Convergence of an operator splitting method on a bounded domain for a convection-diffusion-reaction system

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Abstract

We solve a convection-diffusion-sorption (reaction) system on a bounded domain with dominant convection using an operator splitting method. The model arises in contaminant transport in groundwater induced by a dual-well, or in controlled laboratory experiments. The operator splitting transforms the original problem to three subproblems: nonlinear convection, nonlinear diffusion, and a reaction problem, each with its own boundary conditions. The transport equation is solved by a Riemann solver, the diffusion one by a finite volume method, and the reaction equation by an approximation of an integral equation. This approach has proved to be very successful in solving the problem, but the convergence properties where not fully known. We show how the boundary conditions must be taken into account, and prove convergence in $L_{1,\mathrm{loc}}$ of the fully discrete splitting procedure to the very weak solution of the original system based on compactness arguments via total variation estimates. Generally, this is the best convergence obtained for this type of approximation. The derivation indicates limitations of the approach, being able to consider only some types of boundary conditions. A sample numerical experiment of a problem with an analytical solution is given, showing the stated efficiency of the method.

Key words: operator splitting, convection-diffusion-reaction problem, nonequilibrium sorption
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1 Introduction

Contaminant transport with nonlinear sorption in a strong flow field gives rise to a nonlinear convection-diffusion-sorption system. Precise mathematical models are available and significant efforts have been made to develop efficient numerical methods, see e.g. [1]. However, in the case of dominant convection many of these methods break down numerically.

The general approach to avoid numerical instability is to use some regularization or smoothing strategy. This is usually an upwind method in a finite element framework. Although they are known to converge to the unique weak solution, the time steps needed are sometimes prohibitively small. To avoid this, the operator splitting method is chosen, which allows to choose the optimal method for each subproblem. This approach avoids high numerical dispersion and increases the sensitivity of the solution to a change of the model parameters. As is shown in other papers of the authors, cf. [2], this gives very good numerical results, but the convergence of the practical scheme has not been proved yet. This will be the main goal of the present paper. It is shown in this paper that due to the operator splitting a total variation approach must be followed in proving convergence of the overall scheme, since one of the subproblems is nonlinear transport. Thus, only $L_{1,\mathrm{loc}}$-convergence for approximations can be obtained and consequently the very weak solution of the original problem has to be considered (that is, the corresponding integral identity doesn't contain the derivatives of the unknown solution). Moreover, an additional problem arises with the interpretation of the boundary conditions for the very weak solution. This will be a weak point of applying the operator splitting method and limitates the future use of operator splitting methods on bounded domains. It implies that applications should test the convergence to the correct boundary conditions as done in this paper.

The general mathematical model that is considered reads as follows

$$\partial_t F(C) + \mathrm{div}(\vec{v}C - \mathbf{D}\nabla C) + \rho\partial_t S = 0 \tag{1}$$

$$\partial_t S = \kappa(\psi_n(C) - S) \tag{2}$$

where $x \in \Omega \subset R^d$, $t \in (0,T)$, $d = 2, 3$. In addition, initial and boundary conditions need to be considered. Here, C represents the concentration of

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contaminant, S is the mass of the adsorbed contaminant per unit mass of the porous medium, $\vec{v}$ is the groundwater velocity, ρ is the bulk density of the porous medium, and $\mathbf{D}$ is the dispersivity tensor. The function F is of the form $F(C) = C + \rho\psi_e(C)$. Functions $\psi_e(C)$ and $\psi_n(C)$ are sorption isotherms characterizing the equilibrium and nonequilibrium sorption. In most cases, they are of the form $\psi(C) = aC^p$, $a, p > 0$ (Freundlich isotherm) or $\psi(C) = \frac{aC}{1+bC}$, $b > 0$ (Langmuir isotherm). Finally, the parameter κ is the kinetic rate of sorption.

For simplicity, we consider a rectangular domain, Ω, defined as $[x^{(1)}, x^{(2)}] \times [y^{(1)}, y^{(2)}]$, with inflow at the top, outflow at the bottom, and no-flow boundaries left and right. As a further simplification, inflow and outflow are considered to be perpendicular to the flow boundaries. These simplifications make the proofs shorter without changing their premises.

Our interest is in the general problem
(P) Find $\{v, w\}$ such that

$$\frac{1}{g(x,y)}\left(\partial_t F(v) + \partial_t w\right) = \vec{h} \cdot \nabla v + \partial_x(a(x,y)\partial_x v) + \partial_y(b(x,y)\partial_y v) \quad \text{in } \Omega_T,$$
$$\partial_t w = \kappa(\psi_n(v) - w) \quad \text{in } \Omega_T,$$

with $\Omega_T := \Omega \times (0,T)$, $\vec{h} = [h_1(x,y), h_2(x,y)]^T$, $0 < T < \infty$, subject to the initial conditions (IC)

$$v(x,y,0) = v^0(x,y), \qquad w(x,y,0) = w^0(x,y),$$

and boundary conditions (BC)

$$b(x,y)\partial_y v + h_2(x,y)v = h_2(x,y)v_I(x,t) \quad \text{for } y = y^{(2)} \text{ (inflow)}, \tag{3}$$
$$\partial_\nu v = 0 \quad \text{elsewhere on } \partial\Omega, \tag{4}$$

with $\vec{\nu}$ the outward normal direction and

$$h_1 = 0 \text{ on } x = x^{(1)} \text{ and } x^{(2)} \text{(no-flow)}. \tag{5}$$

The functions g, h, a and b are positive, bounded and smooth, F is such that F and F^{-1} are Lipschitz continuous, monotone increasing with $F(0) = 0$, $F(s) < C_L$ if $s < L$. In particular, F is taken to be of the form: $F(v) = v + \psi_e(v)$. We have that ψ_e and ψ_n are continuous, ψ_e is monotone increasing, so $F(v) \geq v \geq 0$, and moreover that ψ_n is Lipschitz continuous. Furthermore, v^0 and v_I are nonnegative, bounded and of bounded total variation. Due to (4)-(5), the flux $\vec{q}_\nu = -\vec{h}v - \mathbf{D}\nabla v$ is orthogonal to the outward normal $\vec{\nu}$ along these (no-flow) boundaries. Outflow boundaries have advection out of the domain, and inflow boundaries advection into the domain. Due to the limitations on $\vec{h}$ this corresponds to $y = y^{(1)}$ and $y = y^{(2)}$, respectively.

The main goal of the paper is to prove convergence of the operator splitting method to a 'very weak' solution as defined below. Problem $(\mathbf{P})$ arises in column test laboratory experiments as well as in the dual-well field experiment. For groundwater flow, the tensor $\mathbf{D} = (D_{ij})$, $i, j = 1$ and 2, from (1) is typically defined as

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

where D_0 is the molecular diffusion coefficient, δ_{ij} the Kronecker symbol and α_L, α_T the longitudinal and transversal dispersivities, respectively. The authors have solved the original problem (1)–(2) in the dual-well setting, [2], under the Dupuit-Forchheimer approximation (vertical flow is neglected) and steady-state flow. Then, applying a bipolar transformation [3], (1)–(2) is transformed into problem $(\mathbf{P})$ with flow $\vec{h} = (0, h_2)$, h_2 a constant.

The development of the numerical operator splitting method and its practical implementation to the dual-well was described in [2], [4]. The numerical experiments confirm small numerical dispersion and its suitability for solving both direct and inverse problems. In spite of the good practical results, the convergence of the method was not yet proved. Here we show that the developed operator splitting method is convergent to a 'very weak' solution.

Definition 1 *A pair of functions $\{v, w\}$ is said to be a very weak solution to* $(\mathbf{P})$ *if it satisfies the identities*

$$\begin{aligned}\int_{\Omega_T} (\partial_t\phi)\frac{F(v)+w}{g} + \int_{\Omega} \frac{F(v^0(x,y)) + w^0(x,y)}{g}\phi(x,y,0) \\ + \int_{\Omega_T} v\left[\partial_x(a\partial_x(\phi)) + \partial_y(b\partial_y(\phi))\right] - \int_{\Omega_T}(\nabla\cdot\vec{h}\phi)v \\ + \int_0^T\int_{x^{(1)}}^{x^{(2)}} h_2 v_I(t)\phi\,dx\,dt|_{y=y^{(2)}} - \int_0^T\int_{x^{(1)}}^{x^{(2)}} h_2 v(t)\phi\,dx\,dt|_{y=y^{(1)}} = 0, \quad (6)\end{aligned}$$

$\forall\phi \in C^\infty(\Omega_T)$, fulfilling $\phi = 0$ at $t = T$, and further $\partial_y\phi = 0$ for $y = y^{(2)}$, $\partial_y\phi = 0$ for $y = y^{(1)}$ and $\partial_x\phi = 0$ on $x = x^{(1)}$ and $x = x^{(2)}$, for $t > 0$, and

$$\int_{\Omega_T} w\partial_t\eta + \kappa(\psi_n(v) - w)\eta + \int_{\Omega} w^0(x,y)\eta(x,y,0) = 0. \quad (7)$$

holds $\forall\eta \in C^\infty(\Omega_T)$, $\eta(T) = 0$.

The very weak solution follows from integration by parts of the standard weak solution. Let us also consider the localized version:

Definition 2 *A pair $\{v, w\}$ is said to be a local, very weak solution to* $(\mathbf{P})$ *if it satisfies the identities (6), (7) for test functions which have compact support* *near* $y = y^{(1)}$ *(the outflow boundary).*

For the local, very weak solution the last term of (6) is zero.

Remark 3 *The problem* **(P)** *has a unique weak solution under the assumptions (i)-(vi) listed in Section 3, see [5–8]. The weak solution is defined by an integral identity which contains first derivatives (in time and space) and is more regular ($v \in L_2((0,T), W_2^1)$, $\partial_t v \in L_2((0,T), L_2)$ - W_2^1 being the Sobolev space). Approximating problem* **(P)** *by the operator splitting method, we can guarantee only $L_{1,\mathrm{loc}}(\Omega_T)$ convergence of the approximations, based on boundedness of the total variation, since a nonlinear transport subproblem is a part of the global approximation. Consequently, we need a notion of a very weak solution containing the unknown without derivatives in the corresponding integral identity.*

To prove convergence, we will use results by Kružkov in his analysis of hyperbolic equations, [9]. Several results exist in the literature, obtained for the splitting procedure in an unbounded domain. In the paper of Crandall and Majda, [10], a detailed analysis was done for the splitting method applied to conservation laws. The same type of problems was investigated in the work of Holden and Risebro, [11]. A splitting method for convection-diffusion problems was analyzed by Holden, Karlsen, Risebro and Lie in [12] and [13]. Karlsen and Lie proved convergence of a splitting procedure for convection-diffusion-reaction problems in [14]. In these papers the authors consider a spatially unbounded domain, i.e. without boundary conditions. There, the a priori estimate for the total variation in the parabolic part has been proved in one dimension, but it seems that this technique cannot be extended to more dimensions. In this paper we develop an argumentation suitable for more space dimensions. This, consequently, leads to a more complicated technique in the proof of the compactness argument.

Furthermore, in this paper we consider a practical implementation for a system of two differential equations, with a nonlinear term in the time derivative, and moreover on a bounded domain, where one of the equations models non-equilibrium sorption. This reaction is of a different type as that considered in [14]. Non-trivial modifications of known results are needed as well as refined and different techniques in the proofs.

2 Operator splitting method

In the following we choose a time step Δt and an integer N such that $N\Delta t = T$. We denote $t_n = n\Delta t$. This choice is only made for convenience, and the convergence can also be proved for a nonuniform time grid (see [15]).

In each time step we split the original problem **(P)** in three different subproblems corresponding to the physical processes included in the mathematical model. Namely, we have the hyperbolic (nonlinear transport) problem with solution operator $\mathcal{T}_t$, the parabolic (dispersion) problem with solution operator $\mathcal{D}_t$ and the sorption problem with solution operator $\mathcal{A}_t$. If we suppose that we have already computed the approximate solution $[v^n, w^n]$, the corresponding mathematical formulation for time interval $(t_n, t_{n+1}]$ reads

$$\partial_t F(v) - \vec{G}(x,y) \cdot \nabla v = 0, \tag{8}$$

where $\vec{G} = g\vec{h}$, along with an inflow and an initial condition

$$v(x, y^{(2)}, t) = v_I(x, y^{(2)}, t), \qquad v(x, y, t_n) = v^n, \tag{9}$$

together with the parabolic problem

$$\partial_t F(v) = g(x,y)\left\{\partial_x(a(x,y)\partial_x v) + \partial_y(b(x,y)\partial_y v)\right\}, \tag{10}$$

along with the initial condition $v(x, y, t_n) = \mathcal{T}_{\Delta t} v^n$ and the boundary condition

$$\partial_\nu v = 0 \quad \text{on} \quad \partial\Omega, \tag{11}$$

and finally

$$\partial_t F(v) + \partial_t w = 0, \quad \text{and} \quad \partial_t w = \kappa(\psi_n(v) - w), \tag{12}$$

with initial conditions $v(x, y, t_n) = \mathcal{D}_{\Delta t}\mathcal{T}_{\Delta t} v^n$ and $w(x, y, t_n) = w^n$. We have that $v^{n+1} = \mathcal{A}_{\Delta t}\mathcal{D}_{\Delta t}\mathcal{T}_{\Delta t} v^n$ and $w^{n+1} = \mathcal{A}_{\Delta t} w^n$. The corresponding (semi-discrete) splitting method reads

$$v^n = \left[\mathcal{A}_{\Delta t} \circ \mathcal{D}_{\Delta t} \circ \mathcal{T}_{\Delta t}\right]^n v^0, \quad w^n = \left[\mathcal{A}_{\Delta t}\right]^n w^0 \quad n = 1, \ldots, N.$$

For the fully discrete formulation, the exact solutions need to be replaced by the corresponding numerical approximations. We use a front tracking method, [5], to approximate $\mathcal{T}_t$ and a finite volume method (FVM), [16], to approximate $\mathcal{D}_t$. The sorption problem $\mathcal{A}_t$ is transformed to an integral equation that is discretized by piecewise linear approximation of the integrand. Let us denote the approximate solution operators by $\mathcal{T}_{\Delta xy,\Delta t}$, $\mathcal{D}_{\Delta xy,\Delta t}$ and $\mathcal{A}_{\Delta xy,\Delta t}$. Here, $\mathcal{T}_{\Delta xy,\Delta t}$ indicates a front tracking method. This means that dimensional splitting is performed with a 1D-front tracking method per dimension, combined with a suitable projection, as in [5], Chapter 4. So $\mathcal{T}_{\Delta xy,\Delta t} = \mathcal{T}_{\Delta x,\Delta t} \circ \pi \circ \mathcal{T}_{\Delta y,\Delta t}$, where π indicates the projection defined below.

