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1. Introduction

1.1. Motivation

ABSTRACT

Denitrification during the sedimentation process in secondary settlers in waste-water treatment plants has been reported to be still a significant problem. The modelling of such a process with the conservation of mass leads to a nonlinear convection–diffusion–reaction partial differential equation, which needs non-standard numerical methods to obtain reliable simulations. The purpose of this study is to provide a first extension of the Bürger–Diehl settler model, which models sedimentation without reactions, to include biological reactions. This is done with a reduced biokinetic model that contains only the relevant particulate and soluble components. Furthermore, the development is limited to batch settling. The final model describes the last settling stage of a sequencing batch reactor with denitrification. The main result of the paper is a numerical scheme that is tested for simulations with several initial conditions.

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Most models of the activated sludge process in wastewater treatment plants (WWTPs) are based on the assumption that all reactions occur in the biological reactor and that there are no reactions in the secondary settling tank (SST) (Gernaey et al., 2014). It is, however, well known that certain biological reactions can occur in the settler. In particular, at long residence times and incomplete denitrification in the upstream bioreactor, denitrification can take place at the bottom of the tank, where the concentration of sludge is high, nitrate levels are substantial, biomass decay operates, and no oxygen is present. Siegrist et al. (1995) and Koch et al. (1999) reported measurements from three plants showing that of the total

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http://dx.doi.org/10.1016/j.compchemeng.2016.04.037 0098-1354/© 2016 Elsevier Ltd. All rights reserved. denitrification in each plant, 15%, 30% and 37% occurred in the settler, respectively. This is problematic since the produced N_2 can lead to bubbles that can attach to the sludge flocs, reduce their density, and lead to floating sludge which is disastrous for a settler. Thus, mathematical models that are able to capture the mechanical sedimentation–compression process in a SST in combination with biological reactions, in particular denitrification, are urgently needed to allow for the simulation of operational scenarios.

We are interested in modelling reactive settling, which is a process where biological conversions and physical sedimentation occur simultaneously. To describe the settling process, a consistent methodology was presented by Bürger et al. (2011) which considers both hindered and compression settling. Biological conversion processes in WWTPs are well known and dedicated models are available (Henze et al., 1987). However, combining biological and settling processes is not straightforward as it requires the extension of existing model equations as well as the development of a numerical method to deal with this extended set of equations.

It is the purpose of this paper to advance a spatially onedimensional, dynamical (time-dependent) deterministic model for this process of "reactive settling", formulated as five scalar coupled partial differential equations (PDEs) that represent the mass balances for two particulate and three soluble components. The presentation includes a detailed description of a method for







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numerical solution of the PDE model, and therefore for numerical simulation of reactive settling.

1.2. Related work

A couple of modelling approaches of reactive settling can be found in the literature. Gernaey et al. (2006) presented a simulation study of two different models to account for the reactions taking place in the settler. Both models use the simulation model by Takács et al. (1991) for the sedimentation process. The first model includes an extra model block in the return sludge line consisting of an empirical, algebraic elimination of oxygen and nitrate to account for the reactions in the settler. It is obvious that this first approach does not model the combination of sedimentation and reactions. The second model consists in placing the entire activated sludge model no. 1 (ASM1) model by Henze et al. (1987), modelling the bioreactions, in each of the 10 layers in the Takács settler model. Improvements in nitrogen removal predictions were obtained and the first model was recommended mainly because of the much larger computational cost for the second one, but also because the second model overestimates the reactive capacity of the settler.

Further studies with the second model type and different ASMx models were reported by Flores-Alsina et al. (2012), Ostace et al. (2012) and Guerrero et al. (2013). To compensate for the overestimation of the 10-layer reactive settler model, Guerrero et al. (2013) introduced a reduction factor to the kinetics. Such factors are not present in the original mass balances and it is therefore not in agreement with a consistent modelling methodology (Bürger et al., 2011) to introduce any such as a compensation for some other phenomenon—in this case the coarse spatial discretization (10 layers) of the settler for the numerical simulation.

Already without reactions, the Takács simulation model is not recommended because of failure of agreement with the solutions of the conservation of mass partial differential equation (PDE) in certain situations (Jeppsson and Diehl, 1996a; Bürger et al., 2011, 2012a), but also for other shortcomings during normal operating conditions specifically during wet weather (Torfs et al., 2015).

A related application is reactive settling occurring in sequencing batch reactors (SBRs), for which modelling approaches without PDEs can be found (Kazmi and Furumai, 2000a,b; Kazmi et al., 2001; Alex et al., 2011). Keller and Yuan (2002) modelled SBRs without reactive settling. SBRs are processes in which the bioreaction and settling processes occur in the same reactor, but sequenced in time, with reactor filling, reaction, settling and draw phases occurring sequentially in time rather than in space.

Convection-diffusion-reaction PDEs arise in many models of physical, chemical and biological processes. For the present nonlinear process of simultaneous sedimentation and reactions, PDE models and appropriate numerical methods are scarce in literature. A related application is a rotating wall vessel bioreactor developed by the National Aeronautics and Space Administration (NASA), USA, and used during the launch and landing of space shuttles to protect cultured cells from high shear forces. For this bioreactor, Chao et al. (2015) presented a two-dimensional convection-diffusion-reaction model, simulated it with available finite-element-method software and validated against experimental data.

1.3. Novelty of this work

When only the settling process is considered, the settling tanks can be modelled by a single PDE describing the change of particulate concentration in depth. However, when biological reactions are added, the sludge can no longer be considered as a single particulate phase as different activated sludge components will be involved in different biological reactions. Moreover, additional equations to describe the concentration of soluble components over the depth of the settling tank need to be added. Hence, moving from a non-reactive settler to a reactive settler model does not only include additional rate expressions to account for biological reactions but also increases the number of state variables from a single particulate concentration to several particulate components in combination with soluble components. In this contribution, the settling model presented by Bürger et al. (2011, 2013), called the Bürger–Diehl model, is extended with a reduced biological model where only denitrification reactions are considered.

The Bürger–Diehl model originates from the conservation of mass and can be stated as a scalar, nonlinear PDE for the sludge concentration as function of depth and time. Moreover, the Bürger–Diehl model has shown to provide a more realistic representation of the sludge blanket height and thus the sludge accumulation in a secondary clarifier (Torfs et al., 2015) which is an important driving factor for the denitrification process. It is the purpose of this contribution to make a first step towards extending these advances for the numerical treatment of non-reactive settling to the reactive case. To this end, we focus on a reduced-order problem for the biological reactions and confine to batch sedimentation in a closed vessel as a first approach.

We are interested in modelling reactive settling with a consistent modelling methodology (Bürger et al., 2011) by starting with the mass balances and using appropriate numerical methods for the discretization of the model PDEs. Despite the simplicity of our reduced model, it accounts for three constitutive assumptions that determine its mathematical nature:

- (i) the hindered settling of the flocculated particles;
- (ii) compression of the flocculated particles at high concentrations when a network is formed;
- (iii) reaction terms containing nonlinear growth rate kinetics and a constant decay rate of biomass.

