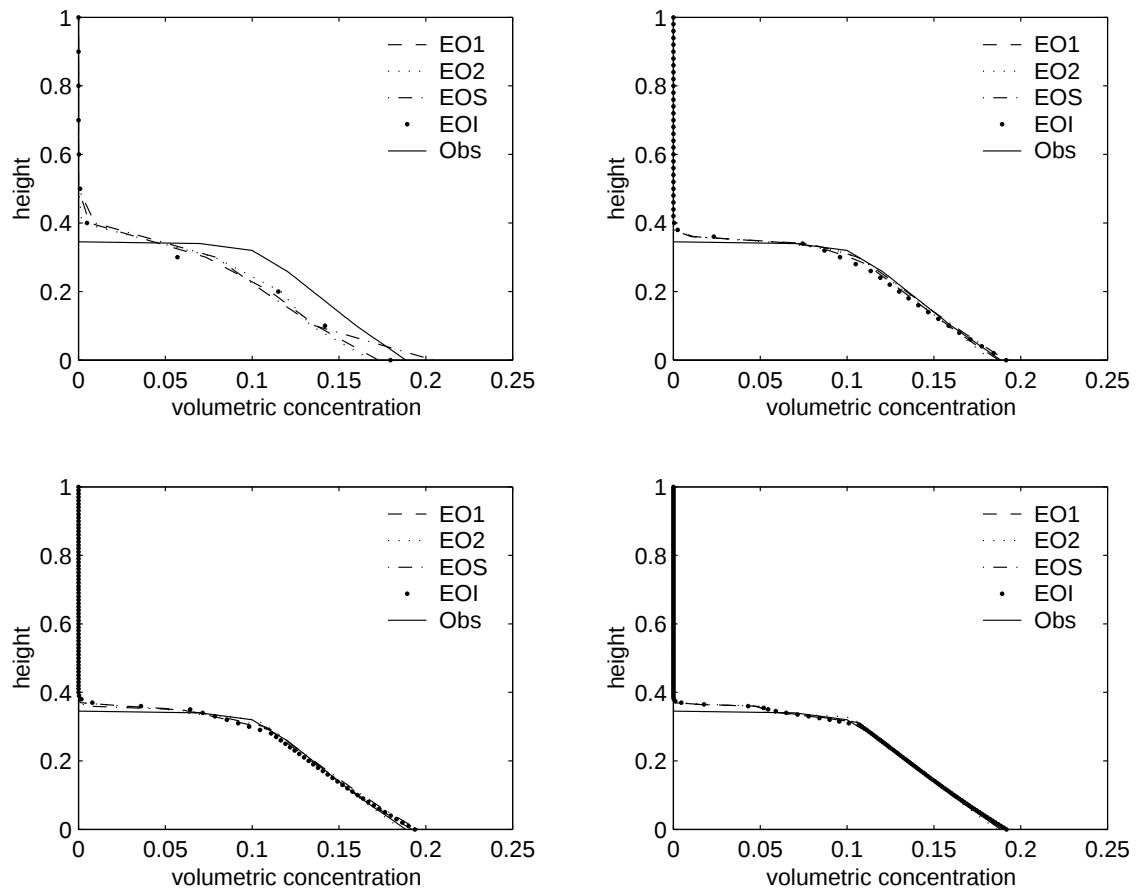


Figure 7. Numerical and observed concentration curves at $T = 12144$ for test 3.

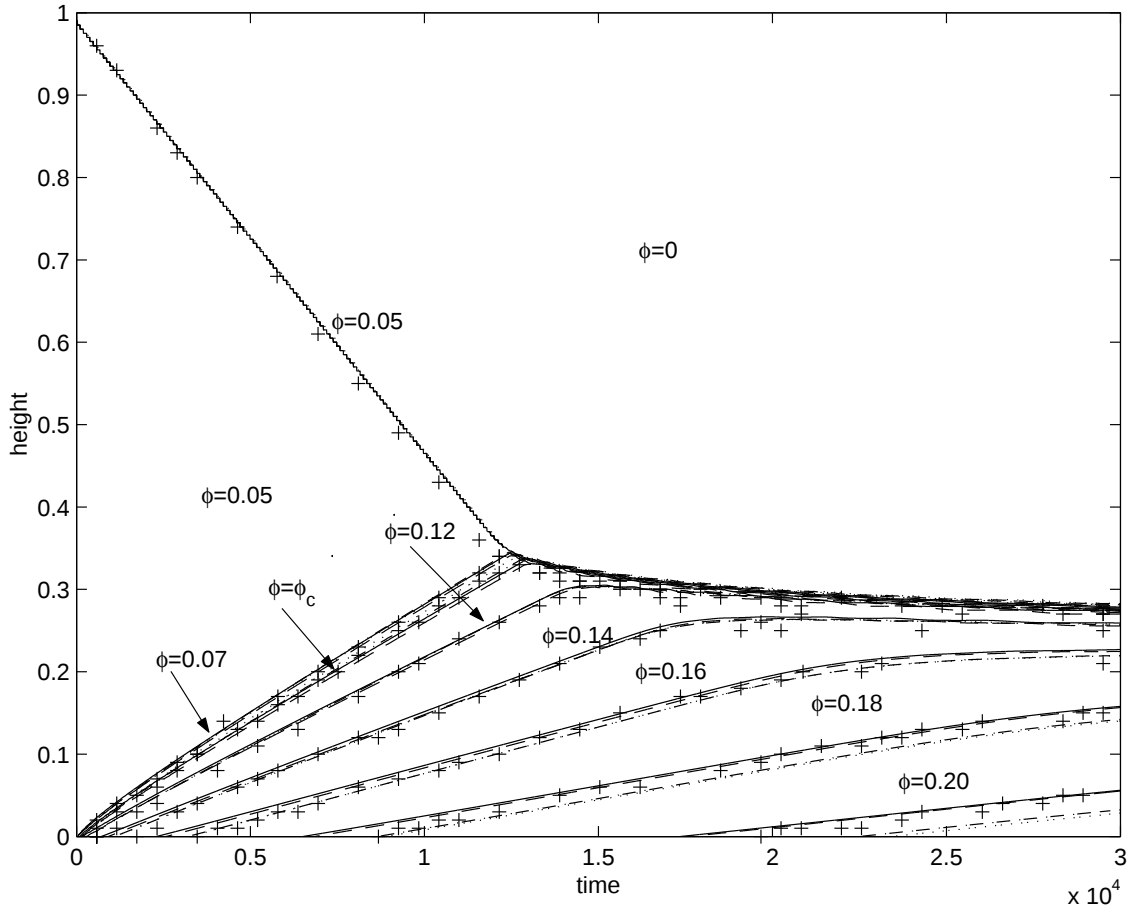


Figure 8. Isoconcentrations curves for test 2 with $M = 200$, $T = 30000$. We denote by $.-.$ the results for EO1, by $\dots$ for EO2, by $-$ for EOS, by $--$ for EOI and by $+++$ for the observation data.