We construct a projection operator as in the Godunov method [17]. The front tracking method used to solve the hyperbolic problem results in a profile that consists of shocks and rarefaction waves. This must be projected onto the fixed Cartesian grid before the diffusion operator can be applied. Let us consider a uniform grid $\{x_i, y_j\}$, with $i = 1, \ldots, N_1$ and $j = 1, \ldots, N_2$. We set $\Delta x = x_{i+1} - x_i$, and analogously for Δy. The projection operator is constructed so that the mass $\int F(v) \mathrm{d}\Omega$ is conserved.

Definition 4 *The projection operators π and $\tilde{\pi}$ are defined by*

$$\pi v(x, y) = F^{-1}\left(\frac{1}{|\Omega_{ij}|}\int_{\Omega_{ij}} F(v(x,y))\, d\Omega\right) = F^{-1}\left(\tilde{\pi}F(v)\right), \quad \textit{for } (x, y) \in \Omega_{ij}, \tag{13}$$

where $\Omega_{ij} = [x_i, x_{i+1}) \times [y_j, y_{j+1})$, with $i = 1, \ldots, N_1 - 1$ and $i = j, \ldots, N_2 - 1$.

The fully discrete splitting method then reads

$$v^n = \left[\mathcal{A}_{\Delta xy,\Delta t} \circ \mathcal{D}_{\Delta xy,\Delta t} \circ \pi \circ \mathcal{T}_{\Delta xy,\Delta t}\right]^n v^0, \quad n = 1, \ldots, N, \tag{14}$$

$$w^n = \left[\mathcal{A}_{\Delta xy,\Delta t}\right]^n w^0, \quad n = 1, \ldots, N, \tag{15}$$

In addition, the sorption part is solved in several substeps with a uniform time step σ, $m\sigma = \Delta t$. The main reason for σ is the different time scaling between convection and diffusion on one hand and the sorption/reaction on the other hand. We write:

$$v^n = \left[\left[\mathcal{A}_{\Delta xy,\sigma}\right]^m \circ \mathcal{D}_{\Delta xy,\Delta t} \circ \pi \circ \mathcal{T}_{\Delta xy,\Delta t}\right]^n v^0, \quad n = 1, \ldots, N, \tag{16}$$

$$w^n = \left[\left[\mathcal{A}_{\Delta xy,\sigma}\right]^m\right]^n w^0, \quad n = 1, \ldots, N, \tag{17}$$

We adopt the following notation:

$$\begin{aligned}\left[\mathcal{A}_{\Delta xy,\Delta t} \circ \mathcal{D}_{\Delta xy,\Delta t} \circ \pi \circ \mathcal{T}_{\Delta xy,\Delta t}\right] v^n &= \mathcal{A}_{\Delta xy,\Delta t} \circ \mathcal{D}_{\Delta xy,\Delta t} \circ \pi \widetilde{v}^{n+\frac{1}{3}} \\ &= \mathcal{A}_{\Delta xy,\Delta t} \circ \mathcal{D}_{\Delta xy,\Delta t} v^{n+\frac{1}{3}} = \mathcal{A}_{\Delta xy,\Delta t} v^{n+\frac{2}{3}} = v^{n+1}\end{aligned} \tag{18}$$

and $\mathcal{A}_{\Delta xy,\Delta t} w^n = w^{n+1}$.

3 Convergence of the operator splitting method

In this section the technique used to prove the convergence of the numerical operator splitting scheme is explained. We start by stating the convergence theorem for problem **(P)**, and next we prove a series of lemmas needed for its proof, which is given in Sec. 3.5. First, we will assume the following conditions to be satisfied throughout the text.

(i) $F(v)$ is nondecreasing
(ii) F and F^{-1} are Lipschitz continuous, hence $0 \leq c \leq F' \leq C$
(iii) $\psi_n(v)$ is nondecreasing and Lipschitz continuous
(iv) functions $g(x, y)$, $h_1(x, y)$, $h_2(x, y)$, $a(x, y)$ and $b(x, y)$ are smooth

(v) $g(x,y) > 0$, $a(x,y) > 0$, $b(x,y) > 0$ for $\forall x, y \in \Omega$
(vi) $v^0(x,y)$, $v_I(x,t)$ and $w^0(x,y)$ are nonnegative, bounded and of bounded total variation

For the norms we use the notations $\|\cdot\|_p$ for the standard norm in $L_p(\Omega)$, the space of measurable p-th power Lesbesgue integrable functions over Ω. By X_{loc}, we indicate the subspace of the function space X where the support of the funcions is contained in Ω. We recall that the 2 dimensional total variation of a function $h(x,y)$ over a rectangular domain is given by

$$TV_{xy}h(x,y) = \int TV_x(h(x,y))\,\mathrm{d}y + \int TV_y(h(x,y))\,\mathrm{d}x.$$

We also consider a numerical scheme satisfying $\Delta t = C\Delta x = C\Delta y$, C fixed as $\Delta t \to 0$.

Definition 5 *Let $v_{\Delta t}(x,y,t)$ be a piecewise constant function in t, $v_{\Delta t}(x,y,t) = v^n(x,y)$ for $t \in (t_{n-1}, t_n)$, and analogously, consider $w_{\Delta t}$.*

The specific approximation methods used will be given below. The result can be summarized in the following theorem.

Theorem 6 (Fully discrete convergence) *Let the conditions (i)–(vi) be satisfied. Then, the numerical approximation $(v_{\Delta t}(x,y,t), w_{\Delta t}(x,y,t))$ obtained by the operator splitting scheme (14)–(15), resp.(16)–(17), applying front tracking for the advection, a finite volume scheme for the diffusion, and a time discretization of the integral equation for the sorption, converges (up to a subsequence) in $L_{1,\text{loc}}$, to a local, very weak solution of the convection-diffusion-reaction problem* **(P)** *for $n \to \infty$, resp. for $n \to \infty$, $\sigma \to \infty$. If the local, very weak solution is unique, the original sequence $(v_{\Delta t}(x,y,t), w_{\Delta t}(x,y,t))$ converges.*

The proof of the theorem is based on application of Riesz-Fréchet-Kolmogorov compactness criterion based on boundedness of total variation.

3.1 Hyperbolic step and projection

The transport problem can be solved by dimensional operator splitting, [11]. Therefore, we first consider only one space dimension. No outflow boundary is set for **(P)** during this transport step. In this section we follow the arguments in [12,11,5,18] and state the results only.

The 1D transport equation is given by

$$\partial_t F(v) - G(x,y)\partial_x v = 0. \tag{19}$$

Generally, there are many weak solutions to (19). One of them is the *entropy solution* v and is physically relevant. It can be interpreted as

$$v := \lim_{\varepsilon \to 0} v_\varepsilon,$$

where v_ε is the solution of a regularized parabolic problem, where $\varepsilon \Delta v$ is added to (19) - for the exact definition see [17]. The front tracking approximation of (19) is based on the solution of the corresponding Riemann problems (piecewise-constant initial profile). The acceptable shocks are moving with Rankine-Hugoniot speed and the unacceptable shocks are split into pieces (discretization), with each piece moving with the corresponding velocity. This leads to a piecewise-constant approximation of the rarefaction waves which develop from nonacceptable shocks.

Remark 7 *As problem* **(P)** *is non-degenerate in the diffusion, no entropy formulation is needed, and standard (very) weak solutions can be used. Therefore, the entropy condition only plays a role in the hyperbolic step.*

Let us recall the following results. Theorem 3.1 of [19] gives an important stability result, based on a Kružkov analysis, see also [12,5]:

Theorem 8 *Let u_1 and u_2 denote the two entropy solutions of*

$$\partial_t u_i + G_i(x,t)\partial_x f_i(u_i) = 0, \quad u_i(x,0) = u_{i,0}, \quad i = 1, 2,$$

with $x \in \mathbb{R}$. Suppose that $\partial_x G_i$ is bounded and f_i satisfies a Lipschitz condition. Then, we have

$$\|u_1(\centerdot, t) - u_2(\centerdot, t)\|_1 \le e^{\gamma t}\|u_{1,0} - u_{2,0}\|_1 + \lambda t e^{\gamma t} \min\left(TV(u_{1,0}), TV(u_{2,0})\right),$$

where

$$\lambda = \|f_1\|_{Lip}\left(\|G_1 - G_2\|_\infty + \nu_t(G_1)\right) + \|G_2\|_\infty \|f_1 - f_2\|_{Lip},$$

$$\gamma = 2\|\partial_x G_1\|_\infty \|f_1\|_{Lip} + \|\partial_x G_2\|_\infty \|f_2\|_{Lip},$$
$$\nu_t(G) = \sup_{0<z<t} \|G(\centerdot, z^+) - G(\centerdot, z^-)\|_\infty,$$

where $G(\centerdot, z^\mp). = \lim_{t \overset{\lessgtr}{\to} z} G(\centerdot, t)$.

This result can be extended to Lipschitz continuous velocity fields G_i. Note that in our setting, $\nu_t(G) = 0$, and that all conditions of this theorem are satisfied in **(P)**, G being smooth and $f = F^{-1}$ being Lipschitz continuous. Along the lines of [12], Lemma 3.1, and [18], Lemma 2.1, we can obtain the following bounds.

Lemma 9 *Let $v(x,t)$ be a solution of (19) obtained by the front tracking method (under any fixed discretization of unacceptable shocks), with G smooth,* *positive and bounded and F and F^{-1} non-decreasing and Lipschitz continuous. Then v satisfies the following estimates*

$$\|F(v(.,t))\|_\infty \leq \max\left(\left\|F(v^0)\right\|_\infty, \|F(v_I(.))\|_\infty\right),$$

$$\|v(.,t)\|_\infty \leq \max\left(\left\|v^0\right\|_\infty, \|v_I(.)\|_\infty\right), \quad \left\|\frac{F(v(.,t)) - F(v^0)}{G}\right\|_1 \leq Ct,$$

$$TV_x F(v(.,t)) \leq TV_x F(v^0) + TV_t F(v_I(.)) \leq TV_x F(v^0) + Ct,$$

where C is a constant depending on the data. The solution can be constructed by front tracking in a finite number of steps for any $t > 0$.

After the transport step in the x- or y-direction, a projection step is done. Passing to 2 space dimensions, if we consider a time step Δt, then starting from $v(x, y, t_n) = v^n$, we arrive after one transport step at $\mathcal{T}_{\Delta xy,\Delta t} v^n = \widetilde{v}^{n+\frac{1}{3}}$. With projection to the fixed grid, we next obtain $\pi\widetilde{v}^{n+\frac{1}{3}} = v^{n+\frac{1}{3}}$. The following lemma is straightforward (see [11]).

Lemma 10 *Let $h(x, y) \in BV(\mathbb{R}^2)$, and let π and $\widetilde{\pi}$ be the projection operators from (13). Then we have*

$$TV_{xy} F(h) \geq TV_{xy} \widetilde{\pi} F(h) = TV_{xy} F(\pi h)$$

We can also derive a result for the variation in time. In the same lines as in [5,11], we obtain

Lemma 11 *If $C = \Delta x/\Delta t = \Delta y/\Delta t$, the projection operator satisfies*

$$\|F(v^{n+\frac{1}{3}}) - F(\widetilde{v}^{n+\frac{1}{3}})\|_1 = \int_\Omega |\widetilde{\pi} F(\widetilde{v}^{n+\frac{1}{3}}) - F(\widetilde{v}^{n+\frac{1}{3}})| \mathrm{d}x\mathrm{d}y \leq C\Delta t TV_{xy} F(\widetilde{v}^{n+\frac{1}{3}}).$$

The above lemma will be useful to relate all errors made to the total variation of the initial condition. Now let us consider the full two dimensional problem. The boundedness is evident. Along the lines of [11], Lemma 2, we prove the following lemma.

Lemma 12 *For $\pi \circ \mathcal{T}_{\Delta x,\Delta t} \circ \pi \circ \mathcal{T}_{\Delta y,\Delta t} v^n = v^{n+\frac{1}{3}}$ we have that*

$$TV_{xy} F(v^{n+\frac{1}{3}}) \leq e^{C_1 \Delta t} \left(TV_{xy} F(v^n) + C_2 \Delta t\right),$$

Here C_1 and C_2 are due to the refined stability estimate given in Theorem 8.

