A DIFFERENCE SCHEME FOR A DEGENERATING CONVECTION-DIFFUSION-REACTION SYSTEM MODELLING CONTINUOUS SEDIMENTATION

RAIMUND BÜRGER¹, STEFAN DIEHL² AND CAMILO MEJÍAS¹

Abstract. Continuously operated settling tanks are used for the gravity separation of solid-liquid suspensions in several industries. Mathematical models of these units form a topic for well-posedness and numerical analysis even in one space dimension due to the spatially discontinuous coefficients of the underlying strongly degenerate parabolic, nonlinear model partial differential equation (PDE). Such a model is extended to describe the sedimentation of multi-component particles that react with several soluble components of the liquid phase. The fundamental balance equations contain the mass percentages of the components of the solid and liquid phases. The equations are reformulated as a system of nonlinear PDEs that can be solved consecutively in each time step by an explicit numerical scheme. This scheme combines a difference scheme for conservation laws with discontinuous flux with an approach of numerical percentage propagation for multi-component flows. The main result is an invariant-region property, which implies that physically relevant numerical solutions are produced. Simulations of denitrification in secondary settling tanks in wastewater treatment illustrate the model and its discretization.

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1. INTRODUCTION

1.1. Scope

The separation of fine solid particles from a liquid by gravity under continuous flows in and out of large tanks is a unit operation in wastewater treatment, mineral processing, hydrometallurgy, and other applications. Since gravity acts in one dimension and computational resources for simulations are limited, spatially onedimensional models are common. The continuous sedimentation of a suspension subject to applied feed and bulk flows, hindered settling and sediment compressibility can be modelled by a nonlinear, strongly degenerate

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 $^{^1~{\}rm CI}^2{\rm MA}$ and Departamento de Ingeniería Matemática, Facultad de Ciencias Físicas y Matemáticas, Universidad de Concepción, Casilla 160-C, Concepción, Chile.

² Centre for Mathematical Sciences, Lund University, P.O. Box 118, S-221 00 Lund, Sweden.

^{*} Corresponding author: diehl@maths.lth.se

parabolic PDE for the solids concentration X = X(z,t) as a function of depth z and time t [12]. This PDE is based on the solid and liquid mass balances, and its coefficients depend discontinuously on z.

Important applications also involve chemical reactions between different components of the solid and liquid phases. In wastewater treatment, there are biokinetic reactions between flocculated activated sludge (bacteria) and substrates (nutrients) dissolved in the liquid. This work combines the model of continuous sedimentation with compression [12] with a description of the transport and reaction of these components. The final model can be written as the system of PDEs

$$\frac{\partial X}{\partial t} + \frac{\partial}{\partial z} \left(\mathcal{F}(X, z, t) - \gamma(z) \partial_z D(X) \right) = \mathcal{A}_X(X, \boldsymbol{p}_X, \bar{\boldsymbol{p}}_L, z, t),$$
(1.1a)

$$\frac{\partial(\boldsymbol{p}_X X)}{\partial t} + \frac{\partial}{\partial z} \Big(\boldsymbol{p}_X \big(\mathcal{F}(X, z, t) - \gamma(z) \partial_z D(X) \big) \Big) = \mathcal{A}_X (X, \boldsymbol{p}_X, \bar{\boldsymbol{p}}_L, z, t),$$
(1.1b)

$$\frac{\partial(\bar{\boldsymbol{p}}_L l_1(X))}{\partial t} + \frac{\partial}{\partial z} \Big(\bar{\boldsymbol{p}}_L l_2 \big(\mathcal{F}(X, z, t) - \gamma(z) \partial_z D(X), z, t \big) \Big) = \mathcal{A}_L(X, \boldsymbol{p}_X, \bar{\boldsymbol{p}}_L, z, t)$$
(1.1c)

for $z \in \mathbb{R}$ and t > 0, along with suitable initial conditions. The convective flux function \mathcal{F} describes the bulk flow and hindered settling, while the function D accounts for sediment compressibility. The characteristic function γ distinguishes between the interior and the exterior of the settling tank, *i.e.*, $\gamma(z) = 1$ if -H < z < B and $\gamma(z) = 0$ outside; see Figure 1a. Both \mathcal{F} and D depend nonlinearly on X and discontinuously on z, and it is assumed that D = 0 on an X-interval of positive length, so the model is strongly degenerate and its solutions will, in general, be discontinuous. Moreover, $\mathbf{p}_X = \mathbf{p}_X(z,t)$ and $\bar{\mathbf{p}}_L = \bar{\mathbf{p}}_L(z,t)$ are vectors of unknown (mass) percentages of components of the solid and liquid phases, l_1 and l_2 are certain given functions, and \mathcal{A}_X , \mathcal{A}_X and \mathcal{A}_L are algebraic expressions that stand for given feed and reaction terms. (Precise definitions and assumptions are provided in Sect. 2.)

We herein derive the new model (1.1) from volume and mass balances and common constitutive assumptions on the relative velocity between the two phases and on the reactions between components. One can insert any suitable constitutive functions that model the effects of hindered settling, compression and biochemical reactions. The model equations are written in a form suitable for explicit numerical methods where the equations in (1.1)are solved consecutively. We derive a difference scheme that combines the approach of [9,12] for the non-reactive case (*i.e.*, suitable for (1.1a) in the absence of reactions) with the numerical percentage transport introduced in [16] for a related multi-component, non-reactive model. The main mathematical result is an invariant-region principle proved under a suitable CFL condition. This result ensures that numerical solutions are physically relevant and, in particular, non-negative. Several examples illustrate the predictions of the new model and the convergence property of the scheme.

1.2. Related work

For the non-reactive case, the first model for the hyperbolic case $(D \equiv 0)$ [15] described hindered settling, and was extended in [12] by a strongly degenerating diffusion function $D \neq 0$ to include sediment compression at high solids concentrations. The discontinuous dependence of \mathcal{F} on z and the presence of $\gamma(z)$ arise from the description of the inlet and outlet streams of the sedimentation tank. Therefore, in the non-reactive case, (1.1a) represents an application of the theory of first-order conservation laws with discontinuous flux and its extensions to degenerate parabolic PDEs. It is well known that solutions of such equations are in general discontinuous and need to be defined as weak solutions along with a selection criterion or entropy condition to ensure uniqueness. The main mathematical issues posed by (1.1a) are to find suitable uniqueness conditions and establish wellposedness [12,14,17,21], as well as to define numerical schemes that provably converge to the unique solution [11]. The well-posedness and numerical analysis of [12] is strongly based on the work by Karlsen, Risebro and Towers [26,28,29]. Versions of the scalar equation (1.1a) are still topic of current research in numerical analysis: adaptive resolution schemes for the case $\mathcal{A}_X \equiv 0$ can be found in [13], monotone entropy stable schemes for the case $D \equiv 0$ and $\mathcal{A}_X \equiv 0$ in [1], and a convergence rate in the case $\mathcal{A}_X \equiv 0$ with several spatial variables is derived in [27].



FIGURE 1. (a) An ideal secondary settling tank (SST) with variables of the feed inlet, effluent and underflow indexed with f, e and u, respectively. The effluent, clarification, thickening, and underflow zones correspond to the respective intervals z < -H, -H < z < 0, 0 < z < B, and z > B. The sludge blanket (concentration discontinuity) separates the hindered settling zone and the compression zone. (b) Aligned illustration of the subdivision of the SST into layers (see Sect. 3). The SST is divided into N internal computational cells, or layers, of depth $\Delta z = (B + H)/N$.

The well-posedness and numerical analysis of the non-reactive version of (1.1a) has led to a recent simulation model for secondary settling tanks (SSTs) in wastewater treatment and an adhering numerical scheme [9, 10]. That model has shown to give more realistic predictions than previous standard models [30, 36].

There are several motivations for extending our previous non-reactive model to the system (1.1). In both mineral processing and wastewater treatment, liquid flocculant added to the suspension sticks to the small particles so that larger flocs are formed and thereby their settling velocity increased. The importance of reactive sedimentation in wastewater treatment has been demonstrated in [2, 19, 20, 23, 24, 31, 32]. Similar phenomena modelled by PDEs are flocculation in mineral processing [34], multi-component two-phase flow in porous media [3,6] and particle-size segregation in granular avalanches [22]. Another application with potential modelling advantages is counter-current "washing" of solids, a process of solvent extraction in hydrometallurgy by coupling a series of clarifier-thickeners [35]. A system of PDEs modelling two-dimensional hydrodynamics coupled to biological reactions for algal growth and a numerical scheme can be found in [5].

A PDE model and numerical scheme for batch sedimentation (closed vessel) of two particulate components including a reduced biokinetic model were presented in [7]. The movements of the substrates were only modelled by simple diffusion. In the examples herein we use the same biokinetic denitrification reactions as in [7].

Positivity preservation of numerical scheme for conservation laws [4, 33] is a challenge in itself. Standard numerical fluxes for finite volume schemes do not preserve the fundamental requirements that the mass per-

centages belong to the interval [0, 1] and their sum is always equal to one [25]. This is, however, handled by our numerical scheme.

1.3. Outline of the remainder of the paper

In Section 2, the model is derived. To this end, we introduce in Section 2.1 the concept of an ideal secondary settling tank (SST) (see Fig. 1), the model variables and some fundamental assumptions. Simplifying assumptions typical of wastewater treatment are collected in Section 2.2. The mathematical model, based on conservation laws, is stated in Section 2.3. To convert it into an equivalent model suitable for simulation, we first replace (in Sect. 2.4) the abstract solid and fluid phase velocities by a mixture bulk velocity, expressed by the given volumetric flows and model variables, and a solid-fluid relative velocity, prescribed by constitutive functions. Next, in Section 2.5 we derive explicit expressions for the total fluxes of the solid and liquid phases, and after further reformulations arrive in Section 2.6 at the model in final, solvable form akin to (1.1). To close the model we introduce in Section 2.7 constitutive functions for hindered and compressive settling, and address in Section 2.8 the choice of initial data and feed input functions for a reactive model of denitrification. In Section 3, a numerical scheme is derived along with a CFL condition and an invariant region property. This is done via a method-of-lines discretization (Sect. 3.1) that combines ingredients from [9] and [16]. A time discretization leading to a fully discrete scheme is introduced in Section 3.2, and the corresponding CFL condition is stated in Section 3.3. Section 4 is devoted to the proof, via several lemmas that appeal to monotonicity arguments, of the main mathematical result, Theorem 4.6, which states that the scheme satisfies an invariant-region principle. In Section 5, we present numerical examples for a reaction model of denitrification. These illustrate the response of the SST to variations of the feed inputs and the impact of different constitutive assumptions. Section 5.5contains estimations of the corresponding error and convergence rate. Conclusions are summarized in Section 6.

2. Model formulation

2.1. Assumptions

In mineral processing and hydrometallurgy, continuously operated sedimentation tanks are usually referred to as "clarifier-thickeners" or simply "thickeners", and in wastewater treatment (our main motivation) as "secondary clarifiers" or "secondary settling tanks" (SSTs). The ideal SST, shown in Figure 1a, has a constant cross-sectional area A. The concentration of each component is assumed to depend only on time t and depth z measured from the feed inlet located at z = 0. The balance laws that make up the model hold for $z \in \mathbb{R}$, have coefficients that are spatially discontinuous at z = -H, 0 and B, and need no boundary condition. The suspension is constituted by the solid phase that consists of particles and the liquid phase that consists of substrates dissolved in water.

The total concentration of particles (or the solid phase) is denoted by X(z,t). Each (flocculated) multicomponent particle is assumed to consist of a number k_X of components described by the (mass) percentage vector

$$\boldsymbol{p}_X = \left(p_X^{(1)}, p_X^{(2)}, \dots, p_X^{(k_X)}\right)^{\mathrm{T}}, \quad \text{where} \quad p_X^{(1)} + \dots + p_X^{(k_X)} = 1.$$
(2.1)

The effluent concentration is $X_{e}(t) := \lim_{\varepsilon \to 0^{+}} X(-H - \varepsilon, t)$. The underflow concentration X_{u} and the percentage vectors $p_{X,e}$ and $p_{X,u}$ are defined analogously. The concentrations of all solid components are

$$\boldsymbol{p}_X X =: \boldsymbol{C} = \left(C^{(1)}, \dots, C^{(k_L)}\right)^{\mathrm{T}}$$

For X = 0 the values of p_X are irrelevant; however, they should always satisfy (2.1).

The total concentration of the liquid phase is denoted by L(z,t). The percentage vector p_L and the concentrations at the in- and outlets are defined in the same way as for the solid phase. We assign the last percentage $p_L^{(k_L)}$ for the water component, which is much larger than the percentages of the soluble components $p_L^{(i)}$, $i = 1, \ldots, k_L - 1$. If the concentrations of the soluble components are contained in the vector

$$\boldsymbol{S} = \left(S^{(1)}, \dots, S^{(k_L-1)}\right)^{\mathrm{T}}$$

and W denotes the water component, then

$$p_L L = \begin{pmatrix} S \\ W \end{pmatrix}$$
, where $W = p_L^{(k_L)} L = \left(1 - \sum_{i=1}^{k_L - 1} p_L^{(i)}\right) L = L - \sum_{i=1}^{k_L - 1} S^{(i)}$. (2.2)

The concentrations $X_{\rm f}$, $L_{\rm f}$, percentage vectors $\boldsymbol{p}_{X,{\rm f}}$, $\boldsymbol{p}_{L,{\rm f}}$, and volumetric flows $Q_{\rm f} \ge Q_{\rm u} > 0$ are given functions of t. It turns out that the effluent volumetric flow $Q_{\rm e}(t; \boldsymbol{C}, \boldsymbol{S})$ generally depends on unknown variables via the reaction terms; see Section 2.4. We define $q_{\rm f} := Q_{\rm f}/A$, $q_{\rm e} := Q_{\rm e}/A$ and $q_{\rm u} := Q_{\rm f}/A$.

The density of the solid phase ρ_X is assumed to be constant and much greater than the maximum packing concentration of the solids X_{max} .