Properties (i) and (ii) are already realized in the Bürger–Diehl model described in a number of previous papers (Bürger et al., 2011, 2013; Torfs et al., 2015). The combination of all three properties (i)–(iii) in the present PDE-based model, and the numerical method presented for its solution constitute, however, a new (original) contribution.

1.4. Outline of the paper

The remainder of this paper is organized as follows. In Section 2 we introduce the governing model, which is defined by a system of convection-diffusion-reaction PDEs supplemented by suitable initial and boundary conditions. (The word "diffusion" is a common mathematical terminology for terms in the PDE with second-order spatial derivative; in our case such terms model either some diffusion or dispersion phenomena or, in the case of the particulate material, the compression of the network of flocculated particles at high concentrations.) Specifically, we first identify the unknown variables (Section 2.1), then state the governing PDEs along with their initial and boundary conditions (Section 2.2), and finally introduce material specific constitutive model functions (Section 2.3), namely the specific growth rate related to biokinetics as well as the hindered settling and effective solid stress functions. In Section 3, the numerical method is introduced. After stating some preliminaries (Section 3.1), we start from discretization in space only (Section 3.2), which is closely related to a system of methodof-lines ordinary differential equations (ODEs). We then outline a fully discrete, explicit scheme in Section 3.3. In Section 3.4 the final method is explained in almost algorithmic form so that it can easily be programmed. A theoretical result stating the method produces non-negative values only is stated in Section 3.5. Next,

in Section 4, we present examples of numerical solutions of the governing model, where we are interested in three types of initial conditions: the traditional Kynch test (KT) (Kynch, 1952), which describes the settling of an initially homogeneous suspension in a column; the Diehl test (Diehl, 2007), in which the suspension is initially located above clear liquid; and the "overcompressed" test (OT), which corresponds to an initial configuration with a highly concentrated layer at the bottom. The initial condition for the Diehl test can be obtained either by a membrane, which is removed at t=0, or by rising the sludge to the top by aeration, e.g., in an SBR. The OT corresponds to a hypothetical initial configuration of a layer of strongly concentrated sediment (e.g., after centrifugation) with clear liquid above where the "pressure" is released at t = 0, allowing the bed to expand. The OT was employed by Bürger and Concha (1998) and Bustos et al. (1999) as an example to illustrate the consequences of modelling sediment compressibility by a nonlinear, possibly degenerate diffusion term under extreme conditions. Since the particle velocities in OT are negative in some regions, contrary to the KT and DT, this experiment is important for testing a numerical scheme. Sections 4.2-4.4 present the numerical results for KT, DT, and OT scenarios, respectively, and are followed by a brief discussion of numerical error and convergence properties of the scheme (Section 4.5). Finally, conclusions arising from the treatment are collected in Section 5.

2. Governing model

2.1. Unknown variables

We study one-dimensional batch sedimentation of suspended particles in water with soluble substrates in a closed vessel with a constant cross-sectional area. The depth *z* is measured from the suspension surface z = 0 downwards to the bottom at z = B. For simplicity, we study the last settling phase of a SBR process where aeration is switched off and the sludge is allowed to settle. We assume that, in addition to particulate biomass, there is still a certain amount of dissolved nitrate (NO₃) in the water. As the biomass decays, readily biodegradable COD is produced, which can be converted to cell biomass using nitrate as electron acceptor and nitrogen gas (N₂) is produced.

The particulate microorganisms are divided into only two components: ordinary heterotrophic organisms (X_{OHO}) and undegradable organics (X_U) since we only need access to those state variables to describe the denitrification process. The total concentration of the flocculated particles is $X := X_{OHO} + X_U$. Each particle is assumed to settle with a velocity $v = v(X, X_z)$ given by constitutive assumptions for hindered and compressive settling involving the local concentration X and its spatial derivative $X_z := \partial X / \partial z$. The notation for the soluble concentrations is S_{NO_3} for the nitrate, S_S for the readily biodegradable substrate and S_{N_2} for nitrogen gas. The small spatial movement of the substrate caused by the settling particles is captured by a single diffusion coefficient $d_{\rm S}$ in the model equations. Hence, particulate components undergo settling and biological reactions whereas soluble components are subject to diffusion and biological reactions. The resulting set of equations is able to describe the evolution of particulate concentrations (X_{OHO} and $X_{\rm U}$) as well as concentrations of soluble components ($S_{\rm NO_3}$, $S_{\rm S}$, $S_{\rm N_2}$) during the settling process.

Summarizing, the unknown variables are the five functions

$$X_{\text{OHO}}(z, t), \quad X_{\text{U}}(z, t), \quad S_{\text{NO}_3}(z, t), \quad S_{\text{S}}(z, t), \quad S_{\text{N}_2}(z, t)$$

sought for $0 \le z \le B$ and $t \ge 0$, and which are determined as solutions of five PDEs, supplied with initial and boundary conditions, stated in the next section.

2.2. Governing partial differential equations, initial and boundary conditions

At the start of settling, the initial concentration distribution of particles may be piecewise constant described by the function $X^0(z)$, whereas we assume that the substrate concentrations are constant: the nitrate concentration $S^0_{NO_3}$, readily biodegradable substrate S^0_S and zero concentration of nitrogen gas. Each particle consists initially of a certain percentage p_0 of heterotrophs and the remainder is undegradable organics. The balance of mass yields the following partial differential equations for 0 < z < B and t > 0:

$$\frac{\partial X_{\text{OHO}}}{\partial t} = -\frac{\partial}{\partial z} (\nu(X, X_z) X_{\text{OHO}}) + (\mu(S_{\text{NO}_3}, S_{\text{S}}) - b) X_{\text{OHO}}, \tag{1}$$

$$\frac{\partial X_{\rm U}}{\partial t} = -\frac{\partial}{\partial z}(\nu(X, X_z)X_{\rm U}) + f_{\rm P}bX_{\rm OHO},\tag{2}$$

$$\frac{\partial S_{\rm NO_3}}{\partial t} = d_{\rm S} \frac{\partial^2 S_{\rm NO_3}}{\partial z^2} - \frac{1 - Y}{2.86Y} \mu(S_{\rm NO_3}, S_{\rm S}) X_{\rm OHO},\tag{3}$$

$$\frac{\partial S_{\rm S}}{\partial t} = d_{\rm S} \frac{\partial^2 S_{\rm S}}{\partial z^2} - \left(\frac{\mu(S_{\rm NO_3}, S_{\rm S})}{Y} - (1 - f_{\rm P})b\right) X_{\rm OHO},\tag{4}$$

$$\frac{\partial S_{N_2}}{\partial t} = d_S \frac{\partial^2 S_{N_2}}{\partial z^2} + \frac{1 - Y}{2.86Y} \mu(S_{NO_3}, S_S) X_{OHO}, \tag{5}$$

which are posed along with the initial conditions

$$\begin{aligned} X_{\text{OHO}}(z,0) &= p_0 X^0(z), \quad X_{\text{U}}(z,0) = (1-p_0) X^0(z), \\ S_{\text{NO}_3}(z,0) &= S_{\text{NO}_3}^0, \quad S_{\text{S}}(z,0) = S_{\text{S}}^0, \quad S_{\text{N}_2}(z,0) = 0, \end{aligned} \tag{6}$$

where $X^0(z)$ is a givn function, p_0 , $S^0_{NO_3}$ and S^0_S are given numbers, and the zero-flux boundary conditions are

$$\begin{aligned} v(X, X_Z)X|_{z=0} &= v(X, X_Z)X|_{z=B} = 0, \\ (S_{NO_3})_z(0, t) &= (S_{NO_3})_z(B, t) = 0, \\ (S_5)_z(0, t) &= (S_5)_z(B, t) = 0, \\ (S_{N_2})_z(0, t) &= (S_{N_2})_z(B, t) = 0. \end{aligned}$$
(7)