Remark 13 *The proof in [11] is given for an unbounded domain and needs to be adapted for our bounded domain. However, the bounded domain considered* *here has only little influence on the proof: no-flow-boundaries have no effect, and the outflow is not accompanied by reflecting waves.*

3.2 The parabolic step

The finite volume approximation scheme is given by

$$\frac{F(v_{i,j}^{n+\frac{2}{3}}) - F(v_{i,j}^{n+\frac{1}{3}})}{g_{ij}} + \left(a_{i+\frac{1}{2},j} + a_{i-\frac{1}{2},j} + b_{i,j+\frac{1}{2}} + b_{i,j-\frac{1}{2}}\right) \frac{\Delta t}{\Delta x^2} v_{i,j}^{n+\frac{2}{3}} - \frac{\Delta t}{\Delta x^2}\left[a_{i-\frac{1}{2},j} v_{i-1,j}^{n+\frac{2}{3}} + a_{i+\frac{1}{2},j} v_{i+1,j}^{n+\frac{2}{3}} + b_{i,j+\frac{1}{2}} v_{i,j+1}^{n+\frac{2}{3}} + b_{i,j-\frac{1}{2}} v_{i,j-1}^{n+\frac{2}{3}}\right] = 0. \quad (20)$$

where $g_{ij} = g(x_i, y_j)$, $a_{i+\frac{1}{2},j} = a(\frac{x_i+x_{i+1}}{2}, y_j)$, $b_{i,j+\frac{1}{2}} = b(x_i, \frac{y_j+y_{j+1}}{2})$. For the sake of brevity and simplicity in the proofs, we choose an equidistant grid, and let $\Delta x = \Delta y$. Taking into account the boundary conditions (11), we put $a_{i-\frac{1}{2},j} \equiv 0$ for the points $\{x_1, y_j\}$ and $a_{i+\frac{1}{2},j} \equiv 0$ for the points $\{x_{N_1}, y_j\}$, $j = 1, \ldots, N_2$. Moreover, for $\{x_i, y_1\}$, $i = 1, \ldots, N_1$, we take $b_{i,j-\frac{1}{2}} \equiv 0$ in (20), and $b_{i,j+\frac{1}{2}} \equiv 0$ for the points $\{x_i, y_{N_2}\}$. For brevity of notation, we introduce $\tilde{\imath} = i - \frac{1}{2}$, $\tilde{\jmath} = j - \frac{1}{2}$. For the boundedness and TV estimates we obtain

Lemma 14 *Let $v_1^{n+\frac{2}{3}}$ and $v_2^{n+\frac{2}{3}}$ be the approximate solutions of (10), generated by the scheme (20) corresponding to the starting points $v_1^{n+\frac{1}{3}}, v_2^{n+\frac{1}{3}}$. Then, one has*

$$\|F(v_1^{n+\frac{2}{3}})\|_\infty \leq \|F(v_1^{n+\frac{1}{3}})\|_\infty, \qquad \left\|\frac{F(v_1^{n+\frac{2}{3}}) - F(v_2^{n+\frac{2}{3}})}{g}\right\|_1 \leq \left\|\frac{F(v_1^{n+\frac{1}{3}}) - F(v_2^{n+\frac{1}{3}})}{g}\right\|_1.$$

PROOF. In (20) we choose $i = l$ and $j = k$, such that $v_{l,k}^{n+\frac{2}{3}} = \max_{ij} v_{ij}^{n+\frac{2}{3}}$. Due to the properties of F, $F(v_{l,k}^{n+\frac{2}{3}}) = \max_{ij} F(v_{ij}^{n+\frac{2}{3}})$. We directly obtain $\max F(v_{i,j}^{n+\frac{2}{3}}) \leq \max F(v_{i,j}^{n+\frac{1}{3}})$, and therefore also $\max v_{i,j}^{n+\frac{2}{3}} \leq \max v_{i,j}^{n+\frac{1}{3}}$. This can be repeated for $\min_{ij} v_{ij}^{n+\frac{2}{3}}$, which proves the first assertion. The second assertion follows by subtracting (20) for v_1 from the same equation for v_2, with $d_{ij} = v_{1,ij}^{n+\frac{2}{3}} - v_{2,ij}^{n+\frac{2}{3}}$. This gives

$$\left[\frac{F(v_{i,j}^{n+\frac{2}{3}}) - F(v_{i,j}^{n+\frac{1}{3}})}{g_{ij} d_{ij}} + (a_{\tilde{\imath}+1,j} + a_{\tilde{\imath}j} + b_{i,\tilde{\jmath}+1} + b_{i\tilde{\jmath}}) \frac{\Delta t}{\Delta x^2}\right] d_{ij}$$
$$= \frac{\Delta t}{\Delta x^2} \left[a_{\tilde{\imath}j} d_{i-1,j} + a_{\tilde{\imath}+1,j} d_{i+1,j} + b_{i,\tilde{\jmath}+1} d_{i,j+1} + b_{ij} d_{i,\tilde{\jmath}-1}\right] + \frac{F(v_{1,i,j}^{n+\frac{1}{3}}) - F(v_{2,i,j}^{n+\frac{1}{3}})}{g_{ij}}.$$

Taking absolute values leads to

$$\left[\frac{F(v_{i,j}^{n+\frac{2}{3}}) - F(v_{i,j}^{n+\frac{1}{3}})}{g_{ij} d_{ij}} + (a_{\tilde{\imath}+1,j} + a_{\tilde{\imath}j} + b_{i,\tilde{\jmath}+1} + b_{i\tilde{\jmath}}) \frac{\Delta t}{\Delta x^2}\right] |d_{ij}| \leq$$
$$\left|\frac{F(v_{1,i,j}^{n+\frac{1}{3}}) - F(v_{2,i,j}^{n+\frac{1}{3}})}{g_{ij}}\right| + \frac{\Delta t}{\Delta x^2} \left[a_{\tilde{\imath}j} |d_{i-1,j}| + a_{\tilde{\imath}+1,j} |d_{i+1,j}| + b_{i,\tilde{\jmath}+1} |d_{i,j+1}| + b_{i\tilde{\jmath}} |d_{i,j-1}|\right],$$

due to condition (i), and the fact that a and b are positive. Summation over i and j, noting that a and b are zero on the boundary, proves the lemma.□

In [12], the bound of total variation is provided in 1D. In higher dimensions, a different approach is needed. The following lemma is sufficient to prove TV boundedness of the scheme (14)–(15). First, rewrite (20) as

$$\frac{F(v_{i,j}^{n+\frac{2}{3}}) - F(v_{i,j}^{n+\frac{1}{3}})}{g_{ij}} = \frac{\Delta t}{\Delta x} \left[a_{\tilde{\imath}+1,j} D_{i+1,j}^{i} v - a_{\tilde{\imath}j} D_{i,j}^{i} v\right] + \frac{\Delta t}{\Delta y} \left[b_{i,\tilde{\jmath}+1} D_{i,j+1}^{j} v - b_{i\tilde{\jmath}} D_{i,j}^{j} v\right], \tag{21}$$

where

$$D_{ij}^{i} v = \frac{v_{i,j}^{n+\frac{2}{3}} - v_{i-1,j}^{n+\frac{2}{3}}}{\Delta x}, \quad D_{ij}^{j} v = \frac{v_{i,j}^{n+\frac{2}{3}} - v_{i,j-1}^{n+\frac{2}{3}}}{\Delta y}.$$

Lemma 15 *Let $v^{n+\frac{2}{3}}$ be the solution of (20) with a and $b \geq \delta > 0$. Then,*

$$\Delta t TV_{xy} v^{n+\frac{2}{3}} \leq C_1 \Delta t - C_2 \sum_{ij} \frac{1}{g_{ij}} \left[F(v_{ij}^{n+\frac{2}{3}}) - F(v_{ij}^{n+\frac{1}{3}})\right] v^{n+\frac{2}{3}} \Delta x \Delta y, \tag{22}$$

where C_1 and $C_2 > 0$.

PROOF. We multiply both sides of (21) with $v_{ij}^{n+\frac{2}{3}}$. We sum over i and j, and apply Abel's summation, $\sum_{k=1}^{m} d_k(c_k - c_{k-1}) = d_m c_m - d_0 c_0 - \sum_{k=1}^{m} (d_k - d_{k-1}) b_{i-1}$ in the rhs, once with $k = i$ and $c_i = a_{i+\frac{1}{2},j} D_{i+1,j}^{i} v$, $d_i = v_{ij}^{n+\frac{2}{3}}$, and once with $k = j$ and $c_j = b_{i,j+\frac{1}{2}} D^j_{i,j+1} v$, $d_j = v_{ij}^{n+\frac{2}{3}}$. Using the boundary conditions ($D^k_{ij} v = 0$, $k = i, j$), we arrive at

$$\sum_{ij} \frac{1}{g_{ij}} \left[F(v_{ij}^{n+\frac{2}{3}}) - F(v_{ij}^{n+\frac{1}{3}}) \right] v_{ij}^{n+\frac{2}{3}} + \Delta t \sum_{ij} \left[a_{i-\frac{1}{2},j} [D^i_{ij} v^{n+\frac{2}{3}}]^2 + b_{i,j-\frac{1}{2}} [D^j_{ij} v^{n+\frac{2}{3}}]^2 \right] = 0. \quad (23)$$

We can now rewrite the total variation. Invoke the inequality $|f| \leq \frac{1}{2} + \frac{1}{2} f^2$. In combination with (23) and the fact that $a_{\tilde{i}j}$ and $b_{i\tilde{j}} \geq \delta > 0$, we obtain

$$\begin{aligned} &\sum_{ij} \left[\left| D^i_{ij} v^{n+\frac{2}{3}} \right| + \left| D^j_{ij} v^{n+\frac{2}{3}} \right| \right] \Delta x \Delta y \qquad (24) \\ &\leq \frac{1}{2} |\Omega| + \frac{1}{2} |\Omega| + \frac{1}{2\delta} \sum_{ij} \left[a_{i-\frac{1}{2},j} [D^i_{ij} v^{n+\frac{2}{3}}]^2 + b_{i,j-\frac{1}{2}} [D^j_{ij} v^{n+\frac{2}{3}}]^2 \right] \Delta x \Delta y \\ &\leq |\Omega| - \frac{1}{2\delta} \frac{1}{\Delta t} \sum_{ij} \frac{1}{g_{ij}} \left[F(v_{ij}^{n+\frac{2}{3}}) - F(v_{ij}^{n+\frac{1}{3}}) \right] v_{ij}^{n+\frac{2}{3}} \Delta x \Delta y. \square \end{aligned}$$

3.3 The sorption step

The sorption has no explicit dependence on space. Whenever possible, for simplicity we only mention the time dependence. From (12) we deduce,

$$F(v(t)) + w(t) = C_0, \quad \text{and} \quad w(t) = w^n e^{-\kappa(t-t_n)} + \kappa \int_{t_n}^{t} e^{-\kappa(t-s)} \psi_n(v(s)) \, ds, \quad (25)$$

where $C_0 = C(x, y) \equiv F(v^{n+\frac{2}{3}}) + w^{n+\frac{2}{3}}$ is a constant in time and where $w^{n+\frac{2}{3}} \equiv w^n$. Consequently, we obtain

$$F(v(t)) = F(v^{n+\frac{2}{3}}) + w^n - w^n e^{-\kappa(t-t_n)} - \kappa \int_{t_n}^{t} e^{-\kappa(t-s)} \psi_n(v(s)) \, ds. \quad (26)$$

This nonlinear integral equation can be solved numerically using l micro-time steps σ, $l\sigma = \Delta t$ in the approximation of the integral. We linearize $\psi_n(s)$ by a piecewise linear function and successively obtain $\widetilde{v}(t)$ by Newton's method, setting $\widetilde{v}(\Delta t) = v^{n+1}$. This can be performed up to a required accuracy. Afterwards, w can be determined from (25). To distinguish the two, we denote by $(v(t), w(t))$ the solution to (25) and by $(v_\sigma(t), w_\sigma(t))$ the numerical approximation. For the details see (57) below.

Lemma 16 *Let $(v(t), w(t))$ be the solution to (25) obtained by the described approximation method. Then,*

$$\|F(v(t))\|_\infty + \|w(t)\|_\infty \leq \left(\|F(v^{n+\frac{2}{3}})\|_\infty + \|w^n\|_\infty\right)(1 + C\Delta t) \tag{27}$$

PROOF. Let us consider the exact solution of (25). By the positivity of F, w and ψ_n, and by the Lipschitz continuity of ψ_n, as well as by $F(v) \geq v \geq 0$, we obtain from (26)

$$\begin{aligned} |F(v(t))| &\leq |F(v^{n+\frac{2}{3}})| + |w^n|(1 - e^{-\kappa(t-t_n)}) + \kappa \int_{t_n}^{t} e^{-\kappa(t-s)} |\psi_n(v(s))|\, ds \\ &\leq |F(v^{n+\frac{2}{3}})| + |w^n|(1 - e^{-\kappa(t-t_n)}) + \kappa L \int_{t_n}^{t} F(v(s))\, ds. \end{aligned}$$

Similarly, from the second equality of (25),

$$|w(t)| \leq |w^n| e^{-\kappa(t-t_n)} + \kappa L \int_{t_n}^{t} F(v(s))\, ds.$$

Adding the two previous estimates gives

$$|F(v(t))| + |w(t)| \leq |F(v^{n+\frac{2}{3}})| + |w^n| + 2\kappa L \int_{t_n}^{t} \left(|F(v(s))| + |w(s)|\right) ds,$$

which allows to apply Gronwall's lemma, resulting in the required inequality for the exact solution. This can be extended to the approximation, see Remark 18.□

Lemma 17 *Let $(v(t), w(t))$ be the solution to (25) obtained by the described approximation method, then, if $\Delta t = C\Delta x = C\Delta y$ and ψ_n is Lipschitz continuous, we have that*

$$TV_{xy}F(v(t)) \leq \left(TV_{xy}F(v^{n+\frac{2}{3}}) + C\Delta t\, TV_{xy}w^n\right)(1 + C\Delta t) \tag{28}$$

$$TV_{xy}w(t) \leq TV_{xy}w^n + C \int_{t_n}^{t_{n+1}} TV_{xy}v(s)\, ds, \tag{29}$$

where C is a positive constant.