The (unknown) solid and liquid phase velocities are denoted by $v_X = v_X(z,t)$ and $v_L = v_L(z,t)$, respectively. Inside the SST, the particles undergo hindered settling and compression according to some constitutive function (see Sect. 2.7) for the relative velocity

$$v_X - v_L =: v_{\rm rel} = v_{\rm rel}(X, \partial X/\partial z).$$
(2.3)

In the effluent and underflow zones, both phases move at the same velocity, *i.e.*,

$$v_{\rm rel} := 0 \quad \text{for } z < -H \text{ and } z \ge B. \tag{2.4}$$

The reaction terms for all particulate and soluble components are collected in the vectors $\mathbf{R}_X(\mathbf{C}, \mathbf{S})$ of length k_X and $\mathbf{R}_L(\mathbf{C}, \mathbf{S})$ of length k_L . We define

$$\tilde{R}_X(C, S) := \sum_{i=1}^{k_X} R_X^{(i)}(C, S), \qquad \tilde{R}_L(C, S) := \sum_{i=1}^{k_L} R_L^{(i)}(C, S).$$

We assume that every volume of the suspension initially contains either of the two phases in the SST and always for the feed input. For a small volume $V = V_X + V_L$ of suspension, where V_X and V_L are the respective volume of each phase, the masses of the two phases in V can be expressed as $\rho_X V_X = XV$ and $\rho_L V_L = LV$, respectively.

Remark 2.1. To allow for defining local values of density, concentration and volume fraction, the volume V should be sufficiently small but contain enough particles to be representative. We refer to [18] for a discussion including different definitions involving, *e.g.*, the average or expected values of V_X and the mass m_X such that the limit $\lim_{V\to 0^+} m_X/V_X$ exists and can define the density ρ_X .

2.2. Specific assumptions for wastewater treatment

The assumptions stated so far refer to any application. The further analysis will, however, rely on some simplifying assumptions typical of wastewater treatment with biological reactions. Since the liquid phase in the feed inlet consists almost entirely of water, the density of the liquid phase ρ_L is assumed to be constant. The water concentration $W = p_L^{(k_L)} L$ does not influence, nor is influenced by, any reaction, so that $R_L^{(k_L)} = 0$.

The water concentration $W = p_L^{(\kappa_L)} L$ does not influence, nor is influenced by, any reaction, so that $R_L^{(\kappa_L)} = 0$. We assume zero growth of bacteria when there is no, *i.e.*, $\mathbf{R}_{X,j}(\mathbf{0}, \mathbf{S}) = \mathbf{0}$, and allow that a zero soluble substrate concentration may increase due to decay of bacteria, that is, $\mathbf{R}_{L,j}(\mathbf{C}, \mathbf{0}) \ge 0$ (non-negative components). We also assume that that if one component is not present, *i.e.* $p_X^{(\kappa)} = 0$, then there cannot vanish any such material, *i.e.*,

$$R_X^{(k)}(\boldsymbol{p}_X X, \boldsymbol{S})\Big|_{p_X^{(k)}=0} \ge 0,$$
 (2.5)

and similarly for the substrate reaction functions R_L . Furthermore, we assume that there is no reaction in the effluent and underflow regions. Finally, the following assumptions are technical but not restrictive for the application:

$$\tilde{R}_X(\boldsymbol{p}_X X_{\max}, \boldsymbol{S}) = 0, \qquad v_{\text{rel}}(X_{\max}, \partial_z X) = 0.$$
(2.6)

The former states that the bacteria cannot grow when they have reached the maximum concentration X_{max} and the latter that the particles follow the liquid flow at X_{max} .

2.3. Balance equations

The fundamental equation that every volume of the suspension contains either of the two phases can be written as

$$V_X + V_L = V \quad \Leftrightarrow \quad \frac{X}{\rho_X} + \frac{L}{\rho_L} = 1 \quad \Leftrightarrow \quad L = \rho_L - rX, \quad \text{where } r := \frac{\rho_L}{\rho_X}.$$
 (2.7)

We assume that this is satisfied at t = 0 within the SST and always for the given feed concentrations; $X_f/\rho_X + L_f/\rho_L = 1$. The assumption $\rho_X > X_{\text{max}}$ implies that always L > 0.

The conservation of mass for each particulate and soluble/liquid component and the requirements of the percentages imply the following system of equations for $z \in \mathbb{R}$ and t > 0, where $\delta(z)$ is the delta function:

$$\frac{\partial(\boldsymbol{p}_X X)}{\partial t} + \frac{\partial(\boldsymbol{p}_X X v_X)}{\partial z} = \delta(z)\boldsymbol{p}_{X,f} X_f q_f + \gamma(z)\boldsymbol{R}_X(\boldsymbol{C},\boldsymbol{S}), \qquad (2.8a)$$

$$\frac{\partial(\boldsymbol{p}_L L)}{\partial t} + \frac{\partial(\boldsymbol{p}_L L v_L)}{\partial z} = \delta(z)\boldsymbol{p}_{L,\mathrm{f}} L_{\mathrm{f}} q_{\mathrm{f}} + \gamma(z)\boldsymbol{R}_L(\boldsymbol{C},\boldsymbol{S}), \qquad (2.8\mathrm{b})$$

$$p_X^{(1)} + \ldots + p_X^{(k_X)} = 1,$$
 (2.8c)

$$p_L^{(1)} + \ldots + p_L^{(k_L)} = 1.$$
 (2.8d)

2.4. Phase, bulk and relative velocities

The full set of $k_X + k_L + 4$ balance equations are (2.3), (2.7) and (2.8), and the unknowns are p_X , X, v_X , p_L , L and v_L . We now reduce the number of equations by eliminating the variables v_X and v_L . To this end, we first replace them by $v_{\rm rel}$ and the average bulk velocity of the suspension q, and then express q in terms of the rest of the unknowns.

Lemma 2.2. Equations (2.8a) and (2.8c) are equivalent to (2.8a) and

$$\frac{\partial X}{\partial t} + \frac{\partial (Xv_X)}{\partial z} = \delta(z)X_{\rm f}q_{\rm f} + \gamma(z)\tilde{R}_X.$$
(2.9)

Analogously, (2.8b) and (2.8d) are equivalent to (2.8b) and

$$\frac{\partial L}{\partial t} + \frac{\partial (Lv_L)}{\partial z} = \delta(z)L_{\rm f}q_{\rm f} + \gamma(z)\tilde{R}_L.$$
(2.10)

Proof. Summing all equations in (2.8a), using (2.8c) and that $p_{X,f}$ satisfies (2.1), we get (2.9). Conversely, summing all equations in (2.8a) and subtracting (2.9) implies (2.8c).

With the volume fraction of the solid phase $\phi := V_X/V$, we have $X = \rho_X \phi$ and $L = \rho_L(1 - \phi)$, cf. (2.7). Analogously, the feed inlet concentrations can be written as $X_f = \rho_X \phi_f$ and $L_f = \rho_L(1 - \phi_f)$. Substituting these expressions into (2.9) and (2.10) and dividing by the constant densities ρ_X and ρ_L , respectively, we get

$$\frac{\partial \phi}{\partial t} + \frac{\partial (\phi v_X)}{\partial z} = \delta(z)\phi_{\rm f}q_{\rm f} + \gamma(z)\frac{R_X}{\rho_X},$$
$$\frac{\partial (1-\phi)}{\partial t} + \frac{\partial ((1-\phi)v_L)}{\partial z} = \delta(z)(1-\phi_{\rm f})q_{\rm f} + \gamma(z)\frac{\tilde{R}_L}{\rho_L}.$$

Adding these two equations and defining the average bulk velocity and a weighted reaction function:

$$q(z,t) := \phi v_X(z,t) + (1-\phi)v_L(z,t), \tag{2.11}$$

$$\mathcal{R}(\boldsymbol{C},\boldsymbol{S}) := \frac{R_X(\boldsymbol{C},\boldsymbol{S})}{\rho_X} + \frac{R_L(\boldsymbol{C},\boldsymbol{S})}{\rho_L},$$
(2.12)

we get an equation without any time derivative:

$$\frac{\partial q}{\partial z} = \delta(z)q_{\rm f} + \gamma(z)\mathcal{R}(\boldsymbol{C},\boldsymbol{S}).$$
(2.13)

We can express v_X and v_L in terms of q and v_{rel} since (2.3) and (2.11) are equivalent to

$$v_X = q + v$$
, where $v := (1 - \phi)v_{\rm rel}$, (2.14)

$$v_L = q - \phi v_{\rm rel}.\tag{2.15}$$

We now derive an explicit expression for q. In view of (2.4), (2.11) implies:

$$q(z,t) = \begin{cases} v_X(z,t) = v_L(z,t) = -q_e(t) & \text{for } z \le -H, \\ v_X(z,t) = v_L(z,t) = q_u(t) & \text{for } z \ge B, \end{cases}$$
(2.16)

where q_u is known and q_e is unknown. We integrate (2.13) from z to B to get

$$q(z,t;\boldsymbol{C},\boldsymbol{S}) = q(B,t) - \int_{z}^{B} \left(\delta(\xi)q_{\mathrm{f}}(t) + \gamma(\xi)\mathcal{R}(\boldsymbol{C}(\xi,t),\boldsymbol{S}(\xi,t)) \right) \mathrm{d}\xi.$$
(2.17)

The following function describes the additional bulk velocity due to the reactions:

$$q^{\text{reac}}(z; \boldsymbol{C}, \boldsymbol{S}) := \int_{z}^{B} \gamma(\xi) \mathcal{R}(\boldsymbol{C}, \boldsymbol{S}) \,\mathrm{d}\xi.$$
(2.18)

Since by (2.16), $q(B,t) = q_u(t)$, we may express q in terms of the unknowns as follows:

$$q(z,t;\boldsymbol{C},\boldsymbol{S}) := \begin{cases} q_{u}(t) - q_{f}(t) - q^{reac}(-H;\boldsymbol{C},\boldsymbol{S}) & \text{for } z \leq -H, \\ q_{u}(t) - q_{f}(t) - q^{reac}(z;\boldsymbol{C},\boldsymbol{S}) & \text{for } -H < z < 0, \\ q_{u}(t) - q^{reac}(z;\boldsymbol{C},\boldsymbol{S}) & \text{for } 0 < z < B, \\ q_{u}(t) & \text{for } z \geq B. \end{cases}$$
(2.19)

Moreover, (2.16) states that $q(z,t) = -q_e(t)$ for $z \leq -H$, so (2.19) defines the effluent bulk velocity in terms of the unknowns: $q_e(t; \mathbf{C}, \mathbf{S}) = q_f(t) - q_u(t) + q^{reac}(-H; \mathbf{C}, \mathbf{S})$.

2.5. Solid and liquid total fluxes

The flux functions of the PDEs (2.9) for X and (2.10) for L can, by means of (2.14) and (2.15), be written as

$$Xv_X = Xq + Xv, \tag{2.20}$$

$$Lv_{L} = \rho_{L}(1-\phi)(q-\phi v_{\rm rel}) = \rho_{L}\left((1-\phi)q-\phi v\right) = \rho_{L}\left(q-\frac{Xq+Xv}{\rho_{X}}\right).$$
 (2.21)

Thus, we define the total fluxes in terms of q and $v = (1 - \phi)v_{rel}$ as follows:

$$F_X := Xq + Xv = Xq + X\left(1 - \frac{X}{\rho_X}\right)v_{\rm rel},\tag{2.22}$$

$$F_L := \rho_L q - rF_X \quad \Leftrightarrow \quad \frac{F_X}{\rho_X} + \frac{F_L}{\rho_L} = q.$$
(2.23)

With q defined by (2.19), F_X by (2.22) and F_L by (2.23) we get the following governing equations, which neither contain v_X nor v_L :

$$\frac{\partial(\boldsymbol{p}_X X)}{\partial t} + \frac{\partial(\boldsymbol{p}_X F_X)}{\partial z} = \delta(z)\boldsymbol{p}_{X,\mathrm{f}} X_{\mathrm{f}} q_{\mathrm{f}} + \gamma(z)\boldsymbol{R}_X(\boldsymbol{C},\boldsymbol{S}), \qquad (2.24\mathrm{a})$$

$$\frac{\partial(\boldsymbol{p}_L L)}{\partial t} + \frac{\partial(\boldsymbol{p}_L F_L)}{\partial z} = \delta(z)\boldsymbol{p}_{L,f}L_f q_f + \gamma(z)\boldsymbol{R}_L(\boldsymbol{C},\boldsymbol{S}), \qquad (2.24b)$$

$$p_X^{(1)} + \ldots + p_X^{(k_X)} = 1,$$
 (2.24c)

$$p_L^{(1)} + \ldots + p_L^{(k_L)} = 1.$$
 (2.24d)

The proof of the following lemma is analogous to that of Lemma 2.2.

Lemma 2.3. Equations (2.24a) and (2.24c) are equivalent to (2.24a) and

$$\frac{\partial X}{\partial t} + \frac{\partial F_X}{\partial z} = \delta(z) X_{\rm f} q_{\rm f} + \gamma(z) \tilde{R}_X.$$
(2.25)

Analogously, (2.24b) and (2.24d) are equivalent to (2.24b) and

$$\frac{\partial L}{\partial t} + \frac{\partial F_L}{\partial z} = \delta(z) L_{\rm f} q_{\rm f} + \gamma(z) \tilde{R}_L.$$
(2.26)

Lemma 2.4. Equations (2.25) and (2.26) are equivalent to (2.25) and (2.7).

Proof. Dividing (2.25) by ρ_X , (2.26) by ρ_L and summing these two equations, we get the following equation which can replace (2.26) (with maintained equivalence):

$$\frac{\partial}{\partial t} \left(\frac{X}{\rho_X} + \frac{L}{\rho_L} \right) + \frac{\partial}{\partial z} \left(\frac{F_X}{\rho_X} + \frac{F_L}{\rho_L} \right) = \delta(z) q_{\rm f} \left(\frac{X_{\rm f}}{\rho_X} + \frac{L_{\rm f}}{\rho_L} \right) + \gamma(z) \left(\frac{\dot{R}_X}{\rho_X} + \frac{\dot{R}_L}{\rho_L} \right)$$

All terms except the first cancel. This is because of the equality (2.23), the expression (2.17) for q and the definition of \mathcal{R} in (2.12). The remaining equation is

$$\frac{\partial}{\partial t} \left(\frac{X}{\rho_X} + \frac{L}{\rho_L} \right) = 0 \quad \Leftrightarrow \quad \frac{\partial}{\partial t} \left(\frac{V_X}{V} + \frac{V_L}{V} \right) = 0 \quad \Leftrightarrow \quad \frac{V_X}{V} + \frac{V_L}{V} = g(z),$$

where the function g(z) must be equal to one, since it is at time t = 0 by assumption. Hence, the remaining equation is equivalent to (2.7).