2.3. Model parameters and constitutive functions

The parameter Y is a dimensionless yield factor and b is the constant decay rate of heterotrophs. The specific growth rate function is the following product of two Monod expressions:

$$\mu(S_{NO_3}, S_S) := \mu_{\max} \frac{S_{NO_3}}{K_{NO_3} + S_{NO_3}} \frac{S_S}{K_S + S_S},$$
(8)

where $\mu_{\text{max}} > b$ is the maximum growth rate and K_{NO_3} , $K_S > 0$ are half-saturation constants (see Table 1). This expresses that denitrification only takes place when favourable conditions for S_{NO_3} and S_S prevail. The constitutive function for the particle velocity $v(X, X_z)$ takes into account both hindered settling and compression and is of the form (Bürger et al., 2011).

$$\nu(X, X_z) = \begin{cases} \nu_{\rm hs}(X) & \text{for } X < X_{\rm c}, \\ \nu_{\rm hs}(X) \left(1 - \frac{\rho_{\rm s} \sigma_{\rm e}'(X)}{Xg\Delta\rho} \frac{\partial X}{\partial z} \right) & \text{for } X > X_{\rm c}. \end{cases}$$
(9)

Here, $v_{hs}(X)$ is the hindered settling velocity function, $\sigma'_e(X) := d\sigma_e(X)/dX$ is the derivative of the effective solids stress function $\sigma_e(X)$, ρ_s the density of the solids, $\Delta \rho$ the density difference between solids and liquid, and X_c is a critical concentration above which the particles touch each other and form a network which can bear a certain stress.

Table 1

Parameter values employed for the simulation of reactive settling.

Model parameter	Symbol	Value and unit
Parameter in hindered settling function $v_{\rm hs}$, cf. (10)	ν_0	$1.76 \times 10^{-3} \text{ m s}^{-1}$
Parameter in hindered settling function v_{hs} , cf. (10)	\overline{X}	$3.87 \text{kg} \text{m}^{-3}$
Parameter in hindered settling function v_{hs} , cf. (10)	q	3.58[-]
Unbiodegradable fraction	$f_{\rm P}$	0.2 [-]
Critical concentration	Xc	5 kg m ⁻³
Parameter in effective stress function σ_{e} , cf. (11)	α	$0.2 \text{ m}^2 \text{ s}^{-2}$
Solid density	$ ho_{s}$	1050 kg m ⁻³
Solid-fluid density difference	$\Delta \rho$	$52 \text{kg} \text{m}^{-3}$
Acceleration of gravity	g	9.81 m s ⁻²
Diffusion coefficient	ds	$1.00\times 10^{-6}\ m^2\ s^{-1}$
Heterotrophic yield	Y	0.67 [-]
Heterotrophic maximal specific growth rate	$\mu_{ m max}$	$4.8d^{-1}$ = $5.56\times10^{-5}s^{-1}$
Heterotropic decay rate	b	$0.6 d^{-1}$ = $6.94 \times 10^{-6} s^{-1}$
Half-saturation coefficient (hsc) for Heterotrophs	Ks	$20\mathrm{g}\mathrm{m}^{-3}$ = 0.02 kg m^{-3}
Hsc for denitrifying heterotrophs	K _{NO3}	$0.5gm^{-3}$ = 5.00 $\times10^{-4}kgm^{-3}$

For the simulations in this paper, we choose (Diehl, 2015; Torfs et al., 2016)

$$v_{\rm hs}(X) = \frac{v_0}{1 + (X/\overline{X})^q},$$
(10)

where the parameters v_0 , \overline{X} and q have the values given in Table 1 (Torfs et al., 2016), and

$$\sigma_{\rm e}(X) = \begin{cases} 0 & \text{for } X < X_{\rm c}, \\ \alpha(X - X_{\rm c}) & \text{for } X > X_{\rm c}, \end{cases}$$
(11)

where the values of α and the critical concentration X_c are indicated in Table 1.

3. Numerical method

3.1. Preliminaries

We define the batch settling flux function $f_b(X) := Xv_{hs}(X)$, set

$$d_{\rm comp}(X) := v_{\rm hs}(X) \frac{\rho_{\rm s} \sigma'_{\rm e}(X)}{g \Delta \rho},\tag{12}$$

and define the primitive

$$D(X) := \int_{X_c}^{X} d_{\text{comp}}(s) \, \mathrm{d}s. \tag{13}$$

The sum of (1) and (2) gives the following equation, which apart from the reaction term only contains derivatives of the total concentration X:

$$\begin{aligned} \frac{\partial X}{\partial t} &= -\frac{\partial}{\partial z} \left(f_{\rm b}(X) - \frac{\partial D(X)}{\partial z} \right) + (\mu(S_{\rm NO_3}, S_{\rm S}) - (1 - f_{\rm P})b)X_{\rm OHO}, \\ 0 &< z < B, \quad t > 0. \end{aligned}$$
(14)

This is in fact the Bürger–Diehl model with a reaction term. As a consequence of (11-13), the PDE (14) is second-order parabolic wherever the solution *X* exceeds X_c and first-order hyperbolic for lower concentration values. Thus, the PDE (14) is called strongly

degenerate parabolic or parabolic–hyperbolic, where the location of the type-change interface is not known beforehand. Moreover, due to the nonlinear and degenerate nature, discontinuities in the solution appear and special techniques for the numerical solution have to be used (which are incorporated in the numerical method outlined herein).