PROOF. We start with the TV_y, denoting by subscript j a grid point on the y-axis. Substract (26) for v_j from the expression for v_{j+1} to obtain

$$\begin{aligned} F(v_{j+1}(t)) - F(v_j(t)) = F(v_{j+1}^{n+\frac{2}{3}}) - F(v_j^{n+\frac{2}{3}}) + (w_{j+1}^n - w_j^n)\left(1 - e^{-\kappa(t-t_n)}\right) \\ - \kappa \int_{t_n}^{t} e^{-\kappa(t-s)} \left(\psi_n(v_{j+1}(s)) - \psi_n(v_j(s))\right) ds. \end{aligned} \tag{30}$$

Taking absolute values, and summing over j, we obtain an expression for TV_y. The same can be done for TV_x, allowing to obtain an expression for TV_{xy}. Assuming Lipschitz continuity of ψ_n and moreover that $\Delta t = C\Delta x = C\Delta y$, it follows that

$$TV_{xy}F(v(t)) \leq TV_{xy}F(v^{n+\frac{2}{3}}) + \left(1 - e^{-\kappa(t-t_n)}\right) TV_{xy}w^n + L\kappa \int_{t_n}^{t} TV_{xy}v(s)\, ds$$
$$\leq TV_{xy}F(v^{n+\frac{2}{3}}) + \left(1 - e^{-\kappa\Delta t}\right) TV_{xy}w^n + L\kappa \int_{t_n}^{t} TV_{xy}F(v(s))\, ds. \quad (31)$$

We used the fact that ψ_e is nondecreasing, and $F(v) = v + \psi_e(v)$ so that $|v_{j+1} - v_j| \leq |F(v_{j+1}) - F(v_j)|$. From (31), using Gronwall's Lemma, we obtain the first assertion. Similarly, (25), gives

$$TV_{xy}w(t) \leq e^{-\kappa(t-t_n)} TV_{xy}w^n + L\kappa \int_{t_n}^{t} TV_{xy}v(s)\, ds \quad (32)$$

The second inequality of the lemma is straightforward. Again this result for the exact solution can be extended to the approximation, see Remark 18.□

Remark 18 *Lemma's 16 and 17 state estimates for the exact solution (v, w) of the sorption problem. We need analogous estimates for the numerical solution $(v_\sigma,\ w_\sigma)$ – σ being the discretization parameter for the reaction part. These analogous estimates can readily be obtained for a practical integration scheme for (25), see eg. [15].*

3.4 The four steps combined

To prove the key issue of total variation boundedness of the numerical solution, we need to define an auxiliary function. Let

$$B(s) := sF(s) - \int_0^s F(z)\, dz.$$

We have that

$$[F(u) - F(v)]\, u \geq B(u) - B(v). \quad (33)$$

Indeed, $[F(u) - F(v)]\, u = F(u)u - F(v)v - (u - v)F(v) \geq F(u)u - F(v)v - \int_v^u F(z)\, dz \equiv B(u) - B(v)$, since $F(u)$ is monotonously increasing. Note also that $B(s) > 0$ if $s > 0$, and $B(0) = 0$, as well as $B'(s) = sF'(s)$. Moreover, the boundedness of B on $(0, L)$ follows from the boundedness of F on $(0, L)$.

We have the following lemma for $v_{\Delta t}$ from Def. 5.

Lemma 19 *The approximation scheme given by (18), with $\Delta t = C\Delta x =$*

$C\Delta y$, satisfies

$$\|v^n\|_\infty + \|w^n\|_\infty \le C, \quad \textit{and} \quad TV_{xy} w_{\Delta t}(t) + \int_0^T TV_{xy} v_{\Delta t}(t)\,\mathrm{d}t \le C,$$

where the constant C is independent of the space and time discretization and only depends on the domain, as well as on a, b, $\|w^0\|_\infty$, $\|v_I\|_\infty$ and $\|v^0\|_\infty$.

PROOF. Lemma 16 in combination with Lemma 9, Lemma 14, and the properties of π, give

$$\|F(v^{n+1})\|_\infty + \|w^{n+1}\|_\infty \le \{\max(\|F(v^n)\|_\infty, \|F(v_I(t))\|_\infty) + \|w^n\|_\infty\}(1 + C\Delta t)$$

Consequently, using $v < F(v)$, and the properties of the initial state w^0, v^0 and the boundary state v_I, the first assertion is true for $n = 0$, and by induction also for all n. For the second inequality, we consider (28) from Lemma 17, we use the Lipschitz continuity of F in the right hand side, and we apply Lemma 15. Furthermore, applying (33), we obtain

$$\begin{aligned}
TV_{xy} F(v(t)) &\le \Big(C_1 L - \frac{C_2 L}{\Delta t} \sum_{ij} \frac{1}{g_{ij}} \Big[F(v_{ij}^{n+\frac{2}{3}}) - F(v_{ij}^{n+\frac{1}{3}})\Big] v_{ij}^{n+\frac{2}{3}} \Delta x \Delta y \\
&\quad + C_3 \Delta t\, TV_{xy} w^n\Big)(1 + C\Delta t) \\
&\le \Big(C_1 L - \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{1}{g_{ij}} \Big[B(v_{ij}^{n+\frac{2}{3}}) - B(v_{ij}^{n+\frac{1}{3}})\Big] \Delta x \Delta y \\
&\quad + C_3 \Delta t\, TV_{xy} w^n\Big)(1 + C\Delta t) \\
&= \Big(C_1 L + C_3 \Delta t\, TV_{xy} w^n - \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{1}{g_{ij}} \displaystyle\int_{\Omega_{ij}} \Big[B(v_{ij}^{n+1}) - B(v_{ij}^n)\Big] \mathrm{d}x\mathrm{d}y \\
&\quad + \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{1}{g_{ij}} \displaystyle\int_{\Omega_{ij}} \Big[B(v_{ij}^{n+1}) - B(v_{ij}^{n+\frac{2}{3}}) + B(v^{n+\frac{1}{3}}(x,y)) - B(\tilde{v}^{n+\frac{1}{3}}(x,y)) \\
&\quad + B(\tilde{v}^{n+\frac{1}{3}}(x,y)) - B(v_{ij}^n)\Big] \mathrm{d}x\mathrm{d}y\Big)(1 + C\Delta t) \\
&\le \Bigg(C_1 L - \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{1}{g_{ij}} \displaystyle\int_{\Omega_{ij}} \Big[B(v_{ij}^{n+1}) - B(v_{ij}^n)\Big] \mathrm{d}x\mathrm{d}y + C_3 \Delta t\, TV_{xy} w^n \\
&\quad + \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{1}{g_{ij}} \displaystyle\int_{\Omega_{ij}} \Big[B(v_{ij}^{n+1}) - B(v_{ij}^{n+\frac{2}{3}})\Big] \mathrm{d}x\mathrm{d}y \\
&\quad + \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{v_{ij}^{n+\frac{1}{3}}}{g_{ij}} \displaystyle\int_{\Omega_{ij}} \Big[F(v_{ij}^{n+\frac{1}{3}}) - F(\tilde{v}^{n+\frac{1}{3}}(x,y))\Big] \mathrm{d}x\mathrm{d}y \\
&\quad + \tfrac{C_2 L}{\Delta t} \textstyle\sum_{ij} \tfrac{1}{g_{ij}} \displaystyle\int_{\Omega_{ij}} \Big[F(\tilde{v}^{n+\frac{1}{3}}(x,y)) - F(v_{ij}^n)\Big] [\tilde{v}^{n+\frac{1}{3}}(x,y)] \mathrm{d}x\mathrm{d}y\Bigg)(1 + C\Delta t).
\end{aligned}$$

Let us denote the last three terms in the first factor by I_1, I_2 and I_3 (contributions due to sorption, projection and transport, respectively). I_2 is zero, as this is exactly the projection (13). I_3 can be estimated by using Lemma 9 (Lipschitz continuity in time and L_∞-diminishing property of the transport part) and the positivity of g. We obtain

$$I_3 \leq C\|F(v^n))\|_\infty + C\|F(v_I(t))\|_\infty \leq C.$$

To estimate I_1, note that (12) yields for every micro time step σ,

$$\frac{F(v^{n,m}) - F(v^{n,m-1})}{\sigma} + \frac{w^{n,m} - w^{n,m-1}}{\sigma} = 0$$

for $m = 1, \dots l$, $l\sigma = \Delta t$, $v^{n,0} = v^{n+\frac{1}{3}}$. Multiplying this equation by σ and using (33) implies

$$B(v^{n,m}) - B(v^{n,m-1}) \leq -(w^{n,m} - w^{n,m-1})F^{-1}(C_0^n - w^{n,m})$$

where we used (25) and $C_0^n = F(v^{n+\frac{2}{3}}) + w^n = F(v^{n,m}) + w^{n,m} = F(v^{n+1}) + w^{n+1}$, $m = 0, 1, \dots l$. After summation over m and integration, we obtain

$$\begin{aligned} I_1 &\leq \frac{C_2 L}{\Delta t} \sum_{ij} \int_{\Omega_{ij}} \left(-\textstyle\sum_{m=1}^{l} \frac{(w^{n,m} - w^{n,m-1})}{\sigma} F^{-1}(C_{0,ij}^n - w^{n,m})\sigma \right) \frac{\mathrm{d}x\mathrm{d}y}{g_{ij}} \\ &\leq \frac{C_2 L}{\Delta t} \sum_{ij} \frac{1}{g_{ij}} \int_{\Omega_{ij}} \left(-\int_{t_n}^{t_{n+1}} (\partial_t w^n(t)) F^{-1}(C_{0,ij}^n - w^n(t))\,\mathrm{d}t + \mathcal{O}(\Delta t) \right) \mathrm{d}x\mathrm{d}y \\ &\leq \frac{C_2 L}{\Delta t} \sum_{ij} \frac{1}{g_{ij}} \int_{\Omega_{ij}} \left(\int_{t_n}^{t_{n+1}} \partial_t [G(C_{0,ij}^n - w^n(t))]\,\mathrm{d}t + \mathcal{O}(\Delta t) \right) \mathrm{d}x\mathrm{d}y, \end{aligned}$$

where we introduced the function G, satisfying $G(s) = \int F^{-1}(s)\,\mathrm{d}s$. Then, one finds

$$\begin{aligned} I_1 \leq \frac{C_2 L}{\Delta t} \sum_{ij} \frac{1}{g_{ij}} \int_{\Omega_{ij}} \left([G(C_{0,ij}^n - w^{n+1}) - G(C_{0,ij}^n - w^n)] + \mathcal{O}(\Delta t) \right) \mathrm{d}x\mathrm{d}y \\ \leq \frac{C}{\Delta t} \sum_{ij} \int_{\Omega_{ij}} |G'|\,|w^{n+1} - w^n| + \frac{\mathcal{O}(\Delta t)}{\Delta t} \leq C. \end{aligned}$$

Here we used that G has bounded derivative and that w is the solution of an integral equation and hence its changes in time are of order $\mathcal{O}(\Delta t)$. Using the estimates of I_1, I_2 and I_3, as well as the relation between v and $F(v)$, we now have

$$\begin{aligned} &TV_{xy} v(t) \leq \\ &\left(C_1 + C_3 \Delta t\, TV_{xy} w^n - \tfrac{C_2}{\Delta t} \textstyle\sum_{ij} \displaystyle\int_{\Omega_{ij}} \frac{1}{g_{ij}} \left[B(v_{ij}^{n+1}) - B(v_{ij}^n) \right] \mathrm{d}x\mathrm{d}y \right) (1 + C\Delta t). \end{aligned} \tag{34}$$

Multiplying this by Δt at $t = t_{n+1}$, and summing over n gives,

$$
\begin{aligned}
&\sum_{n=1}^{N} [\Delta t\, TV_{xy} v^n] \qquad (35)\\
&\leq C(1 + C\Delta t)T - C_2(1 + C\Delta t) \textstyle\sum_{ij} \frac{1}{g_{ij}} \left[B(v_{ij}^N) - B(v_{ij}^0)\right] \Delta x \Delta y \\
&\quad + (1 + C\Delta t)\Delta t C_3 \sum_{n=1}^{N} \Delta t\, TV_{xy} w^n \\
&\leq CT + C \textstyle\sum_{ij} \frac{1}{g_{ij}} B(v_{ij}^0)\Delta x \Delta y + C \leq CT + C \frac{\|F(v^0)\|_\infty \|v^0\|_\infty}{\epsilon} \|\Omega\| + C \leq C,
\end{aligned}
$$

where we used $0 \leq B(v^0) \leq \|F(v^0)\|_\infty \|v^0\|_\infty$ and

$$
\Delta t \sum_{n=1}^{N} \Delta t\, TV_{xy} w^n \leq C \sum_n \sum_{ij} \left(\left| w_{i+1,j}^n - w_{i,j}^n \right| + \left| w_{i,j+1}^n - w_{i,j}^n \right| \right) \Delta x \Delta y \Delta t \leq C,
$$

due to the uniform boundedness of w_{ij}^n and $\Delta t = C\Delta x = C\Delta y$. Estimating $TV_{xy} w$, we substitute (34) into (29), to obtain

$$
\begin{aligned}
&TV_{xy} w(t) \leq TV_{xy} w^n + \\
&C\Delta t \left(C_1 + C_3 \Delta t\, TV_{xy} w^n - \tfrac{C_2}{\Delta t} \textstyle\sum_{ij} \displaystyle\int_{\Omega_{ij}} \frac{1}{g_{ij}} \left[B(v_{ij}^{n+1}) - B(v_{ij}^n) \right] \mathrm{d}x\mathrm{d}y \right) (1 + C\Delta t).
\end{aligned}
$$

Putting $t = t_N$, applying recursion on n and applying the same techniques as before gives

$$
TV_{xy} w^N \leq TV_{xy} w^0 + C \leq C. \; \square \qquad (36)
$$

The TV boundedness property of Lemma 19 can be rephrased as follows.