Lemma 2.5. Equations (2.3), (2.7) and (2.8) are equivalent to the governing equations (2.24).

Proof. Lemma 2.2 states that (2.8c) and (2.8d) can be replaced (keeping the equivalence) by (2.9) and (2.10). Equations (2.3) and (2.7) imply via (2.20)–(2.23) that $Xv_X = F_X$ and $Lv_L = F_L$. Hence, (2.9) and (2.10) are equivalent to (2.25) and (2.26), which by Lemma 2.3 can be replaced by (2.24c) and (2.24d). For the other implication, we should prove that (2.3), (2.7), $F_X = Xv_X$ and $F_L = Lv_L$ hold. Lemma 2.3 implies first that (2.24c) and (2.24d) can be replaced by (2.25) and (2.26). Then Lemma 2.4 implies (2.7). By (2.14) and (2.15), (2.3) is directly satisfied and $F_X = X(q + v) = Xv_X$. With this equality and $\phi = X/\rho_X$, we obtain from (2.11) $F_X/\rho_X + (1 - X/\rho_X)v_L = q$. Substituting this into the definition of F_L (2.23), we get $F_L = \rho_L(q - rF_X) = (\rho_L - rX)v_L = Lv_L$, where the last equality follows from (2.7).

2.6. Model equations in final form

We observe that the last scalar equation of (2.24b) determines $p_L^{(k_L)}$ for the water component of the liquid. This variable does not appear in any other equation. A simpler equation to determine $p_L^{(k_L)}$ is (2.24d). Let the notation with a bar \bar{p}_L denote the first $k_L - 1$ components of p_L .

Theorem 2.6. The balance equations (2.3) and (2.8) are equivalent to the following set of model equations defined for $z \in \mathbb{R}$ and t > 0:

$$\frac{\partial X}{\partial t} + \frac{\partial F_X}{\partial z} = \delta(z) X_{\rm f} q_{\rm f} + \gamma(z) \tilde{R}_X, \qquad (2.27a)$$

$$\frac{\partial(\boldsymbol{p}_X X)}{\partial t} + \frac{\partial(\boldsymbol{p}_X F_X)}{\partial z} = \delta(z)\boldsymbol{p}_{X,f} X_f q_f + \gamma(z)\boldsymbol{R}_X, \qquad (2.27b)$$

$$L = \rho_L - rX, \tag{2.27c}$$

$$\frac{\partial(\boldsymbol{p}_L L)}{\partial t} + \frac{\partial(\boldsymbol{p}_L F_L)}{\partial z} = \delta(z)\bar{\boldsymbol{p}}_{L,f}L_f q_f + \gamma(z)\bar{\boldsymbol{R}}_L, \quad \text{where } F_L = \rho_L q - rF_X, \quad (2.27d)$$

$$p_L^{(k_L)} = 1 - (p_L^{(1)} + \ldots + p_L^{(k_L-1)}).$$
 (2.27e)

Proof. We apply Lemmas 2.5, 2.3 and 2.4 (in that order) to obtain equivalently (2.27a)–(2.27c) and (2.24b). It remains to prove that (2.24b) can be split into (2.27d) and (2.27e). Lemma 2.4 states that we can replace (2.27c) by (2.26), which in turn by Lemma 2.3 can be replaced by (2.27e). Conversely, summing the equations in (2.27d), recalling that $R_L^{(k_L)} = 0$ and using (2.27e), we get

$$\frac{\partial}{\partial t} \left((1 - p_L^{(k_L)})L \right) + \frac{\partial}{\partial z} \left((1 - p_L^{(k_L)})F_L \right) = \delta(z)(1 - p_{L,f}^{(k_L)})L_f q_f + \gamma(z)\tilde{R}_L$$

Now subtract (2.26) to obtain the last equation of (2.24b).

The formulation (2.27) has two advantages. Firstly, for a numerical method with explicit time stepping, the new value of X is obtained by solving (2.27a) only. Then p_X is updated by (2.27b), etc. Secondly, this form of the governing equations yields the invariant-region property of the numerical scheme (see Theorem 4.6), which states that the solution stays in the following region (vectors in inequalities should be interpreted component-wise):

$$\Omega := \{ \boldsymbol{\mathcal{U}} \in \mathbb{R}^{k_X + k_L + 2} : 0 \le \boldsymbol{p}_X, \boldsymbol{p}_L \le 1, \ 0 \le X \le X_{\max}, \\ \rho_L - rX_{\max} \le L \le \rho_L, \ p_X^{(1)} + \ldots + p_X^{(k_X)} = 1, \ p_L^{(1)} + \ldots + p_L^{(k_L)} = 1 \}.$$

We have no proof that an *exact* solution of system (2.27) stays in Ω if the initial datum is since the wellposedness (existence and uniqueness) analysis of the model is not yet concluded, and a suitable concept of a (discontinuous) exact solution is not yet established. However, it is reasonable to expect that an exact solution of (2.27) should also assume values within Ω . To support this conjecture, we mention first that the invariant region property proved herein holds uniformly for approximate solutions, and therefore will hold for any limit to which the scheme converges as discretization parameters tend to zero. In fact, in some previous work on related models the existence of an exact solution is proved by convergence of a suitable numerical scheme [11, 12, 28], where the convergence proofs involve a uniform L^{∞} bound, that is, a simple form of an invariant-region principle. For instance, consider the Cauchy problem for the scalar equation (2.27a) without the reaction term ($\bar{R}_X \equiv 0$). Bürger *et al.* [12] proved the existence of a solution X = X(z, t), which has the interval [0, X_{max}] as invariant region, via the convergence of an explicit numerical scheme. With the properties of the reaction term here, namely that $\tilde{R}_X = 0$ if X = 0 or $X = X_{max}$, the invariance property of the numerical scheme follows with the arguments of the proof of Lemma 4.3 (in Sect. 4). The convergence of that scheme with a reaction term being a function of X only (and utilizing that it is zero for X = 0 or $X = X_{max}$) can be established by modifying the proof in [12].

Another important property of (2.27) is its hyberbolicity, that is, in those regions where the governing system of PDEs reduces to a first-order system of conservation laws, the corresponding flux Jacobian should have real eigenvalues only. To verify satisfaction of this property here, we assume for a moment that F_X is a convective flux function, *i.e.*, a function of X only (v_{rel} is a function of X only; see (2.22)). Then the system (2.27) is of first order where the Jacobian is the same as for the homogeneous system

$$\frac{\partial}{\partial t} \begin{pmatrix} X \\ \boldsymbol{p}_X X \\ \bar{\boldsymbol{p}}_L L \end{pmatrix} + \frac{\partial}{\partial z} \begin{pmatrix} F_X \\ (\boldsymbol{p}_X X) \frac{F_X}{X} \\ (\bar{\boldsymbol{p}}_L L) \frac{F_L}{L} \end{pmatrix} = \mathbf{0},$$

that is, since F_X , F_L and L are functions of X, its Jacobian is a lower triangular matrix with the diagonal

$$\left(F'_X(X), \frac{F_X(X)}{X}, \dots, \frac{F_X(X)}{X}, \frac{F_L(X)}{L}, \dots, \frac{F_L(X)}{L}\right)$$

Since these entries are real, the system is hyperbolic. In the next subsection, we will assume a constitutive assumption that implies that the system (2.27) in addition to the convective flux has second-order derivatives.

2.7. Constitutive assumptions for hindered and compressive settling

Consistently with [7, 10, 12] we assume that $v_{\rm rel} = v/(1-\phi)$, where

$$v = v(X, \partial X/\partial z, z) := \gamma(z)v_{\rm hs}(X) \left(1 - \frac{\rho_X \sigma'_{\rm e}(X)}{Xg(\rho_X - \rho_L)} \frac{\partial X}{\partial z}\right).$$

Here, $v_{\rm hs}$ is the hindered settling velocity and $\sigma_{\rm e}$ the effective solids stress, for which constitutive functions are needed; see Section 5. We require that $\sigma_{\rm e}(X) = 0$ for $X < X_{\rm c}$, where $X_{\rm c}$ is a critical concentration above which the particles form a network, and $\sigma'_{\rm e}(X) \ge 0$ for $X > X_{\rm c}$ (see [12]). It is convenient to define

$$f_{\rm b}(X) := X v_{\rm hs}(X), \qquad d(X) := v_{\rm hs}(X) \frac{\rho_X \sigma'_{\rm e}(X)}{g(\rho_X - \rho_L)}, \qquad D(X) := \int_{X_c}^X d(s) \,\mathrm{d}s.$$

With the batch settling flux function $f_{\rm b}(X)$, the total particulate flux (2.22) becomes

$$F_X(X,\partial X/\partial z, z, t) = Xq(z, t) + \gamma(z) \left(f_{\rm b}(X) - \frac{\partial D(X)}{\partial z} \right).$$
(2.28)

Remark 2.7. We verify that the final model can be expressed as (1.1) when the reactive bulk velocity is neglected, *i.e.*, $q^{\text{reac}} := 0$. Then (2.19) implies that q = q(z,t), and comparing (1.1a) with (2.27a) and (2.28), we get $\mathcal{F}(X, z, t) = Xq(z, t) + \gamma(z)f_{\rm b}(X)$. Moreover, by (2.7) we can express $L = l_1(X) := \rho_L - rX$. Thus, all variables \mathbf{p}_X , X, \mathbf{p}_L , L, S and C can be expressed in terms of \mathbf{p}_X , $\bar{\mathbf{p}}_L$ and X, so that the right-hand sides of (2.27a), (2.27b) and (2.27d) can be written as functions \mathcal{A}_X , \mathcal{A}_X and \mathcal{A}_L , respectively, of $(X, \mathbf{p}_X, \bar{\mathbf{p}}_X, z, t)$. Finally, (2.23) gives $F_L = l_2(F_X, z, t) := \rho_L q(z, t) - rF_X$.

2.8. Initial data and feed input functions

Initial data at t = 0, namely

$$X(z,0) = X^{0}(z), \quad \boldsymbol{p}_{X}(z,0) = \boldsymbol{p}_{X}^{0}(z), \quad \boldsymbol{p}_{L}(z,0) = \boldsymbol{p}_{L}^{0}(z), \quad L(z,0) = L^{0}(z), \quad z \in \mathbb{R}$$

are obtained either from direct information on the particulate total concentration $X^0(z)$ and the percentage vector $p_X^0(z)$, or from given component concentrations:

$$\boldsymbol{p}_X^0 X^0 = \boldsymbol{C}^0 = \left(C^{(1),0}, \dots, C^{(k_X),0} \right)^{\mathrm{T}}.$$

In the latter case, summation yields

$$X^{0} = X^{0} \left(p_{X}^{(1),0} + \ldots + p_{X}^{(k_{X}),0} \right) = C^{(1),0} + \ldots + C^{(k_{X}),0} \quad \text{and} \quad \boldsymbol{p}_{X}^{0} = \boldsymbol{C}^{0} / X^{0}.$$

If $S^0 = (S^{(1),0}, S^{(2),0}, \dots, S^{(k_L-1),0})^T$ denotes the initial soluble concentrations, then (2.7) and (2.2) give $L^0 = \rho_L - rX^0$ and

$$m{p}_L^0 = egin{pmatrix} m{S}^0/L^0 \ 1 - \sum_{i=1}^{k_L - 1} S^{(i),0}/L^0 \end{pmatrix}$$

The feed input functions $p_{X,f}(t)$, $X_f(t)$, $p_{L,f}(t)$ and $L_f(t)$ are defined analogously.

3. A NUMERICAL SCHEME

As in [9], we divide the SST into N internal computational cells, or layers, of depth $\Delta z = (B + H)/N$; see Figure 1b. The midpoint of layer j is assumed to have the coordinate z_j , hence the layer is the interval $[z_{j-1/2}, z_{j+1/2}]$. Layer 1, the top layer in the clarification zone, is thus $[z_{1/2}, z_{3/2}] = [-H, -H + \Delta z]$, and the bottom location is $z = z_{N+1/2} = B$. We define j_f to be the smallest integer larger than or equal to $H/\Delta z$, *i.e.*, $j_f := \lceil H/\Delta z \rceil$. Then the feed inlet (z = 0) is located in layer j_f (the feed layer). Layers -1 and N + 1 have been added to obtain the correct effluent and underflow concentrations, respectively. The average values of the unknowns in each layer j are denoted by $P_{X,j} = P_{X,j}(t)$, $X_j = X_j(t)$, etc. The unknown output functions at the effluent and underflow are $X_e(t) := X_0(t)$, $X_u(t) := X_{N+1}(t)$, etc. To simplify formulas below, we use two mirror cells and set $X_{-1} := X_0$, $X_{N+2} := X_{N+1}$ and analogously for the other variables.