The total flux within the parenthesis on the right-hand side of (14) is

$$v(X, X_z)X = f_{\rm b}(X) - \frac{\partial D(X)}{\partial z}.$$
(15)

This means that for (14) we can utilize ingredients of the numerical method by Bürger et al. (2013) with the addition of the reaction term. To find numerical updates for the two portions X_{OHO} and X_U of X, we use the idea by Diehl (1997) and Jeppsson and Diehl (1996b). To this end, we introduce the percentage $p := X_{OHO}/X$ when X > 0, so that $X_{OHO} = pX$ and $X_U = (1 - p)X$, and rewrite Eq. (1) as

$$\frac{\partial(pX)}{\partial t} = -\frac{\partial}{\partial z}(\nu(X, X_z)pX) + (\mu(S_{NO_3}, S_S) - b)pX, \qquad 0 < z < B, \quad t > 0.$$
(16)

The idea of the numerical method is the following. In each discrete time step, *X* is first updated via a discretized version of (14). This means that the flux (15) is known during this time step, which is essential for any finite volume numerical method. Since the flux of (16) is *p* times the known flux (15), it is only the variable *p* that needs to be updated, and this can be achieved by a discretized version of (16). Then the concentration of the second particulate component is simply $X_U = (1 - p)X$. The numerical updates of S_{NO_3} , S_S and S_{N_2} are then straightforward for the corresponding equations (3)–(5).

3.2. Spatial discretization

We introduce the spatial discretization by dividing the interval (0, B) into N layers and set $\Delta z := B/N$. Let $X_j = X_j(t)$, $S_{NO_3,j} = S_{NO_3,j}(t)$, etc. denote the approximate concentrations in layer j and likewise $P_j = P_j(t)$ the approximation of p. The numerical fluxes between layer j and j + 1 (therefore indexed by j + 1/2) are defined as follows. The convective flux f_b is discretized by the standard Godunov numerical flux, i.e.,

$$G_{j+1/2} := \begin{cases} \min_{X_j \le X \le X_{j+1}} f_{\mathbf{b}}(X) & \text{if } X_j \le X_{j+1}, \\ \max_{X_j \ge X \ge X_{j+1}} f_{\mathbf{b}}(X) & \text{if } X_j > X_{j+1}. \end{cases}$$
(17)

If the numerical compressive flux is defined as

$$J_{j+1/2} := \frac{D(X_{j+1}) - D(X_j)}{\Delta z},$$
(18)

then the total flux (15) between layers *j* and *j*+1 is approximated by $F_{j+1/2} := G_{j+1/2} - J_{j+1/2}$. The corresponding flux of (16) is $P_{j+1/2}(G_{j+1/2} - J_{j+1/2})$, where $P_{j+1/2}$ needs to be defined. We use the idea of Diehl (1997), which is the following. If the total flux $F_{j+1/2}$ is positive, this means that particles move in the direction of the *z*-axis over the boundary between layer *j* to *j*+1. Consequently, the value of $P_{j+1/2}$ at the boundary between the layers is the one in the layer above, i.e. P_j . If $F_{j+1/2} \le 0$, then the value is P_{j+1} , i.e.

$$P_{j+1/2} = \begin{cases} P_{j+1} & \text{if } F_{j+1/2} \le 0, \\ P_j & \text{if } F_{j+1/2} > 0. \end{cases}$$
(19)

Moreover, we define the soluble component diffusive fluxes

$$\mathcal{D}_{\Upsilon,j+1/2} := d_{S} \frac{S_{\Upsilon,j+1} - S_{\Upsilon,j}}{\Delta z}, \quad j = 1, \dots, N-1,$$

$$\Upsilon \in \{NO_{3}, S, N_{2}\}$$
(20)

and finally introduce the zero boundary fluxes and percentages

small Δz) is due to the second-order spatial derivatives in the compression term (Bürger et al., 2005, 2012a) and in the diffusion term for the solubles. Let X_{max} denote the maximally possible particle concentration. The CFL condition for explicit Euler and batch sedimentation is

$$\Delta t \le \frac{1}{\max\{k_1, k_2\}},\tag{26}$$

with

$$k_{1} := \frac{1}{\Delta z} \max_{0 \le X \le X_{\max}} |f'_{b}(X)| + \frac{1}{\Delta z^{2}} \max_{0 \le X \le X_{\max}} d_{comp}(X) + \max\{\mu_{\max} - (1 - f_{P})b, (1 - f_{P})b\} + \max\left\{\frac{\rho_{L}\mu_{\max}X_{\max}}{\rho_{X}K_{NO_{3}}}, \mu_{\max} - b, b\right\}$$

$$k_{2} := \frac{2d_{S}}{\Delta z^{2}} + \frac{\mu_{\max}X_{\max}}{K_{NO_{3}}} \left(\frac{\rho_{L}}{\rho_{X}} + 1\right).$$

$$\begin{split} G_{1/2} &= G_{N+1/2} = J_{1/2} = J_{N+1/2} = P_{1/2} = P_{N+1/2} = 0, \ \mathcal{D}_{\Upsilon, 1/2} \\ &= \mathcal{D}_{\Upsilon, N+1/2} = 0, \quad \Upsilon \in \{\text{NO}_3, \text{S}, \text{N}_2\}. \end{split}$$

We then obtain the following semi-discretized ODE system for the PDEs:

$$\frac{\mathrm{d}X_j}{\mathrm{d}t} = -\frac{F_{j+1/2} - F_{j-1/2}}{\Delta z} + (\mu(S_{\mathrm{NO}_3, j}, S_{\mathrm{S}, j}) - (1 - f_{\mathrm{P}})b)X_{\mathrm{OHO}, j}, \quad (21)$$

$$\frac{\mathrm{d}(P_{j}X_{j})}{\mathrm{d}t} = -\frac{P_{j+1/2}F_{j+1/2} - P_{j-1/2}F_{j-1/2}}{\Delta z} + (\mu(S_{\mathrm{NO}_{3},j},S_{\mathrm{S},j}) - b)X_{\mathrm{OHO},j},$$
(22)

$$\frac{\mathrm{d}S_{\mathrm{NO}_{3},j}}{\mathrm{d}t} = \frac{\mathcal{D}_{\mathrm{NO}_{3},j+1/2} - \mathcal{D}_{\mathrm{NO}_{3},j-1/2}}{\Delta z} - \frac{1-Y}{2.86Y}\mu(S_{\mathrm{NO}_{3},j},S_{\mathrm{S},j})X_{\mathrm{OHO},j},$$
(23)

$$\frac{\mathrm{d}S_{\mathrm{S},j}}{\mathrm{d}t} = \frac{\mathcal{D}_{\mathrm{S},j+1/2} - \mathcal{D}_{\mathrm{S},j-1/2}}{\Delta z} - \left(\frac{\mu(S_{\mathrm{NO}_3,j},S_{\mathrm{S},j})}{Y} - (1-f_{\mathrm{P}})b\right)X_{\mathrm{OHO},j},\tag{24}$$

$$\frac{\mathrm{d}S_{N_2,j}}{\mathrm{d}t} = \frac{\mathcal{D}_{N_2,j+1/2} - \mathcal{D}_{N_2,j-1/2}}{\Delta z} + \frac{1 - Y}{2.86Y} \mu(S_{NO_3,j}, S_{S,j}) X_{OHO,j}, \quad (25)$$