Lemma 20 *Let $v_{\Delta t}$ denote the approximate solution defined by Def. 5. Then*

$$
\int_0^T \int_\Omega |v_{\Delta t}(x + k\Delta x, y + l\Delta y, t) - v_{\Delta t}(x, y, t)| \,\mathrm{d}x\mathrm{d}y\mathrm{d}t \leq C(k\Delta x + l\Delta y), \quad (37)
$$

holds for $k, l = 1, 2, \ldots$. H,ere C only depends on the domain, on a and b, and on $\|w^0\|_\infty$, $\|v_I\|_\infty$ and $\|v^0\|_\infty$.

With respect to the t-variable, the following L_1-Hölder continuity can be proved.

Lemma 21 *Let $v_{\Delta t}, w_{\Delta t}$ denote the approximate solution defined by Definition 5, (15). Then*

$$\int_0^T \int_\Omega |v_{\Delta t}(x,y,t+k\Delta t) - v_{\Delta t}(x,y,t)| \,\mathrm{d}x\mathrm{d}y\mathrm{d}t \le C\sqrt{k\Delta t}, \tag{38}$$

$$\int_0^T \int_\Omega |w_{\Delta t}(x,y,t+k\Delta t) - w_{\Delta t}(x,y,t)| \,\mathrm{d}x\mathrm{d}y\mathrm{d}t \le Ck\Delta t. \tag{39}$$

uniformly for k, where C only depends on the domain, on a and b and on $\|v_I\|_\infty$ and $\|v^0\|_\infty$.

PROOF. The result for w follows directly from (25). The proof for v is based on the Kružkov argument in [5]. Due to the strong Lipschitz continuity of the solution of the hyperbolic problem and the properties of the projection, (13), we have that

$$\sum_{ij} \int_{\Omega_{ij}} \frac{1}{g_{ij}} \left[F(v_{ij}^{n+\frac{1}{3}}) - F(\widetilde{v}^{n+\frac{1}{3}}(x,y)) \right] \phi_h \mathrm{d}x\mathrm{d}y = 0, \tag{40}$$

and

$$\sum_{ij} \int_{\Omega_{ij}} \frac{1}{g_{ij}} \left[F(\widetilde{v}^{n+\frac{1}{3}}(x,y)) - F(v_{ij}^{n}) \right] \phi_h \mathrm{d}x\mathrm{d}y \le C\|\phi\|_\infty \Delta t, \tag{41}$$

where ϕ is a smooth function and where we consider its piecewise constant approximation $\phi_h \equiv \phi_{\Delta x,\Delta t} = \phi_{ij}$, for $(x,y) \in \Omega_{ij}$. Now, for the parabolic step we multiply both sides of (21) by ϕ_{ij} and sum up over i and j. Using the notation (18) and applying Abel's summation, we get

$$\begin{aligned}
&\sum_{ij} \int_{\Omega_{ij}} \frac{1}{g_{ij}} \left[F(v_{ij}^{n+\frac{2}{3}}) - F(v_{ij}^{n+\frac{1}{3}}) \right] \phi_h \mathrm{d}x\mathrm{d}y && (42)\\
&\le \Delta t \left| \sum_{ij} \left[a_{ij} [D_{ij}^i v^{n+\frac{2}{3}}] D_{ij}^i \phi_h + b_{ij} [D_{ij}^j v^{n+\frac{2}{3}}] D_{ij}^j \phi_h \right] \Delta x \Delta y \right| \\
&\le \Delta t C \max\left(\|D^x \phi_h\|_\infty, \|D^y \phi_h\|_\infty \right) TV_{xy} v^{n+\frac{2}{3}} \\
&\le C\Delta t \|\nabla \phi_h\|_\infty TV_{xy} v^{n+\frac{2}{3}} \le C\Delta t \|\nabla \phi\|_\infty TV_{xy} v^{n+\frac{2}{3}}. && (43)
\end{aligned}$$

Here, we used the properties of a and b, and the fact that $\phi_h \to \phi$ for $\Delta t \to 0$, dropping higher order terms in Δt. It remains to consider the sorption. From (26), by the Lipschitz continuity of ψ_n and by the boundedness of v and w, it follows

$$\begin{aligned}
F(v(t_{n+1}) - F(v^{n+\frac{2}{3}}) \le |F(v(t_{n+1}) - F(v^{n+\frac{2}{3}})| \le |w^n|(1 - e^{-\kappa \Delta t}) \\
+ \kappa L \int_{t_n}^{t_{n+1}} e^{-\kappa(t-s)} |v(s)| \,\mathrm{d}s \le \kappa(1+L) C \Delta t. \quad (44)
\end{aligned}$$

The above is valid for the exact solution $v(t_{n+1})$ of the integral equation. However, the same holds for the numerical approximation v^{n+1} as the linear interpolant of $\psi_n(v(s))$ can be bounded in the same way. Therefore, we have $\|F(v^{n+1}) - F(v^{n+\frac{2}{3}})\|_1 \le C\Delta t$ and

$$\sum_{ij}\int_{\Omega_{ij}} \frac{1}{g_{ij}}\left[F(v_{ij}^{n+1}) - F(v_{ij}^{n+\frac{2}{3}})\right]\phi_h \mathrm{d}x\mathrm{d}y \le C\|\phi\|_\infty \Delta t. \tag{45}$$

From the first equality of (25) it immediately follows that also $\|w^{n+1} - w^n\|_1 \le C\Delta t$. We used $w^{n+1} \equiv w^{n+\frac{2}{3}}$, $w^{n+\frac{1}{3}} \equiv w^n$. Combining the four steps (43), (40), (41) and (45) and repeating the argument for time steps $n+1,\dots,n+k$, we find,

$$\sum_{ij}\int_{\Omega_{ij}} \frac{\phi_h}{g_{ij}}\left[F(v_{ij}^{n+k}) - F(v_{ij}^{n})\right]\mathrm{d}x\mathrm{d}y \le C\Delta t(\|\phi\|_\infty k + \|\nabla\phi\|_\infty \sum_{i=1}^{k} TV(v^{n+i-\frac{1}{3}})).$$

Multiplying by Δt, summing on n, we get

$$\int_0^T\int_\Omega \frac{\phi}{g}\left[F(v_{\Delta t}(x,y,t+k\Delta t)) - F(v_{\Delta t}(x,y,t))\right]\mathrm{d}x\mathrm{d}y\mathrm{d}t \le C(\|\phi\|_\infty + \|\nabla\phi\|_\infty)k\Delta t. \tag{46}$$

Here, we used the fact that $\sum_{i=1}^k \Delta t \sum_{n=1}^N TV_{xy} v^{n+i-\frac{1}{3}}\Delta t \le kC\Delta t$, which can be obtained applying the same reasoning as was used in Lemma 19. Changing the summation into integrals, numerical errors are introduced (e.g. when g_{ij} is replaced by $g(x,y)$). However, these go to zero as $\Delta x \to 0$.

For a special choice of ϕ (see [13,9]), (46) results in

$$\int_0^T\int_\Omega \frac{1}{g}\left|F(v_{\Delta t}(x,y,t+k\Delta t)) - F(v_{\Delta t}(x,y,t))\right|\mathrm{d}x\mathrm{d}y\mathrm{d}t \le C\sqrt{k\Delta t}.$$

Recall that $v_{\Delta t}$ is bounded. Use the fact that $TV_{xy}v \le C\,TV_{xy}F(v)$, $(F'(v) \ge \frac{1}{C})$, and notice that $g < C$. We conclude that

$$\int_0^T\int_\Omega \left|v_{\Delta t}(x,y,t+k\Delta t) - v_{\Delta t}(x,y,t)\right|\mathrm{d}x\mathrm{d}y\mathrm{d}t \le C\sqrt{k\Delta t}. \ \square$$

3.5 Compactness

Now we modify $v_{\Delta t}$ and $w_{\Delta t}$ by new functions which reflect the realization of all phenomena (transport, diffusion, reaction) in the time interval Δt. We define $v_\nu(x,y,t)$ as (see [10])

$$v_\nu(x,y,t) = \begin{cases} \mathcal{T}_{\Delta xy}(3(t-t_n))v^n(x,y), & t \in [t_n, t_{n+\frac{1}{3}}) \\ \mathcal{D}_{\Delta xy}(3(t-t_{n+\frac{1}{3}}))v^{n+\frac{1}{3}}(x,y), & t \in [t_{n+\frac{1}{3}}, t_{n+\frac{2}{3}}), \\ \mathcal{A}_{\Delta xy}(3(t-t_{n+\frac{2}{3}}))v^{n+\frac{2}{3}}(x,y), & t \in [t_{n+\frac{2}{3}}, t_{n+1}), \end{cases}$$

for $n = 0, \ldots, N-1$,where v^n is the solution obtained at time t_n and $v^{n+\frac{1}{3}} = \pi \mathcal{T}_{\Delta xy}(3(t_{n+\frac{1}{3}} - t_n))v^n(x,y) = \pi \widetilde{v}^{n+\frac{1}{3}}(x,y)$. Here, we indicate by ν the discretization parameters, $\nu \equiv \nu(\Delta t)$. Furthermore, $t_{n+\frac{1}{3}} = t_n + (t_{n+1} - t_n)/3$, $t_{n+\frac{2}{3}} = t_n + 2(t_{n+1} - t_n)/3$. Next, define $w_\nu(x,y,t)$ as

$$w_\nu(x,y,t) = \begin{cases} \mathcal{T}_{\Delta xy}(3(t-t_n))w^n(x,y) \equiv w^n(x,y), & t \in [t_n, t_{n+\frac{1}{3}}) \\ \mathcal{D}_{\Delta xy}(3(t-t_{n+\frac{1}{3}}))w^n(x,y) \equiv w^n(x,y), & t \in [t_{n+\frac{1}{3}}, t_{n+\frac{2}{3}}) \\ \mathcal{A}_{\Delta xy}(3(t-t_{n+\frac{2}{3}}))w^n(x,y), & t \in [t_{n+\frac{2}{3}}, t_{n+1}), \end{cases}$$

where w^n is the solution obtained at time t_n and $w^{n+1} = \mathcal{A}_{\Delta xy}(3(t_{n+1} - t_{n+\frac{2}{3}}))w^n(x,y)$. This definition corresponds to the fact that the unknown w is changing only in one part of the splitting process. We further write $\tau_n = t_{n+1} - t_n$. All results obtained for $(v_{\Delta t}, w_{\Delta t})$ are also valid for (v_ν, w_ν). We can state:

Lemma 22 *If $\Delta t \to 0$, then there exists a subsequence $v_{\nu_j}(x,y,t)$ of the sequence $v_\nu(x,y,t)$ such that $v_{\nu_j} \to v$ for $j \to \infty$ in $L_{1,\mathrm{loc}}(\Omega \times I)$, $\Omega \times I = (x^{(1)}, x^{(2)}) \times (y^{(1)}, y^{(2)}) \times (0,T)$. Similarly, we can find a subsequence $w_{\nu_j}(x,y,t)$ of $w_\nu(x,y,t)$ such that $w_{\nu_j} \to w$ for $j \to \infty$ in $L_{1,\mathrm{loc}}(\Omega \times I)$*

PROOF. Lemma 19 implies that $v_\nu(x,y,t)$ is uniformly bounded. From Lemmas 19-21 it follows that $\int_0^T \int_\Omega |v_\nu(x+k\Delta x, y+l\Delta y, t+m\Delta t) - v_\nu(x,y,t)| \mathrm{d}x\mathrm{d}y\mathrm{d}t \leq C(k\Delta x + l\Delta y + \sqrt{m\Delta t})$,. Thus, the condition of the compactness criterion in the Riesz-Fréchet-Kolmogorov theorem is satisfied. Consequently, there exists a subsequence $v_{\nu_j}(x,y,t)$ that converges to some $v(x,y,t)$ in $L_{1,\mathrm{loc}}(\Omega \times I)$.

Lemmas 19, 21 give all necessary results for w_ν too. Then, in an analogous way, we can prove the existence of $w_{\nu_j}(x,y,t)$ converging to some $w(x,y,t)$ in $L_{1,\mathrm{loc}}(\Omega \times I)$. $\square$

Remark 23 *We emphasize the fact that the convergence is in $L_{1,\mathrm{loc}}(\Omega \times I)$. Hence, nothing can be said on the value of v on the boundary or about its derivatives. Therefore, the local, very weak formulation is consistent with our approach for proving the convergence result.*

We now prove Theorem 6:

PROOF. Lemma 22 states that subsequences $\{v_\nu\}_{\Delta_t>0}$ and $\{w_\nu\}_{\Delta_t>0}$ converge to some $v(x,y,t)$ and $w(x,y,t)$, respectively. To complete the convergence proof (in the case of a unique local, very weak solution of **(P)**) for the splitting procedure, it is now sufficient to show that this limit is the very weak solution (6)-(7) of problem **(P)**.

Consider test functions $\phi(x,y,t) \in C^\infty(\Omega \times I)$, with compact support away from the the outflow boundary. At the inflow boundary, $y = y^{(2)}$, we impose $\partial_y \phi\Big|_{y=y^{(2)}} = 0$ and at the no-flow boundary we impose $\partial_x \phi\Big|_{x=x^{(1)}} = 0 = \partial_x \phi\Big|_{x=x^{(2)}}$. Furthermore, we require $\phi(x,y,T) = 0$. We also consider the test functions $\eta \in C^\infty(\Omega \times I)$ with $\eta(T) = 0$. The variational formulation is then given by (6)-(7), adapted as mentioned in Def. 2. We have to show that the limit functions $v(x,y,t)$ and $w(x,y,t)$ satisfy (6)-(7). We use ideas from [10,5].