3.1. Spatial discretization

The computational domain is composed of N + 2 intervals and one needs to define numerical fluxes for N + 3 layer boundaries. Except for the reaction term, (2.27a) is a model for which a working numerical scheme is available [9]. The reaction term depends on all variables, and is strongly coupled to the other equations via the total flux (2.28), which contains the bulk velocity q = q(z, t, C, S), which, in contrast to the non-reactive case, depends on the unknown concentrations via q^{reac} in (2.18) and (2.19). This function is well defined at $z_{j+1/2}$ because of the integration in (2.18). For piecewise constant functions in each layer, *i.e.* $X(z,t) = X_j$, $z \in (z_{j-1/2}, z_{j+1/2}]$, etc., we obtain

$$q_{j+1/2}^{\text{reac}} := q^{\text{reac}}(z_{j+1/2}) := \begin{cases} \sum_{i=j+1}^{N} \gamma_i \mathcal{R}_i \Delta z & \text{for} \quad j = -1, \dots, N-1, \\ 0 & \text{for} \quad j = N, N+1, \end{cases}$$
(3.1)

where we recall that $\mathcal{R} = 0$ outside the SST, and then define $q_{j+1/2} := q(z_{j+1/2}, t)$ in accordance with (2.19):

$$q_{j+1/2} = \begin{cases} q_{u}(t) - q_{f}(t) - \sum_{i=j+1}^{N} \mathcal{R}_{i} \Delta z & \text{for} \quad j = -1, \dots, j_{f} - 1, \\ q_{u}(t) - \sum_{i=j+1}^{N} \mathcal{R}_{i} \Delta z & \text{for} \quad j = j_{f}, \dots, N - 1, \\ q_{u}(t) & \text{for} \quad j = N, N + 1. \end{cases}$$
(3.2)

The first bulk flow term qX of (2.28) can be handled by a standard upwind flux:

$$\mathcal{B}_{j+1/2} := \begin{cases} q_{j+1/2} X_{j+1} & \text{if } q_{j+1/2} \le 0, \\ q_{j+1/2} X_j & \text{if } q_{j+1/2} > 0, \end{cases} \qquad j = -1, \dots, N+1.$$
(3.3)

The rest of the terms of (2.28) are only non-zero (strictly) inside the SST. We define $\gamma_{j+1/2} := \gamma(z_{j+1/2})$ (recall that $\gamma(-H) = \gamma(B) = 0$) and define the numerical convective flux $G_{j+1/2}$ for $j = -1, \ldots, N+1$ by means of

the Godunov flux \mathcal{G} :

$$G_{j+1/2} := \gamma_{j+1/2} \mathcal{G}(X_j, X_{j+1}), \quad \text{where} \quad \mathcal{G}(u, v) := \begin{cases} \min_{\substack{u \le X \le v}} f_{\mathrm{b}}(X) & \text{if} \quad u \le v, \\ \max_{\substack{u \ge X \ge v}} f_{\mathrm{b}}(X) & \text{if} \quad u > v. \end{cases}$$
(3.4)

Analogously, the numerical diffusive flux (modelling compression in sedimentation) is

$$J_{j+1/2} := \gamma_{j+1/2} \frac{D(X_{j+1}) - D(X_j)}{\Delta z}, \quad j = -1, \dots, N+1.$$

Then the total flux (2.28) between cells j and j + 1 is approximated by

$$F_{X,j+1/2} := \mathcal{B}_{j+1/2} + G_{j+1/2} - J_{j+1/2}, \qquad j = -1, \dots, N+1.$$

The corresponding flux of (2.27b) is $P_{X,j+1/2}F_{X,j+1/2}$, where $P_{X,j+1/2}$ needs to be defined. If $F_{X,j+1/2} > 0$, then particles move in the direction of the z-axis over the boundary $z_{j+1/2}$, *i.e.* downwards. Then the values of $P_{X,j+1/2}$ at the cell boundary are those coming from the left cell, *i.e.* $P_{X,j}$. If $F_{X,j+1/2} \leq 0$, then the particles move upwards and the values are $P_{X,j+1}$. Consequently, following [16] we define

$$\boldsymbol{P}_{X,j+1/2} := \begin{cases} \boldsymbol{P}_{X,j+1} & \text{if} \quad F_{X,j+1/2} \le 0, \\ \boldsymbol{P}_{X,j} & \text{if} \quad F_{X,j+1/2} > 0, \end{cases} \qquad j = -1, \dots, N+1$$

For the liquid percentage vector appearing in (2.27d), we use the same principle. By (2.23), we define $F_{L,j+1/2} := \rho_L q_{j+1/2} - rF_{X,j+1/2}$ for $j = -1, \ldots, N+1$ and

$$\boldsymbol{P}_{L,j+1/2} := \begin{cases} \boldsymbol{P}_{L,j+1} & \text{if} \quad F_{L,j+1/2} \leq 0, \\ \boldsymbol{P}_{L,j} & \text{if} \quad F_{L,j+1/2} > 0, \end{cases} \qquad j = -1, \dots, N+1$$

We introduce the notation $[\Delta F]_j := F_{j+1/2} - F_{j-1/2}$ and let δ_{j,j_f} denote the Kronecker delta, which is 1 if $j = j_f$ and zero otherwise. The conservation of mass for each layer gives the following method-of-lines equations (for j = 0, ..., N + 1):

$$\frac{\mathrm{d}X_j}{\mathrm{d}t} = -\frac{[\Delta F_X]_j}{\Delta z} + \delta_{j,j_\mathrm{f}} \frac{X_\mathrm{f} q_\mathrm{f}}{\Delta z} + \gamma_j \tilde{R}_{X,j},\tag{3.5a}$$

$$\frac{\mathrm{d}(\boldsymbol{P}_{X,j}X_j)}{\mathrm{d}t} = -\frac{[\Delta(\boldsymbol{P}_XF_X)]_j}{\Delta z} + \delta_{j,j_\mathrm{f}}\frac{\boldsymbol{p}_{X,\mathrm{f}}X_\mathrm{f}q_\mathrm{f}}{\Delta z} + \gamma_j \boldsymbol{R}_{X,j}, \qquad (3.5b)$$
$$L_j = \rho_L - rX_j,$$

$$F_{L,j+1/2} = \rho_L q_{j+1/2} - r F_{X,j+1/2},$$

$$\frac{\mathrm{d}(\boldsymbol{P}_{L,j}L_j)}{\mathrm{d}t} = -\frac{[\Delta(\boldsymbol{P}_L F_L)]_j}{\Delta z} + \delta_{j,j_f} \frac{\boldsymbol{p}_{L,f} L_f q_f}{\Delta z} + \gamma_j \boldsymbol{R}_{L,j},$$
(3.5c)

$$P_L^{(k_L)} = 1 - \left(P_L^{(1)} + \dots + P_L^{(k_L-1)}\right).$$
(3.5d)

If $X_j = 0$, *i.e.* there are no solids in layer j, then the value of $\mathbf{P}_{X,j}$ is irrelevant. Furthermore, note that in (3.5a) we have $\tilde{R}_{X,j} = \tilde{R}_X(\mathbf{C}_j, \mathbf{S}_j)$, where $\mathbf{C}_j = \mathbf{P}_{X,j}X_j$ and $\mathbf{S}_j = \bar{\mathbf{P}}_{L,j}L_j = \bar{\mathbf{P}}_{L,j}(\rho_L - rX_j)$, where $\bar{\mathbf{P}}_{L,j}$ is a vector containing the first $k_L - 1$ components of $\mathbf{P}_{L,j}$. The same holds for each component of $\mathbf{R}_{X,j}$ and $\mathbf{R}_{L,j}$. In (3.5c) and similar formulas below for the computation of \mathbf{P}_L we skip the notation with a bar over all vectors. It is understood that the last equation of (3.5c) is replaced by (3.5d).

3.2. Explicit fully discrete scheme

First, we recall that the initial data for any (one-step) time discretization method can be obtained as is shown in Section 2.8. If the final simulation time is T, we let t_n , $n = 0, 1, \ldots, n_T$, denote the discrete time points and $\Delta t = T/n_T$ the time step that should satisfy a certain CFL condition depending on the chosen time-integration method. Set $\lambda := \Delta t/\Delta z$. For explicit schemes, the right-hand sides of the equations are evaluated at time t_n . The value of a variable at time t_n is denoted by an upper index, *e.g.*, X_j^n . For explicit Euler time integration of (3.5a)-(3.5c), we note in particular the approximation

$$\frac{\mathrm{d}(\boldsymbol{P}_{X,j}X_j)}{\mathrm{d}t} \approx \frac{\boldsymbol{P}_{X,j}^{n+1}X_j^{n+1} - \boldsymbol{P}_{X,j}^nX_j^n}{\Delta t}$$

which implies the following explicit scheme (recall that always $L_i^{n+1} > 0$):

$$X_j^{n+1} = X_j^n + \lambda \left(-\left[\Delta F_X^n\right]_j + \delta_{j,j_f} X_f^n q_f^n \right) + \Delta t \, \gamma_j \tilde{R}_{X,j}^n, \tag{3.6a}$$

$$\boldsymbol{P}_{X,j}^{n+1} = \begin{cases} \text{irrelevant, } e.g. \ \boldsymbol{P}_{X,j}^{n} \\ \frac{1}{X_{j}^{n+1}} \Big[\boldsymbol{P}_{X,j}^{n} X_{j}^{n} + \lambda \Big(- [\Delta(\boldsymbol{P}_{X}^{n} F_{X}^{n})]_{j} + \delta_{j,j_{\mathrm{f}}} \boldsymbol{p}_{X,\mathrm{f}}^{n} X_{\mathrm{f}}^{n} q_{\mathrm{f}}^{n} \Big) + \Delta t \, \gamma_{j} \boldsymbol{R}_{X,j}^{n} \Big] & \text{if } X_{j}^{n+1} > 0, \end{cases}$$
(3.6b)

$$L_{j}^{n+1} = \rho_{L} - rX_{j}^{n+1}, \tag{3.6c}$$

$$F_{L,j+1/2}^n = \rho_L q_{j+1/2}^n - r F_{X,j+1/2}^n, \tag{3.6d}$$

$$\boldsymbol{P}_{L,j}^{n+1} = \frac{1}{L_j^{n+1}} \Big[\boldsymbol{P}_{L,j}^n L_j^n + \lambda \Big(- [\Delta(\boldsymbol{P}_L^n F_L^n)]_j + \delta_{j,j_{\mathrm{f}}} \boldsymbol{p}_{L,\mathrm{f}}^n L_{\mathrm{f}}^n \boldsymbol{q}_{\mathrm{f}}^n \Big) + \Delta t \, \gamma_j \boldsymbol{R}_{L,j}^n \Big], \tag{3.6e}$$

$$P_{L,j}^{(k_L),n+1} = 1 - \left(P_{L,j}^{(1),n+1} + \ldots + P_{L,j}^{(k_L-1),n+1}\right).$$
(3.6f)

The biological reactions do not only influence the variables locally via the reaction terms, but also globally via the additional bulk velocity term $q_{j+1/2}^{\text{reac},n}$. In fact, a local volume increase or decrease at $z = z_0$ has an immediate influence for all $z < z_0$. In other words, the bulk velocity change $q^{\text{reac}}(z; \boldsymbol{C}, \boldsymbol{S})$ given by (2.18) depends on the reactions in the interval [z, B]. For the numerical scheme, this means that the update formulas for the concentrations in a layer j_0 contain the other concentrations in all layers $j > j_0$; see (3.2). We will see in Section 4 that this unfortunately means that the scheme is not monotone. The terms \mathcal{R}_j , $j = 1, \ldots, N$ in (3.1) destroy the monotonicity. Since these are negligible in wastewater treatment (see Sect. 5), we define $q_{j+1/2}^{\text{reac}} := 0$ instead of (3.1).

3.3. CFL condition

We define the vector of unknowns $\mathcal{U} := (\mathbf{p}_X, X, \mathbf{p}_L, L)$ and the following bounds (which are assumed to be finite):

$$\begin{split} \|f_{\mathbf{b}}\|_{\infty} &:= \max_{0 \le X \le X_{\max}} |f_{\mathbf{b}}(X)|, \quad \|q\|_{\infty} := \max_{0 \le t \le T} q_{\mathbf{f}}(t), \\ M_{C} &:= \sup_{\substack{\boldsymbol{u} \in \Omega \\ 1 \le k \le k_{X}}} \left| \frac{\partial \tilde{R}_{X}}{\partial C^{(k)}} \right|, \quad M_{S} := \sup_{\substack{\boldsymbol{u} \in \Omega, 1 \le k \le k_{L} - 1 \\ \mathbf{u} \in \Omega, 1 \le k \le k_{L} - 1}} \left| \frac{\partial \tilde{R}_{X}}{\partial S^{(k)}} \right| \\ M_{C}^{X} &:= \sup_{\substack{\boldsymbol{u} \in \Omega \\ 1 \le k \le k_{X}}} \left| \frac{\partial R_{X}^{(k)}}{\partial C^{(k)}} \right|, \quad M_{S}^{L} := \sup_{\substack{\boldsymbol{u} \in \Omega \\ 1 \le k \le k_{L} - 1}} \left| \frac{\partial R_{L}^{(k)}}{\partial S^{(k)}} \right| \end{split}$$

along with $M := M_C + rM_S$. The CFL condition is

$$\Delta t \left(\frac{\|q\|_{\infty}}{\Delta z} + \max(\beta_X, \beta_{\boldsymbol{P}_X}, \beta_{\boldsymbol{P}_L}) \right) \le 1,$$
 (CFL)

where

$$\beta_{X} := \frac{\|f_{b}'\|_{\infty}}{\Delta z} + \frac{2\|d\|_{\infty}}{\Delta z^{2}} + M, \qquad \beta_{P_{X}} := \frac{\|f_{b}'\|_{\infty}}{\Delta z} + \frac{2\|d\|_{\infty}}{\Delta z^{2}} + M_{C}^{X}, \qquad (3.7)$$
$$\beta_{P_{L}} := \frac{\|f_{b}\|_{\infty}}{\Delta z(\rho_{X} - X_{\max})} + \frac{2D(X_{\max})}{\Delta z^{2}(\rho_{X} - X_{\max})} + M_{S}^{L}.$$

4. Properties of the numerical scheme

With $\eta := \lambda/\Delta z = \Delta t/\Delta z^2$ the update formula (3.6a) reads for each layer:

$$\begin{split} X_{0}^{n+1} &= X_{0}^{n} - \lambda [\Delta \mathcal{B}^{n}]_{0}, \\ X_{1}^{n+1} &= X_{1}^{n} - \lambda ([\Delta \mathcal{B}^{n}]_{1} + \mathcal{G}(X_{1}^{n}, X_{2}^{n})) + \eta (D(X_{2}^{n}) - D(X_{1}^{n})) + \Delta t \, \tilde{R}_{X,1}^{n}, \\ X_{j}^{n+1} &= X_{j}^{n} - \lambda ([\Delta \mathcal{B}^{n}]_{j} + \mathcal{G}(X_{j}^{n}, X_{j+1}^{n}) - \mathcal{G}(X_{j-1}^{n}, X_{j}^{n})) \\ &\quad + \eta (D(X_{j+1}^{n}) - 2D(X_{j}^{n}) + D(X_{j-1}^{n})) + \lambda \delta_{j,j_{f}} X_{f}^{n} q_{f}^{n} + \Delta t \, \tilde{R}_{X,j}^{n}, \quad j = 2, \dots, N-1, \\ X_{N}^{n+1} &= X_{N}^{n} - \lambda ([\Delta \mathcal{B}^{n}]_{N} - \mathcal{G}(X_{N-1}^{n}, X_{N}^{n})) - \eta (D(X_{N}^{n}) - D(X_{N-1}^{n})) + \Delta t \, \tilde{R}_{X,N}^{n} \\ X_{N+1}^{n+1} &= X_{N+1}^{n} - \lambda [\Delta \mathcal{B}^{n}]_{N+1}. \end{split}$$

To be able to prove an invariant region property for each variable, we want every formula to be a monotone function of each argument, *i.e.*, we wish to have $\partial X_j^{n+1}/\partial X_k^n \geq 0$ for all j, k. For j = k, this can be achieved by invoking (CFL). The problematic terms above are $\lambda[\Delta \mathcal{B}^n]_j$ since they contain the bulk velocity reaction function q^{reac} in (2.18). To see this, we let the characteristic function χ_I be equal to 1 if the statement I is true, otherwise 0. Then

$$\mathcal{B}_{j+1/2} = X_{j+1}q_{j+1/2}\chi_{q_{j+1/2} \le 0} + X_j q_{j+1/2}\chi_{q_{j+1/2} > 0}$$
(4.1)

and hence, for j = 0, ..., N - 1 and k = j + 2, ..., N + 1, we have

$$\begin{aligned} \frac{\partial X_j^{n+1}}{\partial X_k} &= -\lambda \frac{\partial [\Delta \mathcal{B}]_j}{\partial X_k} \\ &= -\lambda \bigg((X_{j+1}\chi_{q_{j+1/2} \le 0} + X_j\chi_{q_{j+1/2} > 0}) \frac{\partial q_{j+1/2}}{\partial X_k} + (X_j\chi_{q_{j-1/2} \le 0} + X_{j-1}\chi_{q_{j-1/2} > 0}) \frac{\partial q_{j-1/2}}{\partial X_k} \bigg) \cdot \end{aligned}$$

The derivatives of $q_{j+1/2}^n$ can have any sign due to the reaction terms. We therefore confine the analysis to the scheme when we set $\mathcal{R}_j := 0, j = 1, ..., N$ in (3.1), *i.e.* $q_{j+1/2}^{\text{reac}} := 0$. Then $q_{j+1/2}$ depends only on time and (3.6) becomes a three-point scheme.