 $X_{\text{OHO},j} = P_j X_j,$

$$X_{\mathrm{U},j} = (1-P_j)X_j,$$

For explicit Euler, the time derivatives on the left-hand side of
$$(21)-(25)$$
 are approximated by the standard finite difference ratio and the right-hand side is evaluated at time t_n . First, Eq. (21) gives the update X_i^{n+1} according to

$$X_{j}^{n+1} = X_{j}^{n} + \Delta t \left(-\frac{F_{j+1/2}^{n} - F_{j-1/2}^{n}}{\Delta z} + (\mu(S_{NO_{3},j}^{n}, S_{S,j}^{n}) - (1 - f_{P})b)X_{OHO,j}^{n} \right).$$
(27)

The equations for the substrates can be written in an analogous way, namely

$$S_{NO_{3},j}^{n+1} = S_{NO_{3},j}^{n} + \Delta t \left(\frac{\mathcal{D}_{NO_{3},j+1/2}^{n} - \mathcal{D}_{NO_{3},j-1/2}^{n}}{\Delta z} - \frac{1 - Y}{2.86Y} \mu(S_{NO_{3},j}^{n}, S_{5,j}^{n}) X_{OHO,j}^{n} \right),$$
(28)

$$S_{S,j}^{n+1} = S_{S,j}^{n+1} + \Delta t \left(\frac{\mathcal{D}_{S,j+1/2}^n - \mathcal{D}_{S,j-1/2}^n}{\Delta z} - \left(\frac{\mu(S_{NO_3,j}^n, S_{S,j}^n)}{Y} - (1 - f_P)b \right) X_{OHO,j}^n \right),$$
(29)

$$S_{N_{2},j}^{n+1} = S_{N_{2},j}^{n} + \Delta t \left(\frac{\mathcal{D}_{N_{2},j+1/2}^{n} - \mathcal{D}_{N_{2},j-1/2}^{n}}{\Delta z} + \frac{1 - Y}{2.86Y} \mu(S_{N_{0},j}^{n}, S_{S,j}^{n}) X_{OHO,j} \right).$$
(30)

As for Eq. (22), the approximation of the time derivative is

$$rac{\mathrm{d}(P_jX_j)}{\mathrm{d}t_n}pprox rac{P_j^{n+1}X_j^{n+1}-P_j^nX_j^n}{\Delta t}.$$

Note that if $X_j^{n+1} = 0$, then there is no particle in layer *j*, hence the value of P_j^{n+1} is irrelevant since $P_j^{n+1}X_j^{n+1} = 0$. We get the following update formula for P_i^{n+1} :

$$P_{j}^{n+1} = \begin{cases} P_{j}^{n} & \text{if } X_{j}^{n+1} = 0, \\ \frac{1}{X_{j}^{n+1}} \left[P_{j}^{n} X_{j}^{n} + \Delta t \left(-\frac{P_{j+1/2}^{n} F_{j+1/2}^{n} - P_{j-1/2}^{n} F_{j-1/2}^{n}}{\Delta z} + (\mu(S_{\text{NO}_{3},j}^{n}, S_{\text{S},j}^{n}) - b) X_{\text{OHO},j}^{n} \right) \right] & \text{if } X_{j}^{n+1} > 0. \end{cases}$$
(31)

where j = 1, ..., N. These equations are thus exact conservation laws for each of the *N* layers. Note that $X_{U,j}$ can be defined after the entire simulation.

3.3. Time discretization

Let t_n , n = 0, 1, ... denote the discrete time points and Δt the time step that should satisfy a certain Courant–Friedrichs–Lewy (CFL) condition depending on the chosen time-integration method. 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., P_n^n . The main restriction of the time step (for

3.4. Numerical method in final form

For the ease of reference, we here summarize the information provided in this section and present the resulting numerical method for the approximate solution of the model (1)-(7), and thereby for the simulation of reactive settling.

- (1) Assume that the solution is sought at time t=T>0. Choose $\Delta z=B/N$ and $\Delta t=T/n_{max}$, N and n_{max} being integers, such that the CFL condition (26) is satisfied.
- (2) Calculate the discrete initial values either by averaging

$$X_j^0 = \frac{1}{\Delta z} \int_{(j-1)\Delta z}^{j\Delta z} X^0(z) \,\mathrm{d}z, \quad j = 1, \dots, N,$$

or by using the value in the mid of each layer:

$$X_j^0 = X^0\left(\left(j-\frac{1}{2}\right)\Delta z\right), \quad j = 1, \dots, N.$$

Then set for $i = 1, \ldots, N$:

$$P_j^0 = p_0, \quad X_{OHO,j}^0 = p_0 X_j^0, \quad S_{NO_3,j}^0 = S_{NO_3}^0, \quad S_{S,j}^0 = S_S^0, \quad S_{N_2,j}^0 = 0$$

(3) For $n = 0, 1, ..., n_{max} - 1$, update the discrete solution values as follows:

- (a) For j = 0, ..., N, calculate the numerical fluxes $G_{i+1/2}^n$ and (a) For j=0, ..., N, calculate the numerical match $X_{j} = X_{j+1/2}^{n}$ and $J_{j+1/2}^{n}$ from (17) and (18), respectively, where $X_{j} = X_{j}^{n}, X_{j+1} = X_{j+1}^{n}$, for j = 1, ..., N-1; and set $G_{1/2}^{n} = G_{N+1/2}^{n} = J_{1/2}^{n} = J_{N+1/2}^{n} = 0$. (b) Calculate the total numerical fluxes $F_{j+1/2}^{n} = G_{j+1/2}^{n} - J_{j+1/2}^{n}, \quad j = 0, ..., N$. (c) Calculate the percentage numerical fluxes

$$P_{j+1/2}^{n} = \begin{cases} P_{j+1}^{n} & \text{if } F_{j+1/2}^{n} \le 0, \\ P_{i}^{n} & \text{if } F_{j+1/2}^{n} = 0, \\ P_{i}^{n} & \text{if } F_{i+1/2}^{n} = 0, \end{cases} \quad j = 0, \dots, N.$$

- (d) Calculate X_{j}^{n+1} for j = 1, ..., N from the update formula (27). (e) Calculate P_{j}^{n+1} for j = 1, ..., N from the update formula (31). (f) Calculate $X_{OHO,j}^{n+1} = P_{j}^{n+1}X_{j}^{n+1}$ for j = 1, ..., N. (g) Calculate $X_{U,j}^{n+1} = (1 P_{j}^{n+1})X_{j}^{n+1}$ for j = 1, ..., N. (This step is optional) optional.)
- (h) For each soluble substrate $\Upsilon \in \{NO_3, S, N_2\}$, calculate the corresponding numerical diffusive fluxes $\mathcal{D}^n_{\Upsilon, j+1/2}$ from (20), where $S_{\Upsilon,j} = S_{\Upsilon,j}^n$ and $S_{\Upsilon,j+1} = S_{\Upsilon,j+1}^n$, for j = 1, ..., N-1, and
- $\mathcal{D}^n_{\Upsilon,1/2} = \mathcal{D}^n_{\Upsilon,N+1/2} = 0.$ (i) Calculate $S_{NO_3,j}^{n+1}$, $S_{S,j}^{n+1}$ and $S_{N_2,j}^{n+1}$ from the update formulas (28) - (30).