We begin with the transport part for $t \in (t_n, t_{n+\frac{1}{3}})$ and consider the new variable $z = 3(t - t_n)$, together with the accompanying transformation of the test function $\overline{\phi}(x,y,z) = \phi(x,y,\frac{z}{3} + t_n)$. Write formally $v_\nu(u,v,t) = v^n_{\mathcal{T}}(3(t-t_n))$, where $v^n_{\mathcal{T}}(t) = \mathcal{T}_{\Delta y}(t) v^n(x,y)$. In the considered time interval, v_ν is the exact solution of the transport problem (8) with as the initial state the piecewise constant function v^n, and with the inflow condition $v(x,y^{(2)},t) = v_I(x,y^{(2)},t)$. We denote by $v_{\Delta t,M,tr}(x,y^{(2)},t)$ the value on the outflow boundary during the transport step. We can write

$$
\begin{aligned}
&\int_\Omega \int_{t_n}^{t_{n+\frac{1}{3}}} \left(\frac{1}{3} \frac{F(v_\nu) + w_\nu}{g} \partial_t \phi - v_\nu \nabla \cdot \left(\vec{h}\phi\right) \right) d\Omega \, dt \\
&= \int_\Omega \int_0^{\tau_n} \left(\frac{F\left(v^n_{\mathcal{T}}(z)\right)}{g} \partial_z \overline{\phi} - v^n_{\mathcal{T}}(z) \nabla \cdot \left(\vec{h}\overline{\phi}\right) \right) d\Omega \, \frac{1}{3} dz \\
&\quad + \int_\Omega \frac{1}{3} \frac{w_n}{g} \int_{t_n}^{t_{n+\frac{1}{3}}} \partial_t \phi \, d\Omega \, dt \\
&= \frac{1}{3} \int_\Omega \frac{F\left(v^n_{\mathcal{T}}(z)\right)}{g} \overline{\phi} \Bigg|_{z=0}^{z=\tau_n} d\Omega - \frac{1}{3} \int_0^{\tau_n} \int_{x^{(1)}}^{x^{(2)}} h_2 v^n_{\mathcal{T}}(z) \overline{\phi} \Bigg|_{y=y^{(1)}}^{y=y^{(2)}} dz \\
&\quad + \frac{1}{3} \int_\Omega \frac{w_n}{g} \left(\phi(t_{n+\frac{1}{3}}) - \phi(t_n) \right) d\Omega
\end{aligned}
$$

$$
\begin{aligned}
&= \frac{1}{3}\int_\Omega \frac{F\left(\widetilde{v}^{n+\frac{1}{3}}\right)}{g}\phi(t_{n+\frac{1}{3}})\,d\Omega - \frac{1}{3}\int_\Omega \frac{F\left(v_\nu(t_n)\right)}{g}\phi(t_n)\,d\Omega \\
&-\frac{1}{3}\int_{t_n}^{t_{n+1}}\int_{x^{(1)}}^{x^{(2)}} h_2 v_I(x,y^{(2)},\tilde{t})\phi(\frac{\tilde{t}-t_n}{3}+t_n)\,dx\,d\tilde{t} \\
&+\frac{1}{3}\int_{t_n}^{t_{n+1}}\int_{x^{(1)}}^{x^{(2)}} h_2 v_{\Delta t,M,tr}(x,y^{(1)},\tilde{t})\phi(\frac{\tilde{t}-t_n}{3}+t_n)\,dx\,d\tilde{t} \\
&+\frac{1}{3}\int_\Omega \frac{w_n}{g}\left(\phi(t_{n+\frac{1}{3}})-\phi(t_n)\right)\,d\Omega. \qquad (47)
\end{aligned}
$$

The term containing $v_{\Delta t,M,tr}$ is 0 due to the compact support of ϕ near the outflow boundary. Above we can replace $\phi(\frac{\tilde{t}-t_n}{3}+t_n)$ by $\phi(\tilde{t})$, adding $\mathcal{O}(\Delta t^2)$ to the equality. For this equality, we use $\tilde{t}=3(t-t_n)+t_n$ and $\phi\in C^1(\Omega\times I)$. Hence, $\phi(\frac{\tilde{t}-t_n}{3}+t_n)=\phi(\tilde{t})+\mathcal{O}(\Delta t)$ for $\tilde{t}\in(t_n,t_{n+1})$. The error goes to zero, even after summation over n (i.e. $\sum_n(\Delta t)^2\to 0$). Therefore, we may drop the error term.

We now turn our attention to the diffusion part over the time interval $(t_{n+\frac{1}{3}}, t_{n+\frac{2}{3}})$ with initial state $v^{n+\frac{1}{3}}$. This corresponds to the scheme (21). Multiply both sides of (21) with $\phi_{ij}=\phi(x_i,y_j,t_{n+\frac{1}{3}})$ and sum over i and j. Using the standard notation (18) and putting $\phi_{ij}^{n+\frac{2}{3}}=\phi(x_i,y_j,t_{n+\frac{2}{3}})$, we obtain that

$$
\begin{aligned}
I := \sum_{i=0}^{N_1}\sum_{j=0}^{N_2}\Bigg[&\frac{\Delta x\Delta y}{g_{ij}}\frac{F(v_{ij}^{n+\frac{2}{3}})-F(v_{ij}^{n+\frac{1}{3}})}{\tau_n}\phi_{ij} - \phi_{ij}\left(a_{i+1,j}\frac{v_{i+1,j}^{n+\frac{2}{3}}-v_{ij}^{n+\frac{2}{3}}}{\Delta x}\Delta y\right. \\
&\left.-a_{i,j}\frac{v_{i,j}^{n+\frac{2}{3}}-v_{i-1,j}^{n+\frac{2}{3}}}{\Delta x}\Delta y\right) - \phi_{ij}\left(b_{i,j+1}\frac{v_{i,j+1}^{n+\frac{2}{3}}-v_{ij}^{n+\frac{2}{3}}}{\Delta x}\Delta x - b_{i,j}\frac{v_{i,j}^{n+\frac{2}{3}}-v_{i,j-1}^{n+\frac{2}{3}}}{\Delta y}\Delta x\right)\Bigg] \\
&= 0.
\end{aligned}
$$

Rearranging the first term and applying Abel's summation on the last two terms, give

$$
\begin{aligned}
I = \sum_{i=0}^{N_1}\sum_{j=0}^{N_2}\frac{\Delta x\Delta y}{g_{ij}}&\left(-\frac{\phi_{ij}^{n+\frac{2}{3}}-\phi_{ij}}{\tau_n}F(v_{ij}^{n+\frac{2}{3}}) + \frac{F(v_{ij}^{n+\frac{2}{3}})\phi_{ij}^{n+\frac{2}{3}}}{\tau_n} - \frac{F(v_{ij}^{n+\frac{1}{3}})\phi_{ij}}{\tau_n}\right) \\
&+\sum_{i=1}^{N_1}\sum_{j=0}^{N_2}\frac{\phi_{ij}-\phi_{i-1,j}}{\Delta x}a_{i,j}\frac{v_{i,j}^{n+\frac{2}{3}}-v_{i-1,j}^{n+\frac{2}{3}}}{\Delta x}\Delta x\Delta y \\
&+\sum_{i=0}^{N_1}\sum_{j=1}^{N_2}\frac{\phi_{ij}-\phi_{i,j-1}}{\Delta y}b_{i,j}\frac{v_{i,j}^{n+\frac{2}{3}}-v_{i,j-1}^{n+\frac{2}{3}}}{\Delta y}\Delta x\Delta y = 0, \qquad (48)
\end{aligned}
$$

where we used $a_{0,j} = a_{N_1+1,j} = 0 = b_{i,0} = b_{i,N_2+1}$ because of the homogeneous Neumann boundary condition. We again apply Abel's summation on the second and third double sum of (48), to obtain

$$
\begin{aligned}
I = &\sum_{i=0}^{N_1}\sum_{j=0}^{N_2} \frac{\Delta x \Delta y}{g_{ij}} \left(-\frac{\phi_{ij}^{n+\frac{2}{3}} - \phi_{ij}}{\tau_n} F(v_{ij}^{n+\frac{2}{3}}) + \frac{F(v_{ij}^{n+\frac{2}{3}})\phi_{ij}^{n+\frac{2}{3}}}{\tau_n} - \frac{F(v_{ij}^{n+\frac{1}{3}})\phi_{ij}}{\tau_n} \right) \\
&- \sum_{i=2}^{N_1}\sum_{j=0}^{N_2} \left(a_{i,j}\frac{\phi_{ij} - \phi_{i-1,j}}{\Delta x} - a_{i-1,j}\frac{\phi_{i-1,j} - \phi_{i-2,j}}{\Delta x} \right) \frac{v_{i-1,j}^{n+\frac{2}{3}}}{\Delta x} \Delta x \Delta y \\
&- \sum_{i=0}^{N_1}\sum_{j=2}^{N_2} \left(b_{i,j}\frac{\phi_{ij} - \phi_{i,j-1}}{\Delta y} - b_{i,j-1}\frac{\phi_{i,j-1} - \phi_{i,j-2}}{\Delta y} \right) \frac{v_{i,j-1}^{n+\frac{2}{3}}}{\Delta y} \Delta x \Delta y \\
&+ \sum_{j=0}^{N_2} a_{N_1,j}\frac{\phi_{N_1,j} - \phi_{N_1-1,j}}{\Delta x}\frac{v_{N_1,j}}{\Delta x} - \sum_{j=0}^{N_2} a_{1,j}\frac{\phi_{1,j} - \phi_{0,j}}{\Delta x}\frac{v_{0,j}^{n+\frac{2}{3}}}{\Delta x} \\
&+ \sum_{i=0}^{N_1} b_{i,N_2}\frac{\phi_{i,N_2} - \phi_{i,N_2-1}}{\Delta y}\frac{v_{i,N_2}^{n+\frac{2}{3}}}{\Delta y} - \sum_{i=0}^{N_1} b_{i,1}\frac{\phi_{i,1} - \phi_{i,0}}{\Delta y}\frac{v_{i,0}^{n+\frac{2}{3}}}{\Delta y} = 0.
\end{aligned} \tag{49}
$$

The four single sums contain values of the solution v on the boundary. These terms are all zero for sufficiently small Δx and Δy due to the choice of ϕ. We therefore have

$$
\begin{aligned}
I = &\sum_{i=0}^{N_1}\sum_{j=0}^{N_2} \frac{\Delta x \Delta y}{g_{ij}} \left(-\frac{\phi_{ij}^{n+\frac{2}{3}} - \phi_{ij}}{\tau_n} F(v_{ij}^{n+\frac{2}{3}}) + \frac{F(v_{ij}^{n+\frac{2}{3}})\phi_{ij}^{n+\frac{2}{3}}}{\tau_n} - \frac{F(v_{ij}^{n+\frac{1}{3}})\phi_{ij}}{\tau_n} \right) \\
&- \sum_{i=1}^{N_1-1}\sum_{j=0}^{N_2} \left(a_{i+1,j}\frac{\phi_{i+1,j} - \phi_{i,j}}{\Delta x} - a_{i,j}\frac{\phi_{i,j} - \phi_{i-1,j}}{\Delta x} \right) \frac{v_{i,j}^{n+\frac{2}{3}}}{\Delta x} \Delta x \Delta y \\
&- \sum_{i=0}^{N_1}\sum_{j=1}^{N_2-1} \left(b_{i,j+1}\frac{\phi_{i,j+1} - \phi_{i,j}}{\Delta y} - b_{i,j}\frac{\phi_{i,j} - \phi_{i,j-1}}{\Delta y} \right) \frac{v_{i,j}^{n+\frac{2}{3}}}{\Delta y} \Delta x \Delta y = 0.
\end{aligned} \tag{50}
$$

By reordering terms, multiplying by τ_n, writing formally $v_\nu(u, v, t) = v_{\mathcal{D}}^n(3(t - t_{n+\frac{1}{3}}))$, with $v_{\mathcal{D}}^n(t) = \mathcal{D}_{\delta,\Delta x,\Delta y}(t) v^{n+\frac{1}{3}}(x, y)$, (50) can be seen as an approximation of the following equality

$$
\begin{aligned}
&\int_\Omega \int_0^{\tau_n} \left[\frac{F(v_{\mathcal{D}}^n(z))}{g} \partial_z \overline{\phi}(z) + v_{\mathcal{D}}^n(z) \left(\partial_x a \partial_x \overline{\phi}(z) - \partial_y b \partial_y \overline{\phi}(z) \right) \right] d\Omega dz \\
&\qquad = \int_\Omega \frac{F(v_{\mathcal{D}}^n(\tau_n))}{g} \overline{\phi}(\tau_n)\, d\Omega - \int_\Omega \frac{F(v_{\mathcal{D}}^n(0))}{g} \overline{\phi}(0)\, d\Omega,
\end{aligned} \tag{51}
$$

where $\overline{\phi}(x,y,z) = \phi(x,y,\frac{z}{3}+t_{n+\frac{1}{3}})$. Errors due to numerical differentiation and integration in time and space occur when passing from (50) to (51). However, these errors go to zero as $\Delta t \to 0$, also after summation on n. Therefore, we need not consider them further. As a last step we rewrite (51) as

$$\int_\Omega \int_{t_{n+\frac{1}{3}}}^{t_{n+\frac{2}{3}}} \left[\frac{1}{3}\frac{F(v_\nu(t)) + w_\nu(t)}{g}\partial_t\phi(t) + v_\nu(t)\left(\partial_x a \partial_x \phi(t) + \partial_y b \partial_y \phi(t)\right)\right] d\Omega dt$$
$$= \frac{1}{3}\int_\Omega \frac{F(v_\nu(t_{n+\frac{2}{3}}))}{g}\phi(t_{n+\frac{2}{3}})\, d\Omega - \frac{1}{3}\int_\Omega \frac{F(v^{n+\frac{1}{3}}))}{g}\phi(t_{n+\frac{1}{3}})\, d\Omega$$
$$+ \frac{1}{3}\int_\Omega \frac{w_n}{g}\left(\phi(t_{n+\frac{2}{3}}) - \phi(t_{n+\frac{1}{3}})\right) d\Omega. \quad (52)$$