Lemma 4.1. Assume that $0 \le X_j \le X_{\text{max}}$ for all j. Then the Godunov flux $\mathcal{G}_{j+1/2} = \mathcal{G}(X_j, X_{j+1})$, see (3.4), applied on $0 \le f_{\text{b}} \in C^1$ satisfies

$$-\|f_{\mathbf{b}}'\|_{\infty} \leq \frac{\partial \mathcal{G}_{j+1/2}}{\partial X_{j+1}} \leq 0 \leq \frac{\partial \mathcal{G}_{j+1/2}}{\partial X_j} \leq \|f_{\mathbf{b}}'\|_{\infty}, \quad \left|\frac{\partial [\Delta \mathcal{G}]_j}{\partial X_j}\right| \leq \|f_{\mathbf{b}}'\|_{\infty}, \quad \frac{\mathcal{G}_{j+1/2}}{X_j} \leq \|f_{\mathbf{b}}'\|_{\infty}, \quad \frac{\mathcal{G}_{j+1/2}}{X_{j+1}} \leq \|f_{\mathbf{b}}'\|_{\infty}.$$

Proof. If $X_j \leq X_{j+1}$, then $\mathcal{G}_{j+1/2} = \min\{f_b(X_j), f_b(\xi), f_b(X_{j+1})\}$, where $\xi \in (X_j, X_{j+1})$ is a (possible) stationary point of f_b . If $\mathcal{G}_{j+1/2} = f_b(X_j)$, then X_j is the minimum point and the left endpoint of the interval, hence $\partial \mathcal{G}_{j+1/2}/\partial X_j = f'_b(X_j) \geq 0$. Otherwise, $\partial \mathcal{G}_{j+1/2}/\partial X_j = 0$ holds. Similarly, if $X_j > X_{j+1}$, then $\partial \mathcal{G}_{j+1/2}/\partial X_j = 0$ or $= f'_b(X_j) \geq 0$ (the right endpoint X_j is a maximum point). Analogously, $\partial \mathcal{G}_{j+1/2}/\partial X_{j+1} = 0$ or $= f'_b(X_{j+1}) \leq 0$. Combining these results, we get

$$\frac{\partial [\Delta \mathcal{G}]_j}{\partial X_j} \in \{f'_{\mathbf{b}}(X_j), 0, -f'_{\mathbf{b}}(X_j)\}.$$

Assume again $X_j \leq X_{j+1}$, so that $\mathcal{G}_{j+1/2} = \min\{f_{\rm b}(X_j), f_{\rm b}(\xi), f_{\rm b}(X_{j+1})\}$. Then $\mathcal{G}_{j+1/2}/X_j \leq f_{\rm b}(X_j)/X_j$ and $\mathcal{G}_{j+1/2}/X_{j+1} \leq f_{\rm b}(X_{j+1})/X_{j+1}$. If $X_j > X_{j+1}$, then $\mathcal{G}_{j+1/2} = \max\{f_{\rm b}(X_j^n), f_{\rm b}(\xi), f_{\rm b}(X_{j+1}^n)\}$ where $\xi \in (X_{j+1}, X_j)$ is a possible stationary point. Then we have

$$\frac{\mathcal{G}_{j+1/2}}{X_{j+1}} \le \frac{\mathcal{G}_{j+1/2}}{X_j} = \begin{cases} \text{either} & f_{\rm b}(X_j)/X_j, \\ \text{or} & f_{\rm b}(\xi)/X_j \le f_{\rm b}(\xi)/\xi, \\ \text{or} & f_{\rm b}(X_{j+1})/X_j \le f_{\rm b}(X_{j+1})/X_{j+1}. \end{cases}$$

For any $X \in (0, X_{\max})$, take $\overline{\xi} \in (0, X)$ according to the mean-value theorem so that

$$\frac{f_{\rm b}(X)}{X} = \frac{f_{\rm b}(X) - f_{\rm b}(0)}{X} = f_{\rm b}'(\bar{\xi}) \le \|f_{\rm b}'\|_{\infty}.$$

We define the vector of unknown discrete variables $\mathcal{U}_{j}^{n} := (\mathcal{P}_{X,j}^{n}, X_{j}^{n}, \mathcal{P}_{L,j}^{n}, L_{j}^{n}).$

Lemma 4.2. Assume that $\mathcal{U}_{j}^{n} \in \Omega$ for all j. Then the following holds for $i = 1, \ldots, k_{X}$:

$$\left| \frac{\partial \tilde{R}_{X,j}}{\partial X_k} \right| \begin{cases} \leq M & \text{if } k = j, \\ = 0 & \text{if } k \neq j, \end{cases} \quad \left| \frac{\partial \tilde{R}_{X,j}}{\partial P_{X,k}^{(i)}} \right| = X_k \left| \frac{\partial \tilde{R}_{X,j}}{\partial C_k^{(i)}} \right| \begin{cases} \leq X_j M_C & \text{if } k = j, \\ = 0 & \text{if } k \neq j. \end{cases}$$

Proof. The cases $k \neq j$ are trivial. Assume that k = j and differentiate

$$\frac{\partial \tilde{R}_{X,j}}{\partial X_k} = \frac{\partial \tilde{R}_{X,j}}{\partial X_k} \left(\boldsymbol{P}_{X,j} X_j, \bar{\boldsymbol{P}}_{L,j} (\rho_L - r X_j) \right) = \boldsymbol{P}_{X,j}^{\mathrm{T}} \nabla_{\boldsymbol{C}} \tilde{R}_X - r \bar{\boldsymbol{P}}_{L,j}^{\mathrm{T}} \nabla_{\boldsymbol{S}} \tilde{R}_X,$$

where

$$|\boldsymbol{P}_{X,j}^{\mathrm{T}} \nabla_{\boldsymbol{C}} \tilde{R}_{X}| \leq \sum_{i=1}^{k_{X}} |P_{X,j}^{(i)}| \left| \frac{\partial \tilde{R}_{X,j}}{\partial C^{(i)}} \right| \leq M_{C} \sum_{i=1}^{k_{X}} |P_{X,j}^{(i)}| = M_{C},$$

and the second term is estimated similarly. The derivative $|\partial \tilde{R}_{X,j} / \partial P_{X,k}^{(i)}|$ is handled similarly.

We define $a^+ := \max\{a, 0\}$ and $a^- := \min\{a, 0\}$.

Lemma 4.3. If $\mathcal{U}_j^n \in \Omega$, $q_{j+1/2}^{\operatorname{reac},n} := 0$ for all j and (CFL) holds, then $0 \leq X_j^{n+1} \leq 1$ for all j. *Proof.* We write the update formula (3.6a) for $j = 0, \ldots, N+1$ as

$$X_j^{n+1} = \mathcal{H}_X\big(X_{j-1}^n, X_j^n, X_{j+1}^n\big),$$

and we shall show that \mathcal{H}_X is a monotone function in each of its variables. We can write (4.1) as

$$\mathcal{B}_{j+1/2}^n = X_{j+1}q_{j+1/2}^{n,-} + X_j q_{j+1/2}^{n,+},$$

so that

$$\frac{\partial [\Delta \mathcal{B}^n]_j}{\partial X_j^n} = \frac{\partial}{\partial X_j^n} \left(\mathcal{B}_{j+1/2}^n - \mathcal{B}_{j-1/2}^n \right) = \frac{\partial}{\partial X_j^n} \left(X_{j+1}^n q_{j+1/2}^{n,-} + X_j^n q_{j+1/2}^{n,+} - X_j^n q_{j-1/2}^{n,-} - X_{j-1}^n q_{j-1/2}^{n,+} \right)$$
$$= q_{j+1/2}^{n,+} - q_{j-1/2}^{n,-} \le q_{j_f+1/2}^{n,+} - q_{j_f-1/2}^{n,-} = q_u^n + q_e^n = q_f^n \le ||q||_{\infty}.$$

Differentiation of (3.6a) and utilization of (CFL) and Lemmas 4.1 and 4.2 imply

$$\begin{split} \frac{\partial X_0^{n+1}}{\partial X_0^n} &= 1 - \lambda \frac{\partial [\Delta \mathcal{B}^n]_0}{\partial X_0^n} \geq 1 - \lambda \|q\|_{\infty} \geq 0, \qquad \frac{\partial X_0^{n+1}}{\partial X_1^n} = -\lambda q_{1/2}^{n,-} \geq 0, \qquad \frac{\partial X_1^{n+1}}{\partial X_0^n} = \lambda q_{1/2}^{n,+} \geq 0, \\ \frac{\partial X_1^{n+1}}{\partial X_1^n} &= 1 - \lambda \left(\frac{\partial [\Delta \mathcal{B}^n]_1}{\partial X_1^n} + \frac{\partial \mathcal{G}(X_1^n, X_2^n)}{\partial X_1^n} \right) - \eta d(X_1^n) + \Delta t \frac{\partial \tilde{R}_{X,1}^n}{\partial X_1^n} \\ &\geq 1 - \left(\lambda (\|q\|_{\infty} + \|f_b\|_{\infty}) + \eta \|d\|_{\infty} + \Delta t M \right) \geq 0, \\ \frac{\partial X_1^{n+1}}{\partial X_2^n} &= \lambda \left(-q_{3/2}^{n,-} - \frac{\partial \mathcal{G}(X_1^n, X_2^n)}{\partial X_2^n} \right) + \eta d(X_2^n) \geq 0, \\ \frac{\partial X_j^{n+1}}{\partial X_{j-1}^n} &= \lambda \left(q_{j-1/2}^{n,+} + \frac{\partial \mathcal{G}(X_j^n, X_j^n)}{\partial X_{j-1}^n} \right) + \eta d(X_2^n) \geq 0, \qquad j = 2, \dots, N-1, \\ \frac{\partial X_j^n}{\partial X_j^n} &= 1 - \lambda \left(\frac{\partial [\Delta \mathcal{B}^n]_j}{\partial X_j^n} + \frac{\partial [\Delta \mathcal{G}^n]_j}{\partial X_j^n} \right) - 2\eta d(X_j^n) + \Delta t \frac{\partial \tilde{R}_{X,j}^n}{\partial X_j^n} \\ &\geq 1 - \left(\lambda (\|q\|_{\infty} + \|f_b\|_{\infty}) + 2\eta \|d\|_{\infty} + \Delta t M \right) \geq 0, \quad j = 2, \dots, N-1, \\ \frac{\partial X_j^{n+1}}{\partial X_{j+1}^n} &= -\lambda \left(q_{j+1/2}^{n,-} + \frac{\partial \mathcal{G}(X_j^n, X_{j+1}^n)}{\partial X_{j+1}^n} \right) + \eta d(X_{j+1}^n) \geq 0, \quad j = 2, \dots, N-1. \end{split}$$

The remaining derivatives at the boundary z = B are symmetric to those at z = -H. The proved monotonicity of \mathcal{H}_X and the assumptions (2.6) imply that, for $j \neq j_{\rm f}$,

$$0 = \mathcal{H}_X(0,0,0) \le X_j^{n+1} = \mathcal{H}_X(X_{j-1}^n, X_j^n, X_{j+1}^n) \le \mathcal{H}_X(X_{\max}, X_{\max}, X_{\max}) = X_{\max}$$

and for $j = j_{\rm f}$ we have

$$0 \leq \Delta t \, X_{\rm f} q_{\rm f} = \mathcal{H}_X(0,0,0) \leq X_j^{n+1} = \mathcal{H}_X(X_{j-1}^n, X_j^n, X_{j+1}^n) \leq \mathcal{H}_X(X_{\rm max}, X_{\rm max}, X_{\rm max}) = X_{\rm max} - \lambda (q_{\rm u} X_{\rm max} - (q_{\rm u} - q_{\rm f}) X_{\rm max}) + \lambda X_{\rm f} q_{\rm f} = X_{\rm max} - \lambda q_{\rm f} (X_{\rm max} - X_{\rm f}) \leq X_{\rm max}.$$