All calculations are based on explicit evaluations of update formulas, so the numerical method can be readily implemented (for instance, in MATLAB or any other programming language). No solution of linear or nonlinear systems is necessary; it is not necessary to appeal to any numerical solver or software (except, of course, for the visualization of results).

3.5. A theoretical result

The analysis behind the CFL condition (26) is not presented here. The idea is that the CFL condition should imply that the right-hand side of the update formula for each variable is a monotone function of the same variables in all layers at the previous time point. For example, the CFL condition (26) implies that the right-hand side of (27) is a monotone function of the arguments X_{j-1}^n, X_j^n and X_{j+1}^n (note that $X_{OHO,j}^n = P_j^n X_j^n$) for any values of the substrate concentrations and P_i^n appearing in the formula. A more comprehensive analysis can be found in (Bürger et al., 2016), which also contains results that imply the following theorem.

Theorem 3.1. Assume that the numerical scheme in Section 3.4 produces $X_i^n \leq X_{max}$ for all j = 1, ..., N and $n = 1, ..., n_{max}$, and that the CFL condition (26) holds. Then the following holds (j = 1, ..., N and $n = 1, \ldots, n_{\max}$):

$$\begin{cases} 0 \leq X_j^n, S_{NO_3,j}^n, S_{S,j}^n, S_{N_2,j}^n, \\ 0 \leq P_j^n \leq 1 \end{cases} \Rightarrow \begin{cases} 0 \leq X_j^{n+1}, S_{NO_3,j}^{n+1}, S_{N_2,j}^{n+1}, S_{N_2,j}^{n+1}, \\ 0 \leq P_j^{n+1} \leq 1. \end{cases}$$

The theorem guarantees that if the variables are positive (rather, non-negative) initially, the numerical method will keep them positive. Likewise, percentage values P_i^n will stay between zero and one.

4. Numerical results

4.1. Preliminaries

For all tests we employ the hindered settling velocity function $v_{\rm hs}$ and effective stress function $\sigma_{\rm e}$ given by (10) and (11), respectively. The heterotrophic specific growth rate μ is given in (8), and all other parameters are indicated in Table 1 (unless otherwise stated). For the KT we simulated three different scenarios differing in the choice of the diffusion coefficient $d_{\rm S}$ (Examples 1–3), while the two scenarios considered for each of the DT (Examples 4 and 5) and OT (Examples 6 and 7) differ in the initial concentration of particles.

In all numerical examples, we employ the explicit scheme with N = 100 layers for a column of height B = 1 m. To properly represent the reaction dynamics we present simulations up to t = T = 2 h, except for one long simulation of the KT, which is run to T = 100 h. (This final time is quite irrealistic since the settling phase in an SBR takes at most one hour. However, in this case we are interested in the long-time predictions of the model and the numerical algorithm.) The time step Δt is chosen by 98% of the bound given in the right-hand side of (26).

The initial values common to all examples are

$$S_{S}^{0} = 9.00 \times 10^{-4} \, \text{kg} \, \text{m}^{-3}$$
 and $S_{NO_{3}}^{0} = 6.00 \times 10^{-3} \, \text{kg} \, \text{m}^{-3}$,

while we recall that by (6), the initial value of S_{N_2} is zero.

4.2. Examples 1–3: Kynch test (batch settling of an initially homogeneous suspension)

In Examples 1-3, we simulate the settling of an initially homogeneous suspension of initial density $X_0 = 3.5$ kg m⁻³, which is divided into heterotrophs and undegradable organics by $p_0 = 5/7 \approx 0.7143$, so that

$$X_{\text{OHO}}(z, 0) = 2.5 \text{ kg m}^{-3}, \quad X_{\text{U}}(z, 0) = 1.0 \text{ kg m}^{-3} \text{ for } 0 < z < B.$$

We employ this configuration to assess the influence of the substrate diffusion coefficient $d_{\rm S}$. Example 1 has been obtained by employing the default value $d_{\rm S} = 10^{-6} \, {\rm m}^2 \, {\rm s}^{-1}$ informed in Table 1. Figs. 1 and 2 show the numerical results for all unknowns for T=2h and T=100h, respectively. We observe that the solids settle downwards to the bottom rapidly and form a sludge blanket with a sharp interface at $X_c = 5 \text{ kg m}^{-3}$. Moreover, the concentration increases downwards gradually until reaching about 20 kg m⁻³ at the bottom. Here, and in Examples 2-7, the solutions for all quantities are bounded and non-negative. The S_{NO3} plot indicates a very rapid degradation of nitrate within the sludge blanket while that same quantity decays only very slowly within the supernatant clear liquid. We observe the formation of readily biodegradable substrate (of concentration S_S) at the bottom of the column through



Fig. 1. Example 1 (Kynch test, $d_5 = 10^{-6} \text{ m}^2 \text{ s}^{-1}$). Here and in Figs. 2–6, 8 and 9, the visual grid used to display the numerical solution is coarser than the computational grid, and the plot of the solution for S_{NO_3} has been rotated.

decay of heterotrophs. This is no longer degraded when all nitrate is depleted. Furthermore, the solution for S_{N_2} has a plateau at $6 \times 10^{-3} \text{ kg m}^{-3}$, which is equal to the initial value of S_{NO_3} . This suggests that within the sludge blanket, almost all soluble nitrate has been converted into nitrogen.

For this particular case we also present a simulation until T = 100 h to study the long-time behaviour of the model. The results shown in Fig. 2 illustrate that the total solids concentration attains a maximum of about 20 kg m⁻³ at the bottom but that this maximum, as well as the total solids mass, decay in time. Moreover,

the proportion of undegradable organics increases in time (as expected). The substrates slowly approach an equilibrium concentration as a consequence of their slow diffusive movement.

Figs. 3 and 4 show the corresponding results for the same scenario but with increased values of the substrate diffusion parameter, namely $d_S = 9 \times 10^{-6} \text{ m}^2 \text{ s}^{-1}$ (Fig. 3) and $d_S = 1.3 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$ (Fig. 4). We observe that the changes in this parameter practically do not affect the solids settling behaviour; the solutions for *X*, *X*_U and *X*_{OHO} are virtually the same as in Example 1. However, differences in the solution behaviour of the substrates



Fig. 2. Example 1 (Kynch test, $d_s = 10^{-6} \text{ m}^2 \text{ s}^{-1}$): long-time simulation (*T* = 100 h).