The procedure is completed by handling the sorption part in a similar way. In doing so we take a local time step σ. Then, the numerical scheme for the sorption problem in point (x_i, y_j) actually has the form:

$$F(v_{ij}^{m+1}) - F(v_{ij}^m) + w_{ij}^{m+1} - w_{ij}^m = 0$$

for $m = 0, \ldots, M-1$, where $\tau_n = M\sigma$. We multiply this equation by ϕ_{ij}^m, where ϕ is a proper test function. Then we can again apply summation by parts and we obtain

$$0 = \sum_{m=0}^{M-1}\left(\frac{F(v_{ij}^{m+1}) - F(v_{ij}^m)}{\sigma} + \frac{w_{ij}^{m+1} - w_{ij}^m}{\sigma}\right)\sigma\phi_{ij}^m = \phi_{ij}^M F(v_{ij}^M) - \phi_{ij}^0 F(v_{ij}^0)$$
$$+ \phi_{ij}^M w_{ij}^M - \phi_{ij}^0 w_{ij}^0 - \sum_{m=0}^{M-1} F(v_{ij}^{m+1})\frac{\phi_{ij}^{m+1} - \phi_{ij}^m}{\sigma}\sigma - \sum_{m=0}^{M-1} w_{ij}^{m+1}\frac{\phi_{ij}^{m+1} - \phi_{ij}^m}{\sigma}\sigma$$

Multiplying by $\frac{\Delta x \Delta y}{g_{ij}}$ and summing over i and j, this can be seen as an approximation of

$$\int_\Omega \int_0^{\tau_n}\left(\frac{F(v_\mathcal{A}^n(z)) + w_\mathcal{A}^n(z)}{g}\partial_t\phi\right) dz\, d\Omega = \int_\Omega \frac{F(v^{n+1})}{g}\phi(\tau_n)\, d\Omega$$
$$- \int_\Omega \frac{F(v^{n+\frac{2}{3}})}{g}\phi(0)\, d\Omega + \int_\Omega \frac{w^{n+1}}{g}\phi(\tau_n)\, d\Omega - \int_\Omega \frac{w^n}{g}\phi(0)\, d\Omega,$$

where we wrote symbolically $v_\mathcal{A}^n(t) = \mathcal{A}(t)v^{n+\frac{2}{3}}$ and $w_\mathcal{A}^n(t) = \mathcal{A}(t)w^n$. Here, we make an error of order $O(1)\tau^2$. We use the same argumentation as in the case of the dispersion problem and we let $\sigma \to 0$. Finally, repeating the procedure from the previous two parts we obtain

$$
\begin{aligned}
&\int_\Omega \int_{t_{n+\frac{2}{3}}}^{t_{n+1}} \frac{1}{3}\left(\frac{F(v_\nu)+w_\nu}{g}\partial_t\phi\right)\,dt\,d\Omega = \frac{1}{3}\int_\Omega \frac{F(v^{n+1})}{g}\phi(t_{n+1})\,d\Omega \\
&-\frac{1}{3}\int_\Omega \frac{F(v^{n+\frac{2}{3}})}{g}\phi(t_{n+\frac{2}{3}})\,d\Omega + \frac{1}{3}\int_\Omega \frac{w^{n+1}}{g}\phi(t_{n+1})\,d\Omega - \frac{1}{3}\int_\Omega \frac{w^n}{g}\phi(t_{n+\frac{2}{3}})\,d\Omega.
\end{aligned} \tag{53}
$$

Combining the three results by adding (47), (52), and (53) for $n = 0,\dots,N-1$, we arrive at

$$
\begin{aligned}
&\int_0^T \int_\Omega \Bigg(\tfrac{1}{3}\frac{F(v_\nu)+w_\nu}{g}\partial_t\phi - \chi_{\mathcal{T}}(t)v_\nu\nabla\cdot\left(\vec{h}\phi\right) \\
&\qquad\qquad + \chi_{\mathcal{D}}(t)v_\nu(t)\left[\partial_x a\partial_x\phi(t)+\partial_y b\partial_y\phi(t)\right]\Bigg)\,d\Omega\,dt \\
&\quad = \frac{1}{3}\int_\Omega \frac{F(v_\nu(T))+w_\nu(T)}{g}\phi(T)\,d\Omega - \frac{1}{3}\int_\Omega \frac{F(v_\nu(0))+w_\nu(0)}{g}\phi(0)\,d\Omega \\
&\qquad\qquad + \frac{1}{3}\sum_{n=0}^{N-1}\int_\Omega\left[F(\tilde{v}^{n+\frac{1}{3}})-F(v^{n+\frac{1}{3}})\right]\frac{\phi(t_{n+\frac{1}{3}})}{g}\,d\Omega \\
&\qquad\qquad\qquad - \frac{1}{3}\int_0^T\int_{x^{(1)}}^{x^{(2)}} h_2 v_I(x,y^{(2)},t)\phi(t)\,dx\,dt.
\end{aligned} \tag{54}
$$

Here, $\chi_{\mathcal{T}}(t)$ and $\chi_{\mathcal{D}}(t)$ are characteristic functions defined as

$$
\chi_{\mathcal{T}}(t) = \begin{cases} 1 \text{ for } t \in \cup_k[t_n, t_{n+\frac{1}{3}}) \\ 0 \text{ otherwise} \end{cases}, \quad \chi_{\mathcal{D}}(t) = \begin{cases} 1 \text{ for } t \in \cup_k[t_{n+\frac{1}{3}}, t_{n+\frac{2}{3}}) \\ 0 \text{ otherwise.} \end{cases}.
$$

We have (see [10,5]) that $\chi_{\mathcal{T}}(t)$ and $\chi_{\mathcal{D}}(t) \rightharpoonup \frac{1}{3}$ in $L_2(0,T)$ for $\Delta t \to 0$.

Recall further that the test function ϕ was chosen so as to satisfy $\phi(T) = 0$. Moreover, for $\Delta t \to 0$, $(n \to \infty)$, the projection error represented by the third term on the rhs of (54), tends to zero. This property follows from

$$
\begin{aligned}
&\tfrac{1}{3}\sum_{n=0}^{N-1}\int_\Omega\left[F(\tilde{v}^{n+\frac{1}{3}})-F(v^{n+\frac{1}{3}})\right]\frac{\phi(t_{n+\frac{1}{3}})}{g}\,d\Omega \\
&\qquad = \tfrac{1}{3}\sum_{n=0}^{N-1}\sum_{ij}\int_{\Omega_{ij}}\left[F(\tilde{v}^{n+\frac{1}{3}})-F(v_{ij}^{n+\frac{1}{3}})\right]\frac{\phi_{ij}(t_{n+\frac{1}{3}})}{g_{ij}}\,d\Omega \\
&+\tfrac{1}{3}\sum_{n=0}^{N-1}\sum_{ij}\int_{\Omega_{ij}}\left[F(\tilde{v}^{n+\frac{1}{3}})-F(v_{ij}^{n+\frac{1}{3}})\right]\left[\frac{\phi(t_{n+\frac{1}{3}})}{g}-\frac{\phi_{ij}(t_{n+\frac{1}{3}})}{g_{ij}}\right]\,d\Omega = I_1 + I_2.
\end{aligned}
$$

By the definition of the projection, (13), we have that $I_1 \equiv 0$, $\forall n$. For I_2 we can use the smoothness of ϕ and g with $g > \epsilon$, together with Lemma 11 and

Lemma 19, to obtain

$$\begin{aligned} I_2 \le & \tfrac{1}{2} \sum_{n=0}^{N-1} \int_\Omega \left| F(\tilde{v}^{n+\frac{1}{3}}) - F(v_{ij}^{n+\frac{1}{3}}) \right| \left[\frac{\|\nabla \phi\|_\infty}{\epsilon} + \frac{\|\phi\|_\infty \|\nabla g\|_\infty}{\epsilon^2} \right] \Delta x \, d\Omega \\ \le & \tfrac{1}{3} \sum_{n=0}^{N-1} C \Delta t \, TV_{xy} F(\tilde{v}^{n+\frac{1}{3}}) \Delta x \le C \Delta x. \end{aligned}$$

We now pass to the limit $\Delta t \to 0$ in (54), with $\Delta t = C\Delta x$. Taking into account the convergence of v_ν and w_ν to v and w in $L_{1,\text{loc}}(\Omega \times I)$, we finally obtain that the limit functions v, w satisfy (6).

We now proceed to prove that $[v, w]$ satisfy (7). We can proceed analogously. As $w_\nu(t)$ remains constant for $t \in (t_n, t_{n+\frac{2}{3}})$, for $n = 0, \dots, N-1$, we get

$$\int_\Omega \int_{t_n}^{t_{n+\frac{1}{3}}} \frac{1}{3} w_\nu \partial_t \eta \, dt \, d\Omega = \frac{1}{3} \int_\Omega \eta(x, y, t_{n+\frac{1}{3}}) w^n \, d\Omega - \frac{1}{3} \int_\Omega \eta(x, y, t_n) w^n \, dv, \quad (55)$$

and similarly

$$\int_\Omega \int_{t_{n+\frac{1}{3}}}^{t_{n+\frac{2}{3}}} \frac{1}{3} w_\nu \partial_t \eta \, dt \, d\Omega = \frac{1}{3} \int_\Omega \eta(x, y, t_{n+\frac{2}{3}}) w^n \, d\Omega - \frac{1}{3} \int_\Omega \eta(x, y, t_{n+\frac{1}{3}}) w^n \, d\Omega. \quad (56)$$

Now recall (26). More in detail, if we solve the sorption problem with a local micro-time step σ, then at any time point $\sigma_m = m\sigma$, $m = 0, \dots, l$, $l\sigma = \Delta t$, we have

$$\begin{aligned} F(v^m) &= F(v^{n+\frac{2}{3}}) + w^n - w^n e^{-\kappa \sigma_m} \qquad (57) \\ &-\kappa \sum_{i=0}^{m-1} \int_{\sigma_i}^{\sigma_{i+1}} e^{-\kappa(\sigma_m - z)} \left(\left(1 - \frac{z - \sigma_i}{\sigma} \right) \psi_n(v^i) + \frac{z - \sigma_i}{\sigma} \psi_n(v^{i+1}) \right) dz \\ w^m &= w^n e^{-\kappa \sigma_m} \\ &+\kappa \sum_{i=0}^{m-1} \int_{\sigma_i}^{\sigma_{i+1}} e^{-\kappa(\sigma_m - z)} \left(\left(1 - \frac{z - \sigma_i}{\sigma} \right) \psi_n(v^i) + \frac{z - \sigma_i}{\sigma} \psi_n(v^{i+1}) \right) dz. \end{aligned}$$

Denote by $L_i(z)$ the linear interpolant of $\psi_n(v)$ on the interval (σ_i, σ_{i+1}). We can compute

$$\begin{aligned} \frac{w^{m+1} - w^m}{\sigma} &= w^n \frac{e^{-\kappa(\sigma_m + \sigma)} - e^{-\kappa \sigma_m}}{\sigma} \\ +\kappa \sum_{i=0}^{m-1} \int_{\sigma_i}^{\sigma_{i+1}} & \frac{e^{-\kappa(\sigma_m + \sigma - z)} - e^{-\kappa(\sigma_m - z)}}{\sigma} L_i(z) \, dz + \frac{\kappa}{\sigma} \int_{\sigma_m}^{\sigma_m + \sigma} e^{-\kappa(\sigma_m + \sigma - z)} L_m(z) \, dz. \end{aligned}$$

In the above we have approximations of derivatives of $e^{-\kappa t}$, namely

$$\frac{e^{-\kappa(\sigma_m+\sigma)} - e^{-\kappa\sigma_m}}{\sigma} = -\kappa e^{-\kappa\sigma_m} + k_1\sigma,$$
$$\frac{e^{-\kappa(\sigma_m+\sigma-z)} - e^{-\kappa(\sigma_m-z)}}{\sigma} = -\kappa e^{-\kappa(\sigma_m-z)} + k_2\sigma.$$

Therefore, we can continue

$$\frac{w^{m+1} - w^m}{\sigma} = -\kappa w^n e^{-\kappa\sigma_m} - \kappa^2 \sum_{i=0}^{m-1} \int_{\sigma_i}^{\sigma_{i+1}} e^{-\kappa(\sigma_m-z)} L_i(z)\, dz$$
$$+ \frac{\kappa}{\sigma} \int_{\sigma_m}^{\sigma_m+\sigma} L_m(z)\, dz + \varepsilon_1(\sigma) + \varepsilon_2(\sigma) + \varepsilon_3(\sigma), \quad (58)$$

where $\varepsilon_1(\sigma) = k_1 w^n \sigma$, $\varepsilon_2(\sigma) = \kappa \sum_{i=0}^{m-1} \int_{\sigma_i}^{\sigma_{i+1}} k_2 \sigma L_i(z)\, dz$, and

$$\varepsilon_3(\sigma) = \frac{\kappa}{\sigma} \int_{\sigma_m}^{\sigma_m+\sigma} \left(e^{-\kappa(\sigma_m+\sigma-z)} - 1 \right) L_m(z)\, dz.$$

If we evaluate the integral of $L_m(z)$ in (58), the equation can be rewritten as

$$\frac{w^{m+1} - w^m}{\sigma} = \kappa \frac{\psi_n(v^{m+1}) + \psi_n(v^m)}{2} - \kappa w^m + \varepsilon_1 + \varepsilon_2 + \varepsilon_3. \quad (59)$$

We consider (59) in the point (x_i, y_j), and multiply it by the test function values η_{ij}^m, by $\Delta x \Delta y$ and by σ. Finally, we sum over i, j and m to obtain

$$\sum_{ij} \sum_{m=0}^{l-1} \frac{w_{ij}^{m+1} - w_{ij}^m}{\sigma} \eta_{ij}^m \sigma \Delta x \Delta y = \sum_{ij} \sum_{m=0}^{l-1} \kappa \frac{\psi_n(v_{ij}^{m+1}) + \psi_n(v_{ij}^m)}{2} \eta_{ij}^m \sigma \Delta x \Delta y$$
$$- \sum_{ij} \sum_{m=0}^{l-1} \kappa w_{ij}^m \eta_{ij}^m \sigma \Delta x \Delta y + e_1 + e_2 + e_3.$$