Lemma 4.4. If $\mathcal{U}_j^n \in \Omega$, $q_{j+1/2}^{\operatorname{reac},n} := 0$ for all j, and (CFL) holds, then $0 \leq \mathbf{P}_{X,j}^{n+1} \leq 1$ for all j. *Proof.* If $X_j^{n+1} = 0$, then $\mathbf{P}_{X,j}^{n+1} := \mathbf{P}_{X,j}^n \in [0,1]$. We assume that $X_j^{n+1} > 0$ and write (3.6b) as

$$\boldsymbol{P}_{X,j}^{n+1} = \frac{\boldsymbol{\Psi}_{X,j}^{n}}{X_{j}^{n+1}}, \quad \text{where} \quad \boldsymbol{\Psi}_{X,j}^{n} := \boldsymbol{P}_{X,j}^{n} X_{j}^{n} + \lambda \Big(- [\Delta(\boldsymbol{P}_{X}^{n} F_{X}^{n})]_{j} + \delta_{j,j_{\mathrm{f}}} \boldsymbol{p}_{X,\mathrm{f}}^{n} X_{\mathrm{f}}^{n} q_{\mathrm{f}}^{n} \Big) + \Delta t \, \gamma_{j} \boldsymbol{R}_{X,j}^{n},$$

and

$$\begin{aligned} [\Delta(\boldsymbol{P}_{X}^{n}F_{X}^{n})]_{j} &= \boldsymbol{P}_{X,j+1/2}^{n}F_{X,j+1/2}^{n} - \boldsymbol{P}_{X,j-1/2}^{n}F_{X,j-1/2}^{n} \\ &= \boldsymbol{P}_{X,j+1}^{n}F_{X,j+1/2}^{n,-} + \boldsymbol{P}_{X,j}^{n}F_{X,j+1/2}^{n,+} - \boldsymbol{P}_{X,j}^{n}F_{X,j-1/2}^{n,-} - \boldsymbol{P}_{X,j-1}^{n}F_{X,j-1/2}^{n,+}. \end{aligned}$$

$$(4.2)$$

Consider $\varPsi_{X,j}^{(k),n}=\varPsi_{X,j}^{(k),n}(P_{X,j}^{(k),n}).$ We have

$$\left(\Psi_{X,j}^{(k),n}\right)'\left(P_{X,j}^{(k),n}\right) = X_j^n - \lambda \left\{F_{X,j+1/2}^{n,+} - F_{X,j-1/2}^{n,-}\right\} + \Delta t \,\gamma_j \frac{\partial R_{X,j}^{(k),n}}{\partial P_{X,j}^{(k),n}}.$$
(4.3)

The last term here is estimated by

$$\Delta t \, \gamma_j \frac{\partial R_{X,j}^{(k),n}}{\partial P_{X,j}^{(i),n}} = X_j^n \Delta t \, \gamma_j \frac{\partial R_{X,j}^{(k),n}}{\partial C_j^{(i),n}} \ge -X_j^n \Delta t \, M_C^X,$$

cf. Lemma 4.2. To estimate the expression within curled brackets in (4.3), we note that $-a^- = (-a)^+$, $(a+b)^+ \le a^+ + b^+$ and start with the first of three terms of $F_X = \mathcal{B} + G - J$:

$$\begin{split} \mathcal{B}_{j+1/2}^{n,+} + (-\mathcal{B}_{j-1/2}^{n})^+ &= \left(X_{j+1}^n q_{j+1/2}^{n,-} + X_j^n q_{j+1/2}^{n,+}\right)^+ + \left(-X_j^n q_{j-1/2}^{n,-} - X_{j-1}^n q_{j-1/2}^{n,+}\right)^+ \\ &\leq X_j^n (q_{j+1/2}^{n,+} - q_{j-1/2}^{n,-}) \leq X_j^n (q_{j_{\rm f}+1/2}^{n,+} - q_{j_{\rm f}+1/2}^{n,-}) \\ &= X_j^n (q_{\rm u}^n + q_{\rm e}^n) = X_j^n q_{\rm f}^n \leq X_j^n \|q\|_{\infty}. \end{split}$$

Since $\mathcal{G}(u, v) > 0$ whenever $f_{\rm b} > 0$ we use Lemma 4.1 to obtain

$$G_{j+1/2}^{n,+} + (-G_{j-1/2}^n)^+ = G_{j+1/2}^{n,+} = G_{j+1/2}^n \le X_j^n \|f_{\rm b}'\|_{\infty}.$$

The term corresponding to -J is estimated by utilizing that D(X) is a non-decreasing function, which is zero for $X \leq X_c$:

$$(-J_{j+1/2}^{n,+})^{+} + J_{j-1/2}^{n,+} = \frac{1}{\Delta z} \left(\left(D(X_{j}^{n}) - D(X_{j+1}^{n}) \right)^{+} + \left(D(X_{j}^{n}) - D(X_{j-1}^{n}) \right)^{+} \right)$$
$$\leq \frac{1}{\Delta z} 2D(X_{j}^{n}) = \frac{2}{\Delta z} \int_{X_{c}}^{X_{j}^{n}} d(s) \, \mathrm{d}s \leq X_{j}^{n} \frac{2\|d\|_{\infty}}{\Delta z}.$$
(4.4)

The CFL condition (CFL) now implies that

$$(\Psi_{X,j}^{(k),n})'(P_{X,j}^{(i),n}) \ge X_j^n \left[1 - \left(\lambda \left(\|q\|_{\infty} + \|f_{\rm b}'\|_{\infty} \right) + 2\eta \|d\|_{\infty} + \Delta t \, M_C^X \right) \right] \ge 0$$

By Assumption (2.5), we have

$$\Psi_{X,j}^{(k),n}(0) = \lambda \left(-P_{X,j+1}^{(k),n} F_{X,j+1/2}^{n,-} + P_{X,j-1}^{(k),n} F_{X,j-1/2}^{n,+} + \delta_{j,j_{\rm f}} p_{X,{\rm f}}^{(k),n} X_{\rm f}^{n} q_{\rm f}^{n} \right) + \Delta t \, \gamma_{j} \left. R_{X,j}^{(k),n} \right|_{P_{X,j}^{(k),n}=0} \ge 0.$$

Hence, $\Psi_{X,j}^{(k),n} = \Psi_{X,j}^{(k),n}(P_{X,j}^{(k),n}) \ge 0$ holds for all $k = 1, ..., k_X$, and since

$$\sum_{k=1}^{k_X} \Psi_{X,j}^{(k),n} = X_j^{n+1}$$

it follows that $\Psi_{X,j}^{(k),n} \leq X_j^{n+1}$. We have proved that $0 \leq \mathbf{P}_{X,j}^{n+1} \leq 1$. **Lemma 4.5.** If $\mathcal{U}_j^n \in \Omega$, $q_{j+1/2}^{\operatorname{reac},n} := 0$ for all j and (CFL) holds, then $0 \leq \mathbf{P}_{L,j}^{n+1} \leq 1$ for all j. *Proof.* We follow the proof of Lemma 4.4 and write (3.6e) as

$$\boldsymbol{P}_{L,j}^{n+1} = \frac{\boldsymbol{\Psi}_{L,j}^{n}}{L_{j}^{n+1}}, \quad \text{where} \quad \boldsymbol{\Psi}_{L,j}^{n} := \boldsymbol{P}_{L,j}^{n} L_{j}^{n} + \lambda \Big(- [\Delta(\boldsymbol{P}_{L}^{n} F_{L}^{n})]_{j} + \delta_{j,j_{\mathrm{f}}} \boldsymbol{p}_{L,\mathrm{f}}^{n} L_{\mathrm{f}}^{n} q_{\mathrm{f}}^{n} \Big) + \Delta t \, \gamma_{j} \boldsymbol{R}_{L,j}^{n}.$$

We consider $\varPsi_{L,j}^{(k),n}=\varPsi_{L,j}^{(k),n}(P_{L,j}^{(k),n})$ and calculate

$$(\Psi_{L,j}^{(k),n})'(P_{L,j}^{(i),n}) = L_j^n - \lambda \left\{ F_{L,j+1/2}^{n,+} - F_{L,j-1/2}^{n,-} \right\} + \Delta t \, \gamma_j \frac{\partial R_{L,j}^{(k),n}}{\partial P_{L,j}^{(k),n}}.$$
(4.5)

For the expression within curled bracket of (4.5), we note that

$$F_{L,j+1/2}^{n,+} = (q_{j+1/2}^n \rho_L - rF_{X,j+1/2}^n)^+$$

= $(q_{j+1/2}^n \rho_L - r\mathcal{B}_{j+1/2}^n - rG_{j+1/2}^n + rJ_{j+1/2}^n)^+ \le \mathcal{T}_1 + rJ_{j+1/2}^{n,+}$

where $\mathcal{T}_1 := (q_{j+1/2}^n \rho_L - r \mathcal{B}_{j+1/2}^n)^+$. Similarly, we obtain

$$(-F_{L,j-1/2}^{n,+})^+ \le \mathcal{T}_2 + rG_{j-1/2}^{n,+} + r(-J_{j-1/2}^n)^+, \quad \mathcal{T}_2 := (-q_{j-1/2}^n\rho_L + r\mathcal{B}_{j-1/2}^n)^+$$

Utilizing $q_{j+1/2}^n = q_{j+1/2}^{n,+} + q_{j+1/2}^{n,-}$ and $\mathcal{B}_{j+1/2}^n = X_{j+1}q_{j+1/2}^{n,-} + X_jq_{j+1/2}^{n,+}$, we get

$$\mathcal{T}_{1} + \mathcal{T}_{2} = \left(q_{j+1/2}^{n,+}(\rho_{L} - rX_{j}^{n}) + q_{j+1/2}^{n,-}(\rho_{L} - rX_{j+1}^{n})\right)^{+} \\ + \left(-q_{j-1/2}^{n,+}(\rho_{L} - rX_{j-1}^{n}) - q_{j-1/2}^{n,-}(\rho_{L} - rX_{j}^{n})\right)^{+} \\ = \left(q_{j+1/2}^{n,+}L_{j}^{n} + q_{j+1/2}^{n,-}L_{j}^{n+1}\right)^{+} + \left(-q_{j-1/2}^{n,+}L_{j-1}^{n} - q_{j-1/2}^{n,-}L_{j}^{n}\right)^{+} \\ \leq \left(q_{j+1/2}^{n,+} - q_{j-1/2}^{n,-}\right)L_{j}^{n} \leq L_{j}^{n} \|q\|_{\infty}.$$

For the rest of the terms, we have from Lemma 4.2 and (4.4):

$$rG_{j-1/2}^{n,+} \le r \|f_{\rm b}\|_{\infty} = \frac{L_j^n}{\rho_L - rX_j^n} r \|f_{\rm b}\|_{\infty} \le \frac{L_j^n}{\rho_X - X_{\rm max}} \|f_{\rm b}\|_{\infty},$$

$$r(-J_{j+1/2}^{n,+})^+ + rJ_{j-1/2}^{n,+} \le \frac{r2D(X_j^n)}{\Delta z} \le \frac{L_j^n}{\rho_X - X_{\rm max}} \frac{2D(X_{\rm max})}{\Delta z}.$$

The reaction term of (4.5) is handled as

$$\Delta t \, \gamma_j \frac{\partial R_{L,j}^{(k),n}}{\partial P_{L,j}^{(k),n}} = \Delta t \, \gamma_j L_j^n \frac{\partial R_{L,j}^{(k),n}}{\partial S_j^{(k),n}} \ge -\Delta t \, L_j^n M_S^L.$$

The CFL condition implies

$$(\Psi_{L,j}^{(k),n})'(P_{L,j}^{(i),n}) \ge L_j^n \left(1 - \lambda \|q\|_{\infty} - \frac{\lambda \|f_{\rm b}\|_{\infty} + 2\eta D(X_{\rm max})}{\rho_X - X_{\rm max}} - \Delta t \, M_S^L\right) \ge 0.$$

As in the proof of Lemma 4.4 we have $\Psi_{L,j}^{(k),n}(0) \ge 0$ by the assumption on $R_L^{(k)}$ corresponding to (2.5). Hence, $\Psi_{L,j}^{(k),n} = \Psi_{L,j}^{(k),n}(P_{L,j}^{(k),n}) \ge 0$ holds for all $k = 1, \ldots, k_X$. Since (see (4.2))

$$\sum_{i=1}^{k_X} [\Delta(P_X^{(i),n}F_X^n)]_j = F_{X,j+1/2}^n - F_{X,j-1/2}^n = [\Delta F_X^n]_j$$

we have, by (3.6c), (3.6d) and (2.18) with $\mathcal{R} = 0$,

$$\sum_{k=1}^{k_L} \Psi_{X,j}^{(k),n} = L_j^n + \lambda \Big(- [\Delta F_L^n]_j + \delta_{j,j_f} L_f^n q_f^n \Big) + \Delta t \gamma_j \tilde{R}_{L,j}^n$$

$$= \rho_L - rX_j^n + \lambda \Big(- \rho_L [\Delta q^n]_j + r[\Delta F_X^n]_j + \delta_{j,j_f} (\rho_L - rX_f^n) q_f^n \Big) - r\Delta t \gamma_j \tilde{R}_{X,j}^n$$

$$= \rho_L - r \Big(X_j^n + \lambda \Big(- [\Delta F_X^n]_j + \delta_{j,j_f} X_f^n q_f^n \Big) + \Delta t \gamma_j \tilde{R}_{X,j}^n \Big) - \lambda \left(\rho_L [\Delta q^n]_j - \delta_{j,j_f} \rho_L q_f^n \right)$$

$$= \rho_L - rX_j^{n+1} - \lambda \rho_L \Big([\Delta q^n]_j - \delta_{j,j_f} q_f^n \Big) = L_j^{n+1} - \lambda \rho_L \Big([\Delta q^n]_j - \delta_{j,j_f} q_f^n \Big) = L_j^{n+1},$$

where we in the latter equality has used (3.2), which implies $[\Delta q^n]_j = 0$ for $j \neq j_f$ and $[\Delta q^n]_{j_f} = q_u^n - (q_u^n - q_f^n) = q_f$. It follows that $\Psi_{L,j}^{(k),n} \leq L_j^{n+1}$ and have proved that $0 \leq \mathbf{P}_{L,j}^{n+1} \leq 1$.

Theorem 4.6. If (2.6) and (CFL) hold, then Ω is invariant under the scheme (3.6) with $q_{j+1/2}^{\text{reac},n} := 0$ for all j and n, i.e., $\mathcal{U}_{j}^{n} \in \Omega \Rightarrow \mathcal{U}_{j}^{n+1} \in \Omega$ for all j and n.