Fig. 4. Example 3 (Kynch test, $d_s = 1.3 \times 10^{-5} \text{ m}^2 \text{ s}^{-1}$).

are appreciable as can be seen for example by the reduction in S_{NO_3} at the top of the settling column at time t=2h when d_S increases. Roughly speaking, since increasing d_S means increasing the diffusive flux of each substrate, that is, the flow rate from regions of high concentration to those of low concentration, we observe that the flux of nitrate into the sludge zone consistently increases when comparing the results of Examples 1–3. Since the degradation of nitrate takes place due to reactions in that zone, we obtain that for this test, increasing d_S produces an overall more rapid denitrification. Corresponding

differencs in solution behaviour are visible with the two other substrates.

4.3. Examples 4 and 5: Diehl test (batch settling of suspension initially located above clear liquid)

We here choose the following initial distribution of the solids:

$$X_0(z) = \begin{cases} 7 \, \text{kg} \, \text{m}^{-3} & \text{for } 0 \, \text{m} < z \le 0.5 \, \text{m}, \\ 0 & \text{for } 0.5 \, \text{m} < z \le 1 \, \text{m} \end{cases}$$



Fig. 5. Example 4 (Diehl test, $X(z, 0) = 7 \text{ kgm}^{-3}$ above z = 0.5 m).

for Example 4, and

$$X_0(z) = \begin{cases} 14 \, \text{kg} \, \text{m}^{-3} & \text{for } 0 \, \text{m} < z \le 0.25 \, \text{m}, \\ 0 & \text{for } 0.25 \, \text{m} < z \le 1 \, \text{m} \end{cases}$$

for Example 5. All other parameters are chosen as in Example 1. Since the initial total solids mass is the same as in Examples 1 to 3, results can be compared. The numerical solutions are shown in Figs. 5 and 6. We observe in both examples that the initial body of sludge dilutes, forming a so-called rarefaction wave, the solids

settle downward, and accumulate at the bottom to form a sludge layer. Under suitable choices of parameters and initial concentrations, the solution behaviour of a Diehl test produces a curved trajectory of the suspension-supernatant interface that does not arise with a Kynch test, and that can be converted into certain portions of the function f_b . While this property has led us to propose a Diehl test as a device for identification of f_b (Diehl, 2007; Bürger and Diehl, 2013; Betancourt et al., 2014), we use this configuration basically to test the numerical method. We see that the solution for S_{NO_3} is non-monotone (as a function of *z* for fixed *t*), which is also



Fig. 6. Example 5 (Diehl test, $X(z, 0) = 14 \text{ kgm}^{-3}$ above z = 0.25 m).



Fig. 7. Examples 1 to 5: evolution of the approximate normalized nitrate inventory $I_{N_2}^{\Delta}(t)$. Examples 1–3 show results of three KTs with increasing diffusion coefficient d_s , while Examples 4–5 show results of two DT with the same value on d_s as in Example 1.

reflected in the solution for S_{N_2} . Comparing the S_{NO_3} plot of Fig. 6 with that of Fig. 1 shows that the total amount of nitrate at T = 2 h is significantly smaller in Examples 4 and 5 than in Example 1. Consequently, the total amount of dissolved nitrogen gas shows the opposite behaviour.

In light of the latter observation we quantify the evolution of N_2 in the system by measuring the time-dependent average N_2 concentration, defined by

$$I_{N_2}(t) := \frac{1}{B} \int_0^B S_{N_2}(z, t) dz.$$

For a given discretization $\Delta := (\Delta z, \Delta t)$ and $t = n \Delta t$ this quantity is approximated by

$$I_{N_2}^{\Delta}(t) := \frac{1}{B} \sum_{j=1}^{N} S_{N_2,j}^n \Delta z = \frac{1}{N} \sum_{j=1}^{N} S_{N_2,j}^n.$$

Fig. 7 displays the evolution of $I_{N_2}^{\Delta}(t)$ for Examples 1–5. Comparing the curves for Examples 1–3, we find confirmed that an increased value of the substrate diffusion coefficient $d_{\rm S}$ accelerates the denitrification process in the setup of the Kynch test. However, $d_{\rm S}$ is a model parameter that is not possible to control, so it is of more practical interest to compare the results of Example 1 (KT) with those of Examples 4 and 5 (DT) (calculated with the same value of d_{S}). Here we observe that the initial rate of fairly rapid denitrification is the same in all of these three examples up to 30 min, but is maintained slightly longer in case of the DT, with the effect that the portions of the curves corresponding to slow rates of denitrification (produced in the consolidation stage after 30 min) lie about 10% and 15%, in the respective cases of the DT Examples 4 and 5, above that of the KT Example 1 for a couple of hours. This result illustrates how the initial placement of solids mass may influence the rate of denitrification. For long times, the right plot in Fig. 7 shows that the curves approach each other, which means that also



Fig. 8. Example 6 (overcompressed test, $X(z, 0) = 20 \text{ kg m}^{-3}$ below z = 0.5 m)



Fig. 9. Example 6 (overcompressed test, $X(z, 0) = 25 \text{ kg m}^{-3}$ below z = 0.9 m)



Fig. 10. Example 1 (Kynch test): comparison between a reference solution (N=3200) and two fastly obtained simple numerical solutions (N=20 and N=50) at simulated times T=4 min (top row) and T=30 min (bottom row), showing results for X (left), S_{NO_3} (middle) and S_S (right).

a small diffusion d_S makes the nitrate slowly move down into the sediment where it is converted to nitrogen gas.

4.4. Examples 6 and 7: overcompressed test (expansion of compressed sludge)

We utilize the same parameters as in Example 1 and place a highly compressed body of sludge near the bottom of the column. Specifically, we choose

$$X(z,\,0) = \begin{cases} 0 & \text{for } 0\,m < z \le 0.7\,m, \\ 20\,kg \ m^{-3} & \text{for } 0.7\,m < z \le 1\,m \end{cases}$$

for Example 6 and

$$X_{\rm OHO}(z,\,0) = \begin{cases} 0 & \mbox{for } 0\,m < z \le 0.9\,m, \\ 25\,kg & m^{-3} & \mbox{for } 0.9\,m < z \le 1\,m. \end{cases}$$



Fig. 11. Example 4 (Diehl test): comparison between a reference solution (N=3200) and two fast obtained simple numerical solutions (N=20 and N=50) at simulated times T=6 min (top row) and T=30 min (bottom row), showing results for X (left), S_{NO_3} (middle) and S_S (right).

for Example 7. The respective numerical results are shown in Figs. 8 and 9. In both cases, the compressed layer expands once the system starts to evolve. These simulations alert to the limitations of modelling sediment compressibility by a nonlinear diffusion term $\frac{\partial^2 D(\phi)}{\partial z^2}$. This approach corresponds to elastic and in a sense reversible material behaviour which is usually not observed with activated sludge in reality. Describing this behaviour in an anomalous situation with more realism calls for an improvement of the constitutive assumptions concerning sediment compressibility. We emphasize, however, that this test produces an upward movement of solid particles, which is associated with negative values of the velocity v defined in (9) allowing to test the numerical scheme under different conditions. The case discrimination in (19), which goes back to the method by Diehl (1997), has precisely been devised to handle this situation. Thus, Figs. 8 and 9 demonstrate that the model is sound, and the numerical scheme works properly, even for settling velocities of variable sign.