We apply summation by parts to the left hand side to get

$$\sum_{ij} w_{ij}^l \eta_{ij}^l \Delta x \Delta y - \sum_{ij} w_{ij}^0 \eta_{ij}^0 \Delta x \Delta y - \sum_{ij} \sum_{m=0}^{l-1} w_{ij}^{m+1} \frac{\eta_{ij}^{m+1} - \eta_{ij}^m}{\sigma} \sigma \Delta x \Delta y$$
$$= \sum_{ij} \sum_{m=0}^{l-1} \kappa \sigma \frac{\psi_n(v_{ij}^{m+1}) + \psi_n(v_{ij}^m)}{2} \eta_{ij}^m \Delta x \Delta y$$
$$- \sum_{ij} \sum_{m=0}^{l-1} \kappa w_{ij}^m \eta_{ij}^m \sigma \Delta x \Delta y + e_1 + e_2 + e_3 \quad (60)$$

This is an approximation of

$$\int_\Omega \int_0^{\tau_n} \left(w_{\mathcal{A}}^n(t) \partial_t \eta + \kappa \left(\psi_n(v_{\mathcal{A}}^n(t)) - w_{\mathcal{A}}^n(t) \right) \eta \right)\, dt\, d\Omega$$
$$= \int_\Omega w^{n+1} \eta(\tau_n)\, d\Omega - \int_\Omega w^n \eta(0)\, d\Omega + e_1 + e_2 + e_3. \quad (61)$$

Using (61), we compute

$$\begin{aligned}
&\int_\Omega \int_{t_{n+\frac{2}{3}}}^{t_{n+1}} \left(\frac{1}{3} w_\nu \partial_t \eta + \kappa \left(\psi_n(v_\nu) - w_\nu\right) \eta\right) dt\, d\Omega \\
&= \frac{1}{3} \int_\Omega \int_0^{\tau_n} \left(w_{\mathcal{A}}^n(\xi) \partial_\tau \bar{\eta} + \kappa \left(\psi_n(v_{\mathcal{A}}^n(\xi)) - w_{\mathcal{A}}^n(\xi)\right) \bar{\eta}\right) d\xi\, d\Omega \qquad (62) \\
&= \frac{1}{3} \int_\Omega \eta(t_{n+1}) w^{n+1}\, dv - \frac{1}{3} \int_\Omega \eta(t_{n+\frac{2}{3}}) w^n\, d\Omega + \frac{1}{3}(e_1 + e_2 + e_3),
\end{aligned}$$

where we have used the substitution $\xi = 3(t - t_{n+\frac{2}{3}})$ and $\bar{\eta}(x, y, t) = \eta(x, y, \xi/3 + t_{n+\frac{2}{3}})$. Finally, we complete the proof by summing up (55) , (56) and (62) for $n = 0, \ldots, N-1$, using $\eta(T) = 0$, to obtain

$$\int_\Omega \int_0^T \left(\frac{1}{3} w_\nu \partial_t \eta + \chi_{\mathcal{A}}(t) \kappa \left(\psi_n(v_\nu) - w_\nu\right) \eta\right) dt\, d\Omega - \frac{1}{3} \int_\Omega w(x, y, 0) \eta(0)\, d\Omega = E_1 + E_2 + E_3, \quad (63)$$

where we make an error of order $O(\tau)$. The characteristic function $\chi_{\mathcal{A}}(t)$ is defined as

$$\chi_{\mathcal{A}}(t) = \begin{cases} 1 \text{ for } t \in \cup_k [t_{n+\frac{2}{3}}, t_{n+1}) \\ 0 \text{ otherwise.} \end{cases}$$

We still have to examine the error terms E_1, E_2 and E_3. These were obtained from $\varepsilon_1(\sigma)$, $\varepsilon_1(\sigma)$ and $\varepsilon_1(\sigma)$ by the same operations that led first from (58) to (60) and next to (63). We have

$$E_1 = \frac{1}{3} \chi_{\mathcal{A}}(t) \sum_{ij} \sum_{m=0}^{l-1} k_1 w^n \eta_{ij}^m \sigma^2 \Delta x \Delta y.$$

As w^n is bounded, this term tends to zero as $\sigma \to 0$. We next consider E_2. Because v^i (and $\psi_n(v^i)$) are bounded we have

$$\begin{aligned}
E_2 &= \frac{1}{3} \chi_{\mathcal{A}}(t) \kappa \sum_{ij} \sum_{m=0}^{l-1} \sum_{k=0}^{m-1} \int_{\sigma_k}^{\sigma_{k+1}} k_2 \sigma L_k(z)\, dz \\
&\le \frac{1}{3} \chi_{\mathcal{A}}(t) \kappa\, C k_2 \sigma \sum_{ij} \sum_{m=0}^{l-1} \sigma_m \eta_{ij}^m \sigma \Delta x \Delta y \le C \sigma \Delta t.
\end{aligned}$$

Finally, for the term E_3 we can write

$$E_3 = \frac{1}{3} \chi_{\mathcal{A}}(t) \kappa \sum_{ij} \sum_{m=0}^{l-1} \eta_{ij}^m \sigma \Delta x \Delta y \int_{\sigma_m}^{\sigma_m + \sigma} \frac{e^{-\kappa(\sigma_m + \sigma - z)} - 1}{\sigma} L_m(z)\, dz.$$

On account of the boundedness of ψ_n we can estimate the integral as follows

$$\int_{\sigma_m}^{\sigma_m+\sigma} \frac{e^{-\kappa(\sigma_m+\sigma-z)}-1}{\sigma} L_m(z)\, dz \leq C \int_{\sigma_m}^{\sigma_m+\sigma} \frac{e^{-\kappa(\sigma_m+\sigma-z)}-1}{\sigma}\, dz = k_3\sigma$$

Therefore, we have

$$E_3 \leq \frac{1}{3}\chi_{\mathcal{A}}(t)\kappa k_3 \sum_{ij}\sum_{m=0}^{l-1} \eta_{ij}^m \sigma^2 \Delta x \Delta y$$

As $\sigma \to 0$, the right hand side approaches zero.

Summarizing, if v and w are the limits of v_ν and w_ν for $\nu \to 0$, from (63) we have the desired equality

$$\int_\Omega \int_0^T (w\partial_t \eta + \kappa\,(\psi_n(v) - w)\,\eta)\; dt\, d\Omega - \int_\Omega w(x,y,0)\eta(x,y,0)\, d\Omega = 0. \; \Box$$

This proves the existence of a local, very weak solution introduced in Def. 2.

Remark 24 *We cannot prove* BC *(4) on the outflow boundary. Instead we have from (47) that our approximate solution converges on the outflow boundary to the unknown limit function* $\lim_{\Delta t\to 0} v_{\Delta t,M,tr} = v_{M,tr}(t)$*, which, generally, cannot be related to* $v(x,y,t)$*, the concentration inside the domain. This corresponds to the natural outflow condition*

$$b\partial_y v + h_2 v = h_2 v_{M,tr},$$

indicating a continuous flux condition. However, it does not exclude that $\partial_y v = 0$*. As we consider dominant convection, we have anyway* $h_2 >> b$*.*

Remark 25 *In some practical situations, the Lipschitz continuity of* ψ_e*, (resp.* F*) cannot be guaranteed. For example, if we use Freundlich sorption isotherms of the form* $\psi(v) = av^q$*,* $0 < q < 1$*, then we have* $\psi'(0) = \infty$ *and the Lipschitz condition is not satisfied. Let us now consider the following sequence for* $\varepsilon > 0$*:*

$$F_\varepsilon(v) = F(v) \;\text{if}\; v > \varepsilon, \quad F_\varepsilon(v) = \frac{F(\varepsilon)}{\varepsilon} v \;\;\text{otherwise.}$$

$F_\varepsilon(v)$ *is Lipschitz continuous for all* ε *and it uniformly converges to* $F(v)$ *as* $\varepsilon \to 0$*. Let* $(v_\varepsilon, w_\varepsilon)$ *be the weak solution of the problem (***P***), where we use* $F_\varepsilon(v)$ *instead of* $F(v)$*. This solution is regular (*$v_\varepsilon \in L_2((0,T), W_2^1)$*,* $\partial_t v_\varepsilon \in L_2((0,T), L_2)$*,* W_2^1 *being the Sobolev space). Along the same lines as in [20] it is possible to find a subsequence* $\{\varepsilon_j\}_{j>0}$ *such that* $(v_{\varepsilon_j}, w_{\varepsilon_j})$ *is convergent in* $L_2(\Omega_T)$*. The limit is the weak solution* (v, w) *of the original problem (***P***).*

4 Numerical experiments

Before an analysis of the method from the theoretical point of view existed, it was extensively tested. A large amount of numerical experiments for both forward and inverse problems was realized. Some of them were published e.g. in [2], [21]. At this point we present only one linear example with non-equilibrium sorption of which the analytical solution is known, as the intention of this paper was to provide the theoretical results. In the experiment presented here, we consider a one-dimensional problem of the form

$$\partial_t C + 2\partial_x C - D\partial_x^2 C + \partial_t S = 0 \quad \partial_t S = \kappa(C - S)$$

with the following boundary conditions and initial conditions

$$C(0,t) = C_I(t) \equiv 1 \qquad C(x,0) = 0, \quad S(x,0) = 0 \tag{64}$$

In this simple case, it is possible to find an analytical solution of the problem (see [22], where the solution is over a semi-infinite domain $[0,\infty)$). The comparison between the splitting scheme and the analytical solution can be seen in Fig. 1. We also add a comparison with two finite difference schemes, namely an implicit upwind and an exponential upwind method. As we can see, the splitting method leads to results with lower numerical dispersion.

As for the parameters, we set the sorption rate coefficient $\kappa = 6.95$ and take as the diffusion coefficients $D = 0.1$ and 0.01, respectively. We use the value 0.08 for the space step for both finite difference and operator splitting schemes. We take an operator splitting time step of $\Delta t = 0.04$ and $\Delta t = 0.02$, respectively. Hence, no projection error occurs after transport for the first experiment, resulting in a very exact approximation. The second experiment clearly shows that even with a projection step adding numerical dispersion, the operator splitting is better suited for the problem at hand than the upwind schemes. In this second experiment, $D << 2$, and numerical dispersion in the upwind methods overshadows the low diffusion coefficient completely.

Next, we present two tables showing the convergence as the mesh size is decreased. For this the Courant number is fixed to be 0.5. In Table 1 the experimental order of convergence (EOC) is given for the operator splitting, as well as for the upwind scheme. The proof of convergence given does not provide a theoretical prediction of the rate of convergence. In this case we can see that it is of order 1. This order is typical for an operator splitting method. Obviously, it is possible to use a higher order upwind scheme, but this does not imply that the operator splitting approach is not suitable for practical applications. In the case of dominant advection, focused upon in the introduction, splitting is a very attractive method to avoid small time steps while retaining high accuracy. Even if the convergence is only of first order, the error made on the

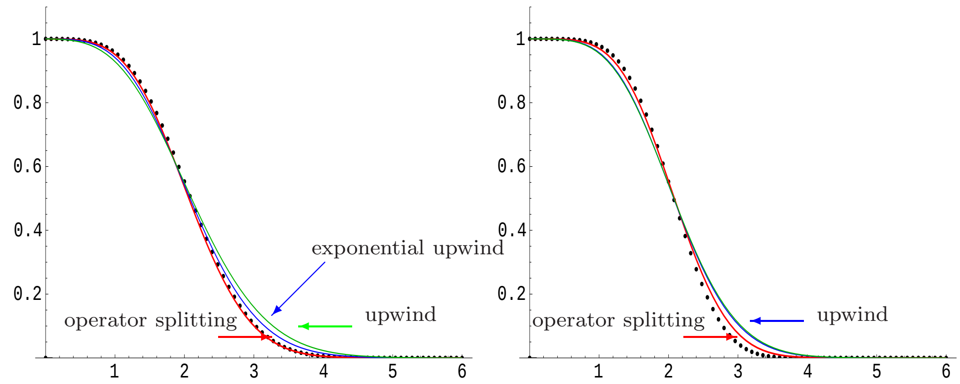

Fig. 1. Comparison of the operator splitting and upwind schemes with the analytical solution (dotted line) at $t = 2s$, $\Delta x = 0.08$. Left: $D = 0.1$, $\Delta t = 0.04$. Right: $D = 0.01$, $\Delta t = 0.02$.

Δx	$L_2((0,T), L_2(\Omega))$-error	EOC
0.08	0.06027	
0.04	0.03084	0.9668
0.02	0.01561	0.9820
0.01	0.00793	0.9771
0.005	0.00401	0.9820

Δx	$L_2((0,T), L_2(\Omega))$-error	EOC
0.08	0.13162	
0.04	0.07037	0.9034
0.02	0.03658	0.9440
0.01	0.01869	0.9688
0.005	0.00948	0.9788

Table 1
Left: Experimental order of convergence for the operator splitting method. Right: Experimental order of convergence for the upwind scheme

larger time step is very small in all subproblems, if higher order methods are applied for those problems. Splitting also has the advantage that well established toolboxes can be used to solve the subproblems, as opposed to codes that solve the global problem.

Remark 26 *The practical implementation in [3,2] benefits strongly from the operator splitting scheme as, in essense, the problem is 1D in the convective part, and 2D in the diffusion. For multi-dimensional flow problems, one could instead use operator splitting between diffusion-convection and adsorption, using an upwind method to control the convective part. Operator splitting between diffusion and convection is possible, but the authors are aware of the fact that multi-dimensional front tracking is more cumbersome and increases the numerical dispersion. Nevertheless, front tracking is used in many practical applications, [5].*

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