Proof. The bounds on X_j^n , $P_{X,j}^n$ and $P_{L,j}^n$ for all j and n were proved in Lemmas 4.3–4.5. We get $\rho_L - rX_{\max} \leq L_j^{n+1} = \rho_L - rX_j^{n+1} \leq \rho_L$. Summing all equations in (3.6b) and using (3.6a), we get

$$\sum_{i=1}^{k_X} P_{X,j}^{(i),n+1} = 1.$$

By definition (3.6f) we have

$$\sum_{i=1}^{k_L} P_{L,j}^{(i),n+1} = 1.$$

5. Numerical examples

5.1. Preliminaries

The biological reactions are those of a model of denitrification, which is conversion of bound nitrogen to free nitrogen (N₂) that occurs in SSTs in wastewater treatment [7]. The $k_X = 2$ particulate concentrations are X_{OHO} (ordinary heterotrophic organisms) and X_U (undegradable organics), and the $k_L - 1 = 3$ soluble concentrations S_{NO_3} (nitrate), S_S (readily biodegradable substrate) and S_{N_2} (nitrogen), so that $\mathbf{p}_X X = \mathbf{C} = (X_{OHO}, X_U)^T$ and $\mathbf{S} = (S_{NO_3}, S_S, S_{N_2})^T$. The reaction terms are

$$\boldsymbol{R}_{X} = X_{\text{OHO}} \begin{pmatrix} \mu(\boldsymbol{S}) - b \\ f_{\text{P}}b \end{pmatrix} Z(X), \qquad \boldsymbol{R}_{L} = X_{\text{OHO}} \begin{pmatrix} -\frac{1-Y}{2.86Y} \mu(\boldsymbol{S}) \\ -\frac{1}{Y} \mu(\boldsymbol{S}) + (1-f_{\text{P}})b \\ \frac{1-Y}{2.86Y} \mu(\boldsymbol{S}) \\ 0 \end{pmatrix}$$

where Y = 0.67 is a yield factor, $b = 6.94 \times 10^{-6} \text{ s}^{-1}$ is the decay rate of heterotrophic organisms and $f_{\rm P} = 0.2$ is the portion of these that decays to undegradable organics. The continuous function Z(X) should be equal to one for low concentrations and decrease to zero at some large concentration so that the second technical assumption in (2.6) is satisfied. The function Z(X) should not influence the condition (CFL). We have used $Z(X) \equiv 1$ for all simulations and still obtained bounded solutions. Hence, after some trial simulations, the maximum concentration $X_{\rm max}$ can be defined and used in (CFL). We have used $X_{\rm max} = 30 \text{ kg/m}^3$. The specific growth rate function is

$$\mu(\mathbf{S}) := \mu_{\max} \frac{S_{\mathrm{NO}_3}}{K_{\mathrm{NO}_3} + S_{\mathrm{NO}_3}} \frac{S_{\mathrm{S}}}{K_{\mathrm{S}} + S_{\mathrm{S}}}$$

where $\mu_{\text{max}} = 5.56 \times 10^{-5} \text{ s}^{-1}$, $K_{\text{NO}_3} = 5 \times 10^{-4} \text{ kg/m}^3$, $K_{\text{S}} = 0.02 \text{ kg/m}^3$. We get

$$\tilde{R}_X = \left(\mu(\boldsymbol{S}) - (1 - f_{\rm P})b\right) X_{\rm OHO} Z(X), \qquad \tilde{R}_L = -\left(\frac{\mu(\boldsymbol{S})}{Y} - (1 - f_{\rm P})b\right) X_{\rm OHO}.$$

In light of (2.12), this implies

$$|\mathcal{R}(\boldsymbol{C},\boldsymbol{S})| \le \left(\mu_{\max} \left| \frac{1}{\rho_X} - \frac{1}{\rho_L Y} \right| + (1 - f_{\mathrm{P}}) b \left| \frac{1}{\rho_X} - \frac{1}{\rho_L} \right| \right) X_{\max} = 7.0792 \times 10^{-7} \text{ m/s},$$

so that q^{reac} is negligibly small in comparison to the bulk velocities q_e and q_u in continuous sedimentation. It is also negligible in batch sedimentation (although $q_e = q_u = 0$), where the interval of settling velocities is $[0, v_0]$ with $v_0 = 1.76 \times 10^{-3}$ m/s.



FIGURE 2. Graphs of the constitutive functions used in Examples 1 and 2 (*dashed blue*) and 3 (*solid red*): (a) hindered settling velocity, (b) batch settling flux, (c) effective solids stress, (d) compression.

For Examples 1 and 2, we choose the constitutive functions for hindered settling and compression (where $Z(X) \equiv 1$ is used in the simulations)

$$v_{\rm hs}(X) = \frac{v_0}{1 + (X/\bar{X})^{\bar{r}}} Z(X), \qquad \sigma_{\rm e}(X) = \begin{cases} 0 & \text{for} \quad X < X_{\rm c}, \\ \alpha(X - X_{\rm c}) & \text{for} \quad X > X_{\rm c}, \end{cases}$$

where $v_0 = 1.76 \times 10^{-3}$ m/s, $\bar{X} = 3.87$ kg/m³, $\bar{r} = 3.58$, $\alpha = 0.2$ m²/s² and $X_c = 5$ kg/m³. Other constants used are A = 400 m², $\rho_X = 1050$ kg/m³, $\rho_L = 998$ kg/m³ and g = 9.81 m/s². For Example 3, we choose the constitutive functions

$$v_{\rm hs}(X) = v_0 e^{-r_{\rm V} X} Z(X), \qquad \sigma_{\rm e}(X) = \begin{cases} 0 & \text{for } X < X_{\rm c}, \\ \tilde{\alpha} \log\left((X - X_{\rm c} + \tilde{\beta})/\tilde{\beta}\right) & \text{for } X > X_{\rm c}, \end{cases}$$

with $r_{\rm V} = 0.55 \text{ m}^3/\text{kg}$, $\tilde{\alpha} = 7.0 \text{ Pa}$ and $\tilde{\beta} = 2.9 \text{ kg/m}^3$. Graphs of the constitutive functions are shown in Figure 2. All other parameters are as in Examples 1 and 2.

All simulations start from a steady state obtained by a long-time simulation. For Examples 1 and 2, $Q_f(0) = 175 \text{ m}^3/\text{h}$, $Q_u(0) = 22 \text{ m}^3/\text{h}$ and $X_f(0) = 3.5 \text{ kg/m}^3$, whereas Example 3 starts from $Q_f(0) = 100 \text{ m}^3/\text{h}$, $Q_u(0) = 25 \text{ m}^3/\text{h}$, and $X_f(0) = 3 \text{ kg/m}^3$. These feed inputs are kept constant for a while, but then varied with time according to Figure 3. The vector of particulate feed percentages is $\mathbf{p}_{X,f}(0) = (5/7, 2/7)^{\text{T}}$ in all examples, and this value is varied only in Example 2; see Figure 3c. The feed substrate concentrations have the following constant values during all simulations: $S_{\text{S},f}(t) = 9.00 \times 10^{-4} \text{ kg/m}^3$, $S_{\text{NO}_3,f}(t) = 6.00 \times 10^{-3} \text{ kg/m}^3$, and $S_{\text{N}_2,f}(t) = 0 \text{ kg/m}^3$. Different simulation times are used and the values of Δt for different N determined from (CFL) are given in Table 1. For fine mesh resolutions, the large values of β_X and β_{P_X} establish the expected fact that the time step Δt is limited by the second-order derivative term modelling compression.

5.2. Example 1: Variations of feed flow and particle concentration

We choose the volume flows $Q_{\rm f}(t)$, $Q_{\rm u}(t)$ and the feed concentration $X_{\rm f}(t)$ as piecewise constant functions of time specified in Figures 3(a) and 3(b), respectively, and we let $p_{X,{\rm f}}$ and $p_{L,{\rm f}}$ be constant in time. We have chosen these extreme variations to test the scheme. The initial steady state is kept during the first hour of the simulation; see Figure 4. There is a sludge blanket, *i.e.*, a discontinuity from a low concentration up to the critical concentration $X_c = 5 \text{ kg/m}^3$ separating the hyperbolic and parabolic regions; see also Figure 5(a). The movement of this discontinuity is of particular interest to model in wastewater treatment. Below the discontinuity, the solution is continuous because of the compression effect. At t = 4 h, the step increase in $Q_{\rm f}(t)$, decrease in $Q_{\rm e}(t)$ and simultaneous increase in the fed bacteria $X_{\rm OHO}$ to the SST imply a rapidly rising sludge



FIGURE 3. Examples 1 (a, b), 2 (c) and 3 (d, e): (a, d, e) volumetric flows, (b) solids feed concentration, (c) particulate feed percentages. The piecewise constant values and time points of changes are indicated.

TABLE 1. Coefficients for the calculation of the CFL condition (CFL), where $\kappa := \|q\|_{\infty}/\Delta z$.

		Examples 1 and 2					Example 3				
		κ	β_X	β_{P_X}	β_{P_L}		κ	β_X	β_{P_X}	β_{P_L}	
N	$\Delta z~[{ m m}]$	$[s^{-1}]$	$[s^{-1}]$	$[s^{-1}]$	$[s^{-1}]$	$\Delta t \ [s]$	$[s^{-1}]$	$[s^{-1}]$	$[s^{-1}]$	$[s^{-1}]$	Δt [s]
10	0.40000	0.001	3.178	0.007	0.166	0.31147	0.001	3.182	0.011	0.166	0.31105
30	0.13333	0.003	3.207	0.037	0.166	0.30841	0.003	3.247	0.076	0.167	0.30469
90	0.04444	0.009	3.420	0.249	0.167	0.28875	0.008	3.776	0.606	0.167	0.26164
270	0.01481	0.027	5.175	2.004	0.171	0.19034	0.023	8.384	5.213	0.173	0.11777
405	0.00988	0.040	7.591	4.420	0.176	0.12974	0.035	14.810	11.640	0.181	0.06669
810	0.00494	0.081	20.494	17.324	0.205	0.04812	0.070	49.373	46.202	0.223	0.02002
2430	0.00165	0.243	156.944	153.774	0.515	0.00630	0.211	416.852	413.681	0.670	0.00237

blanket that reaches the top of the SST around t = 7 h, which means that the SST becomes overloaded with solids leaving also through the effluent. The fast reactions imply that the soluble nitrate (NO₃) is quickly converted to N₂ in regions where the bacteria OHO are present, which is below the sludge blanket. At the end of the simulation, this phenomenon is clearly seen by the peak near z = 0 in Figure 4(d) and the corresponding dip in Figures 4(f) and 5(f).

5.3. Example 2: Variations of the feed percentages

In this case $Q_{\rm f}$, $Q_{\rm u}$, $X_{\rm f}$ and $p_{L,\rm f}$ are kept the same constants as for the initial steady-state solution. Only $p_{X,\rm f}(t)$ is chosen as a periodically varying function of time as shown in Figure 3(c). The resulting waves in the particle components through from the feed to the bottom are shown in Figures 6(b) and 6(c). A part of the incoming nitrate (NO₃) is transported upwards to the effluent without undergoing any reaction since there



FIGURE 4. Example 1: Simulation of reactive settling in an SST starting from a stationary state followed by variations of the volumetric flows $Q_{\rm u}$ and $Q_{\rm f}$ and of the solids feed concentration $X_{\rm f}$. Here and in Figures 6 and 8, the solution displayed is the reference solution obtained with $N = N_{\rm ref} = 2430$ projected onto a coarser visual grid, and plots (d) and (g) have been rotated.

is no solids in the clarification zone. The need for a high mesh resolution for such extremely varying particle concentrations can be seen in Figures 7(a)-7(c).

5.4. Example 3: Transitions between steady states

In this simulation, shown in Figures 8 and 9, only the volumetric flows $Q_f(t)$ and $Q_u(t)$ are varied in a piecewise constant way according to Figures 3(d) and 3(e). After 7 h the volumetric flows are set to constant values slightly different from the initial ones and a new steady state arises after a transient period with a sludge blanket rising into the clarification zone above the feed inlet. The rise of this discontinuity ends at t = 3 h where $Q_f(t)$ is lowered substantially. After t = 4 h, the sludge blanket sinks because of the increased volumetric underflow $Q_u(t)$. The transport of N₂ in the thickening zone is in accordance with the changes of the bulk flows. The short appearance of particulate bacteria in the clarification zone implies that some of the otherwise non-reacted overflow of nitrate (NO₃) is converted to N₂; see Figures 8(d) and 8(f).

5.5. Approximate errors

For a given spatial discretization $\Delta z = (B + H)/N$, we denote by $X_{\text{OHO},N}$ the piecewiese constant function with $X_{\text{OHO},N}(z,t) = P_{X,j}^{(1),n}X_j^n$ if $z \in (z_{j-1/2}, z_{j+1/2}]$ and $t \in (t_{n-1}, t_n]$, and define the approximate relative L^1



FIGURE 5. Example 1: Numerical solutions for coarse discretizations (N = 10, 30, 90) at (a), (d) t = 3 h, (b, e) t = 5 h, (c), (f) t = 7 h. The reference solution $(N = N_{\text{ref}} = 2430)$ is included.



FIGURE 6. Example 2: Simulation starting from a stationary state followed by variations of the feed percentages of the substrates.



FIGURE 7. Example 2: Numerical solutions for coarse discretizations (N = 10, 30, 90) at (a), (d) t = 8 h, (b), (e) t = 12 h and (c), (f) t = 18 h. The reference solution $(N = N_{ref} = 2430)$ is included.



FIGURE 8. Example 3: Simulation starting and ending in two different steady states.



FIGURE 9. Example 3: Numerical solutions for coarse discretizations (N = 10, 30, 90) at (a), (d) t = 3 h, (b), (e) t = 5 h and (c), (f) t = 10 h. The reference solution $(N = N_{ref} = 2430)$ is included.

TABLE 2. Total approximate relative L^1 errors $e_N^{\text{rel}}(t)$, convergence rates $\theta(t)$ and CPU times for selected examples and indicated simulated times.