4.5. Numerical solution versus discretization

To illustrate the accuracy of the method, we plot in Figs. 10 and 11 solutions of Examples 1 and 4 obtained at two different times with fairly coarse discretizations, N = 20 and N = 50, against a reference solution obtained with N = 3200 subintervals. We observe that smooth portions of the solution profiles are approximated quite well by approximate solutions at these coarse discretizations. Nevertheless, discontinuities appear smeared out. Furthermore, to gain some systematic insight into how the numerical solution behaves versus discretization, we calculated the approximate relative error, defined at a fixed time point *T*, by adding the relative errors of the individual components. The latter are obtained by dividing with the average masses at times zero and *T* for the reference solution:

$$m_{\text{OHO}}^{\text{ref}}(T) := \frac{1}{2} (\|X_{\text{OHO}}^{\text{ref}}(\cdot, 0)\|_{L^1} + \|X_{\text{OHO}}^{\text{ref}}(\cdot, T)\|_{L^1}),$$

where $\|h\|_{L^1} := \int_0^B h(z) \, \mathrm{d}z,$

and similarly for the other variables. Both the masses at times zero and *T* are used as some component may be zero at either of those two time points because of the reactions. We define the normalized relative error

$$\begin{split} e_N^{\text{rel}}(T) &:= \frac{\|(X_{\text{OHO}} - X_{\text{OHO}}^{\text{ref}})(\cdot, T)\|_{L^1}}{m_{\text{OHO}}^{\text{ref}}(T)} + \frac{\|(X_{\text{U}} - X_{\text{U}}^{\text{ref}})(\cdot, T)\|_{L^1}}{m_{\text{U}}^{\text{ref}}(T)} \\ &+ \frac{\|(S_{\text{NO}_3} - S_{\text{NO}_3}^{\text{ref}})(\cdot, T)\|_{L^1}}{m_{\text{NO}_3}^{\text{ref}}(T)} + \frac{\|(S_{\text{N}_2} - S_{\text{N}_2}^{\text{ref}})(\cdot, T)\|_{L^1}}{m_{\text{N}_2}^{\text{ref}}(T)} \\ &+ \frac{\|(S_{\text{S}} - S_{\text{S}}^{\text{ref}})(\cdot, T)\|_{L^1}}{m_{\text{S}}^{\text{ref}}(T)}, \end{split}$$

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

Table 2

Examples 1 and 4: approximate relative errors e_N^{rel} , convergence rates θ (calculated between neighboring values of *N*) and CPU times for two different simulated times (cf. Figs. 10 and 11).

Ν	Exam	Example 1, T=4 min			Example 1, T=30 min		
	$e_N^{\rm rel}$	θ	CPU[s]	$e_N^{\rm rel}$	θ	CPU[s]	
20	0.066	_	0.0076	0.195	-	0.0163	
50	0.020	1.765	0.0255	0.073	1.423	0.1533	
100	0.011	0.788	0.1770	0.037	0.980	1.2127	
200	0.005	1.262	1.3987	0.017	1.117	8.8516	
400	0.002	1.191	9.5642	0.008	1.077	56.3849	
800	0.001	0.783	63.8714	0.003	1.210	432.2561	
Ν	Example	ample 4, T=6 min			Example 4, T=30 min		
	$e_N^{\rm rel}$	θ	CPU[s]	$e_N^{\rm rel}$	θ	CPU[s]	
20	0.147	-	0.0016	0.087	-	0.0132	
50	0.077	0.925	0.0148	0.035	1.309	0.1512	
100	0.047	0.727	0.1141	0.021	0.777	1.1988	
200	0.028	0.759	0.8956	0.011	0.944	9.8084	
400	0.015	0.868	7.1999	0.006	0.916	55.8816	
800	0.008	1.003	39.6432	0.003	1.127	423.4776	

$$\theta := \frac{-\log(e_{N_1}^{\mathrm{rel}}/e_{N_2}^{\mathrm{rel}})}{\log(N_1/N_2)}$$

Our results, collected in Table 2, are consistent with the fact that the scheme is formally first-order accurate in space and time, and moreover the approximate solutions exhibit discontinuities. Of course, while these results suggest that the scheme converges to a definite limit function, a rigorous convergence proof is still lacking. Furthermore, the CFL condition (26), which determines the admissible time step Δt for a given spatial discretization Δz , essentially imposes that $\Delta t \sim \Delta z^2$. This means that if one halves the spatial discretization Δz , or equivalently, doubles *N* (to increase accuracy) and chooses Δt according to (26), then one should expect that the total CPU time to solve the problem to a final time increases by a factor of eight. The CPU times reported in Table 2 indicate that this is indeed the case.

5. Conclusions

A reduced model of simultaneous biological reactions and sedimentation of flocculated particles in batch operation is written as a system of convection-diffusion-reaction PDEs, and a numerical scheme for its simulation is suggested. The idea of introducing a percentage vector for the composition of the flocculated particles (Diehl, 1997) can be used in a natural way also when the effects of compression and reactions are included in the equations. In the present reduced model, with only two particulate components, this vector is simply $(p, 1-p)^{T}$. The advantage of this approach is that since the vector appears linearly in each term of the equations for the particle concentrations, the sum of these equations yields an equation of the total suspended solids concentration X except for a reaction term. This equation is the Bürger-Diehl settler model equation with an additional reaction term. Consequently, we can utilize the ingredients by Bürger et al. (2013) for a correct spatial discretization into computational cells (layers). The time discretization utilizes that X can be updated first, so that the numerical fluxes between the layers are known, which is then utilized in the updates of the percentage vectors.

Numerical examples for the modelling of the last stage of an SBR process, where denitrification occurs, indicate that the suggested numerical scheme works well and the expected denitrification process is simulated correctly. Furthermore, numerical tests with other initial data, resulting in non-monotone concentration profiles and movement of particles upwards, indicate that the numerical method could be extended to the case of continuous sedimentation in secondary settlers of WWTPs. The latter is an obvious continuation of this initial work on reactive settling for batch sedimentation. Other potential improvements are: a more accurate modelling of the liquid, in which the substrates are dissolved; the extension to include a full activated sludge model for the biokinetic reactions; an analysis of the convergence properties of the numerical scheme; the development of more efficient time discretizations; and the extension of the model to polydisperse particles and several space dimensions.

Concerning the latter two points, we finally mention that more rigorous mathematical and numerical treatments are available in the non-reactive case (Berres et al., 2003; Bürger et al., 2012b, 2015) that in particular deal with the necessity to solve additional equations for the motion of the mixture in several space dimensions. On the other hand, the non-spatial ASM1 model (Henze et al., 1987) is more involved than the reactive model incorporated into our model. However, this paper does not present a simpler version of any more rigorous published model since the *combined* description of the mechanical sedimentation–compression process with biological reactions is new.

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