	Example 1, $t = 3 \mathrm{h}$			Exa	mple 1, t	$=5 \mathrm{h}$	Example 1, $t = 7 \mathrm{h}$			
N	$e_N^{\rm rel}(t)$	$\theta(t)$	$\mathrm{CPU}\left[s \right]$	$e_N^{\rm rel}(t)$	$\theta(t)$	$\mathrm{CPU}\left[s \right]$	$e_N^{\rm rel}(t)$	$\theta(t)$	$\mathrm{CPU}\left[s \right]$	
10	0.570	-	0.08	0.639	_	0.13	0.257	_	0.17	
30	0.233	0.812	0.19	0.324	0.618	0.31	0.133	0.598	0.43	
90	0.085	0.924	0.56	0.136	0.791	0.92	0.056	0.789	1.26	
270	0.029	0.973	2.41	0.047	0.971	4.03	0.024	0.772	5.44	
405	0.018	1.190	5.28	0.031	1.045	8.66	0.018	0.732	11.97	
810	0.007	1.264	28.18	0.012	1.306	47.35	0.007	1.276	65.06	
	Example 2, $t = 8 \mathrm{h}$			Exar	nple 2, t	= 12 h	Example 2, $t = 18 \mathrm{h}$			
10	0.679	-	0.24	0.646	—	0.30	0.722	—	0.55	
30	0.497	0.284	0.48	0.711	-0.087	0.72	0.789	-0.080	1.04	
90	0.317	0.410	1.40	0.537	0.255	2.08	0.632	0.201	3.10	
270	0.156	0.643	6.05	0.293	0.553	9.07	0.373	0.480	13.42	
405	0.113	0.797	13.61	0.212	0.801	20.26	0.276	0.744	30.25	
810	0.056	1.003	75.02	0.105	1.006	110.58	0.138	1.004	167.98	
	Exa	mple 3, t	= 3 h	Exa	mple 3, t	$=5\mathrm{h}$	Example 3, $t = 10 \mathrm{h}$			
10	0.302	-	0.05	0.381	-	0.08	0.332	-	0.15	
30	0.102	0.990	0.12	0.226	0.477	0.19	0.183	0.540	0.35	
90	0.053	0.599	0.32	0.120	0.572	0.50	0.072	0.855	0.92	
270	0.020	0.878	0.94	0.054	0.722	1.50	0.029	0.817	2.78	
405	0.012	1.299	1.53	0.039	0.809	2.41	0.022	0.735	4.37	
810	0.005	1.220	3.96	0.018	1.107	6.28	0.009	1.207	11.64	

error

$$e_{N,X_{\text{OHO}}}^{\text{rel}}(t) := \frac{\|(X_{\text{OHO},N} - X_{\text{OHO},N_{\text{ref}}})(\cdot,t)\|_{L^{1}(-H,B)}}{\|X_{\text{OHO},N_{\text{ref}}}(\cdot,t)\|_{L^{1}(-H,B)}},$$

where $N_{\rm ref} = 2430$. The corresponding quantities for $X_{\rm U}$, $S_{\rm NO_3}$, $S_{\rm N_2}$ and $S_{\rm S}$ are defined in the same way. We define the total approximate relative error

$$e_{N}^{\rm rel}(t) := e_{N,X_{\rm OHO}}^{\rm rel}(t) + e_{N,X_{\rm U}}^{\rm rel}(t) + e_{N,S_{\rm NO_3}}^{\rm rel}(t) + e_{N,S_{\rm N_2}}^{\rm rel}(t) + e_{N,S_{\rm S}}^{\rm rel}(t)$$

and the observed convergence rate between two discretizations $N = N_1$ and $N = N_2$,

$$\theta(t) := -\frac{\log\left(e_{N_1}^{\text{rel}}(t)/e_{N_2}^{\text{rel}}(t)\right)}{\log(N_1/N_2)}$$

Table 2 shows values of $e_N^{\text{rel}}(t)$, $\theta(t)$ and corresponding CPU times, for selected examples and times of those used in Figures 5, 7 and 9. We observe that all approximate total relative errors tend to zero as N is increased. The rates θ assume values between zero and one for $N \leq 270$ (among the selected values of N), as should be expected for a first-order discretization in time and for the convective flux (see [11, 12] for comparable results). The values $\theta > 1$ observed for N = 810 do, however, alert to the limitations of error analysis via a reference solution with $N_{\text{ref}} = 2430$.

6. Concluding Remarks

The one-dimensional model equations (1.1) for continuous sedimentation of multi-component solid particles in a liquid, containing several soluble components, with possible biochemical reactions have been derived. Previous model ingredients such as hindered settling and compression at high concentrations have been complemented with the transport and reactions of components. Focus has been laid on the application to wastewater treatment, for which special simplifying model assumptions have been made. One assumption is that the solid and liquid phases have constant densities. This is not restrictive in wastewater treatment, where the concentrations of the soluble substrates are negligible in the water component.

Although there are only two densities, their difference and the reactions cause a volume change of the suspension; see the bulk velocity component due to reactions q^{reac} of the total bulk velocity q in (2.19). In wastewater treatment, q^{reac} seems to be negligible. Hence, our numerical scheme will produce very similar solutions when setting $q^{\text{reac}} = 0$. The latter was, however, done to obtain a three-point explicit scheme with the monotonicity properties that lead to the invariant-region property; see Theorem 4.6. For other applications with larger q^{reac} , our scheme can still be used.

While this paper is focussed on the model formulation, the development of a numerical scheme and its applications, the well-posedness analysis is still open. The basic difficulties associated with the model (1.1) are discussed in Section 1.2. The numerical results confirm that solutions are discontinuous due to changes in the definitions of fluxes across the inlet z = 0 and outlets z = -H, B (visible, for instance, in Figure 4a at z = 0), the nonlinearity of the flux as a function of X, and the strongly degenerating behaviour of D. The combined effect of both becomes visible, for instance, in the sharpness of the solution at the typical sludge blanket in Figure 4a, which moves up into the clarification zone and eventually overloads the SST. Moreover, the invariant-region principle (Thm. 4.6) is not only an asset in itself for practical purposes (concentrations are nonnegative and percentages satisfy their natural requirements, properties that are not automatically built into finite volume schemes [25]), but along with the underlying monotonicity could also form an important step towards proving existence of a weak solution of the problem via convergence of a scheme, as was done in [11, 12, 28] and many other works for related problems.

Our numerical scheme entails the well-known drastic growth of CPU time concomitant with mesh refinement for explicit discretizations of convection-diffusion-reaction problems. It is therefore highly desirable to develop more efficient solvers for the model, for example, a semi-implicit variant of the scheme that would limit this

growth [8]. Such a scheme would be based on an implicit discretization of the diffusive terms arising in the fully discrete formulation (3.6), with the consequence that the corresponding CFL condition imposes a limitation on $\Delta t/\Delta z$ instead of $\Delta t/\Delta z^2$ as in the present treatment (cf. (CFL), (3.7)). While parts of the analysis related to the invariant-region principle can easily be adapted to such an implicit treatment (for instance, Lem. 4.3 can be adapted to a semi-implicit scheme by following [8], (Lem. 3.2)), it is not obvious how to define (in the semi-implicit case) several quantities, for instance the analogue of $F_{X,j+1/2}^n$, that arise in the update formulas for the percentage vectors, (3.6b) and (3.6e). We therefore leave the definition of efficient semi-implicit or implicit-explicit (IMEX) schemes as an open research problem.

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References

- R. Adimurthi, Dutta, G.D. Veerappa Gowda and J. Jaffré, Monotone (A, B) entropy stable numerical scheme for scalar conservation laws with discontinuous flux. ESAIM: M2AN 48 (2014) 1725–1755.
- [2] J. Alex, S.G.E. Rönner-Holm, M. Hunze and N. C. Holm, A combined hydraulic and biological SBR model. Wat. Sci. Tech. 64 (2011) 1025–1031
- [3] T. Arbogast, C.-S. Huang and T.F. Russell, A locally conservative Eulerian-Lagrangian method for a model two-phase flow problem in a one-dimensional porous medium. SIAM J. Sci. Comput. 34 (2012) A1950–A1974.
- [4] J. Balbás and G. Hernández-Dueñas, A positivity preserving central scheme for shallow water flows in channels with wet-dry states. ESAIM: M2AN 48 (2014) 665–696.
- [5] O. Bernard, A.-C. Boulanger, M.-O. Bristeau and J. Sainte-Marie, A 2d model for hydrodynamics and biology coupling applied to algae growth simulations. ESAIM: M2AN 47 (2013) 1387–1412.
- S. Borazjani, A.J. Roberts and P. Bedrikovetsky, Splitting in systems of PDEs for two-phase multicomponent flow in porous media. Appl. Math. Letters 53 (2016) 25–32.
- [7] R. Bürger, J. Careaga, S. Diehl, C. Mejías, I. Nopens and P.A. Vanrolleghem, Simulations of reactive settling of activated sludge with a reduced biokinetic model. *Comput. Chem. Eng.* 92 (2016) 216–229.
- [8] R. Bürger, A. Coronel and M. Sepúlveda, A semi-implicit monotone difference scheme for an initial-boundary value problem of a strongly degenerate parabolic equation modeling sedimentation-consolidation processes. Math. Comput. 75 (2006) 91–112.
- [9] R. Bürger, S. Diehl, S. Farås, I. Nopens and E. Torfs, A consistent modelling methodology for secondary settling tanks: A reliable numerical method. *Water Sci. Tech.* 68 (2013) 192–208.
- [10] R. Bürger, S. Diehl and I. Nopens, A consistent modelling methodology for secondary settling tanks in wastewater treatment. Water Res. 45 (2011) 2247–2260.
- [11] R. Bürger, K.H. Karlsen, N.H. Risebro and J.D. Towers, Well-posedness in BV_t and convergence of a difference scheme for continuous sedimentation in ideal clarifier-thickener units. Numer. Math. 97 (2004) 25–65.
- [12] R. Bürger, K.H. Karlsen and J.D. Towers, A model of continuous sedimentation of flocculated suspensions in clarifier-thickener units. SIAM J. Appl. Math. 65 (2005) 882–940.
- [13] R. Bürger, R. Ruiz, K. Schneider and M. Sepúlveda, Fully adaptive multiresolution schemes for strongly degenerate parabolic equations in one space dimension. ESAIM: Math. Modell. Num. Anal. 42 (2008) 535–563.
- [14] S. Diehl, On scalar conservation laws with point source and discontinuous flux function. SIAM J. Math. Anal. 26 (1995) 1425–1451.
- [15] S. Diehl, A conservation law with point source and discontinuous flux function modelling continuous sedimentation. SIAM J. Appl. Math. 56 (1996) 388–419.
- [16] S. Diehl, Continuous sedimentation of multi-component particles. Math. Meth. Appl. Sci. 20 (1997) 1345–1364.
- [17] S. Diehl, A uniqueness condition for nonlinear convection-diffusion equations with discontinuous coefficients. J. Hyperbolic Diff. Equ. 6 (2009) 127–159.
- [18] D.A. Drew and S.L. Passman. Theory of Multicomponent Fluids, volume 135, Springer-Verlag, New York (1999).
- [19] X. Flores-Alsina, K.V. Gernaey and U. Jeppsson, Benchmarking biological nutrient removal in wastewater treatment plants: Influence of mathematical model assumptions. Water Sci. Tech. 65 (2012) 1496–1505.
- [20] K.V. Gernaey, U. Jeppsson, D.J. Batstone and P. Ingildsen, Impact of reactive settler models on simulated WWTP performance. Water Sci. Tech. 53 (2006) 159–167.
- [21] T. Gimse and N.H. Risebro, Solution of the Cauchy problem for a conservation law with a discontinuous flux function. SIAM J. Math. Anal. 23 (1992) 635–648.
- [22] J.M.N.T. Gray and C. Ancey, Multi-component particle-size segregation in shallow granular avalanches. J. Fluid Mech. 678 (2011) 535–588.

- [23] J. Guerrero, X. Flores-Alsina, A. Guisasola, J.A. Baeza and K.V. Gernaey, Effect of nitrite, limited reactive settler and plant design configuration on the predicted performance of simultaneous C/N/P removal WWTPs. *Bioresource Tech.* 136 (2013) 680–688.
- [24] J. Hamilton, R. Jain, P. Antoniou, S.A. Svoronos, B. Koopman and G. Lyberatos, Modeling and pilot-scale experimental verification for predenitrification process. J. Environ. Eng. 118 (1992) 38–55.
- [25] S. Jaouen and F. Lagoutière, Numerical transport of an arbitrary number of components. Computer Methods Appl. Mech. Eng. 196 (2007) 3127–3140.
- [26] K.H. Karlsen and N.H. Risebro, On the uniqueness and stability of entropy solutions of nonlinear degenerate parabolic equations with rough coefficients. Discrete Continuous Dynamical Syst. 9 (2003) 1081–1104.
- [27] K.H. Karlsen, N.H. Risebro and E.B. Storrøsten, On the convergence rate of finite difference methods for degenerate convectiondiffusion equations in several space dimensions. ESAIM: M2AN 50 (2016) 499–539.
- [28] K.H. Karlsen, N.H. Risebro and J.D. Towers, Upwind difference approximations for degenerate parabolic convection-diffusion equations with a discontinuous coefficient. IMA J. Numer. Anal. 22 (2002) 623–664.
- [29] K.H. Karlsen, N.H. Risebro and J.D. Towers, L¹ stability for entropy solutions of nonlinear degenerate parabolic convectiondiffusion equations with discontinuous coefficients. Trans. Royal Norwegian Society Sci. Letters (Skr. K. Nor. Vidensk. Selsk.) 3 (2003) 49.
- [30] B. Li and M.K. Stenstrom, Practical identifiability and uncertainty analysis of the one-dimensional hindered-compression continuous settling model. Water Res. 90 (2016) 235–246.
- [31] Z. Li, R. Qi, B. Wang, Z. Zou, G. Wei and M. Yang, Cost-performance analysis of nutrient removal in a full-scale oxidation ditch process based on kinetic modeling. J. Environ. Sci. 25 (2013) 26–32.
- [32] G.S. Ostace, V.M. Cristea and P.S. Agachi, Evaluation of different control strategies of the waste water treatment plant based on a modified activated sludge model no. 3. Environ. Eng. Manag. J. 11 (2012) 147–164.
- [33] B. Parent, Positivity-preserving high-resolution schemes for systems of conservation laws. J. Comp. Phys. 231 (2012) 173–189.
- [34] V.V. Shelukhin, Quasistationary sedimentation with adsorption. J. Appl. Mech. Tech. Phys. 46 (2005) 513–522.
- [35] L. Svarovsky, Countercurrent washing of solids, Edited by Ladislav Svarovsky. In: Solid-Liquid Separation, chap. 15. Butterworth Heinemann, Oxford, 4th edition edition (2001), 442–475.
- [36] E. Torfs, T. Maere, R. Bürger, S. Diehl and I. Nopens, Impact on sludge inventory and control strategies using the benchmark simulation model no. 1 with the Bürger-Diehl settler model. *Water Sci. Tech.* 71 (2015) 1524–1535.