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A REDUCED MODEL AND SIMULATIONS OF REACTIVE SETTLING OF ACTIVATED SLUDGE

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ABSTRACT. Denitrification during the sedimentation process in secondary settlers in wastewater treatment plants has been reported to be significant. The modelling of such a process with the conservation of mass leads to a nonliner convection-diffusion-reaction partial differential equation, which needs non-standard numerical methods to obtain reliable simulations. The purpose of this study is to present how the Bürger-Diehl settler model, which models the sedimentation-consolidation process without reactions, can be extended to include biological reactions. This is done with a reduced model, having few particulate and soluble components, which can be seen as a model of the last stage of a sequencing batch reactor (SBR) process during which denitrification occurs. The main result is a numerical scheme, which has been used for simulations with different initial conditions. One outcome of the simulations is that the initial distribution of activated sludge, which in principle can be controlled by the operator of an SBR, can have a significant impact on the reduction of nitrate.

1. INTRODUCTION

A well-accepted model for the sedimentation process of the secondary clarifier, or settler, in the activated sludge process of wastewater treatment plants originates from the conservation of mass and can be stated as a scalar, nonlinear partial differential equation (PDE) for the sludge concentration as function of depth and time (Bürger et al., 2011, 2013). 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 batch sedimentation as a first approach.

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Most models of the activated sludge process 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 biological reactions do occur in the settler. In particular, denitrification occurs at the bottom of the tank, where the concentration of sludge is high and there is no supply of oxygen. Siegrist et al. (1995) and Koch et al. (1999) reported measurements from three plants showing that of the total denitrification in each plant, 15%, 30% and 37% occurred in the settler, respectively.

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 reaction 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. 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 PDE in certain situations (Jeppsson and Diehl, 1996a; Bürger et al., 2011, 2012), but also for other shortcomings during normal operating conditions (Torfs et al., 2015a).

A related application is the reactive settling occurring in sequencing batch reactors (SBRs), for which some heuristic modelling approaches can be found (Alex et al., 2011; Kazmi and Furumai, 2000a,b). Keller and Yuan (2002) modelled SBRs without reactive settling.

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 (Bürger et al., 2011, 2013; Torfs et al., 2015a).

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 partial differential equation (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.) Moreover, the material specific model functions, namely the hindered settling and effective solid stress functions, are introduced. In Section 3 the numerical method is introduced, starting from discretization in space only (Section 3.1), which is closely related to a system of method-of-lines ordinary differential equations (ODEs). A fully discrete, explicit scheme is outlined in Section 3.2. In Section 4, we present 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. Such an initial condition 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 third initial condition gives the "overcompressed test" (OT), which corresponds to a hypothetical initial configuration of a layer of strongly concentrated sediment 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, 4.3 and 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

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 we assume that, in addition to particulate biomass and inert matter, there is still a certain amount of dissolved nitrate (NO₃) in the water. As the biomass decays, readily biodegradable COD is produced, which reacts with the nitrate, and nitrogen gas (N₂) is produced in such low concentrations that it is dissolved in the water.

The particulate microorganisms are divided into only two components, which we for simplicity call active biomass and inert matter, having the concentrations $X_{\rm a}$ and $X_{\rm i}$, respectively. These could typically be ordinary heterotrophic organisms ($X_{\rm OHO}$) and unbiodegradable particulate matter ($X_{\rm U}$), respectively. The total concentration of the flocculated particles is $X := X_{\rm a} + X_{\rm i}$. 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 are $S_{\rm NO_3}$ for the nitrate, $S_{\rm S}$ for the readily biodegradable substrate and $S_{\rm N_2}$ for nitrogen gas. The small spatial movement of the substrate caused by the settling particles is assumed to be captured by a single diffusion coefficient $d_{\rm S}$ in the model equations. At the start of the settling, we assume a homogeneous suspension of particles with concentration X_0 , nitrate at the concentration $S^0_{NO_3}$, readily biodegradable substrates at S^0_S and a zero concentration of nitrogen gas. Each particle consists initially of a certain percentage p_0 of active biomass and the remainder is inert. The balance of mass yields the following partial differential equations for 0 < z < B and t > 0:

$$\frac{\partial X_{\rm a}}{\partial t} = -\frac{\partial}{\partial z} \left(v(X, X_z) X_{\rm a} \right) + \left(\mu(S_{\rm NO_3}, S_{\rm S}) - b \right) X_{\rm a},\tag{1}$$

$$\frac{\partial X_{\rm i}}{\partial t} = -\frac{\partial}{\partial z} \left(v(X, X_z) X_{\rm i} \right) + f_{\rm P} b X_{\rm a},\tag{2}$$

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

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

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

which are posed along with the initial conditions

$$X_{\rm a}(z,0) = p_0 X_0, \quad X_{\rm i}(z,0) = (1-p_0) X_0, S_{\rm NO_3}(z,0) = S^0_{\rm NO_3}, \quad S_{\rm S}(z,0) = S^0_{\rm S}, \quad S_{\rm N_2}(z,0) = 0,$$
(6)

where $S_{NO_3}^0$ and S_S^0 are given numbers, and the zero-flux boundary conditions

$$v(X, X_z)X|_{z=0} = v(X, X_z)X|_{z=B} = 0,$$

$$(S_{\text{NO}_3})_z(0, t) = (S_{\text{NO}_3})_z(B, t) = 0,$$

$$(S_{\text{S}})_z(0, t) = (S_{\text{S}})_z(B, t) = 0,$$

$$(S_{\text{N}_2})_z(0, t) = (S_{\text{N}_2})_z(B, t) = 0.$$

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

$$\mu(S_{\rm NO_3}, S_{\rm S}) := \mu_{\rm max} \frac{S_{\rm NO_3}}{K_{\rm NO_3} + S_{\rm NO_3}} \frac{S_{\rm S}}{K_{\rm S} + S_{\rm S}},\tag{7}$$

where μ_{max} is the maximum growth rate and $K_{\text{NO}_3}, K_{\text{S}} \geq 0$ are half-saturation constants (see Table 1). The constitutive function for the particle velocity $v(X, X_z)$ is assumed to take into account both hindered settling and compression and is of the following form (Bürger et al., 2011):

$$v(X, X_z) = \begin{cases} v_{\rm hs}(X) & \text{for } X < X_{\rm c}, \\ v_{\rm hs}(X) \left(1 - \frac{\rho_{\rm s} \sigma_{\rm e}'(X)}{Xg\Delta\rho} \frac{\partial X}{\partial z} \right) & \text{for } X > X_{\rm c}. \end{cases}$$
(8)

Here, $v_{\rm hs}(X)$ is the hindered settling velocity function, $\sigma_{\rm e}$ the effective solids stress, $\rho_{\rm s}$ the density of the solids, $\Delta \rho$ the density difference between solids and liquid, and $X_{\rm c}$ is a critical concentration above which the particles touch each other and form a network which can bear a certain stress.

Model parameter	symbol	value and unit
parameter in hindered settling function $v_{\rm hs}$, cf. (9)	v_0	$1.76 \times 10^{-3} \mathrm{m \ s^{-1}}$
parameter in hindered settling function $v_{\rm hs}$, cf. (9)	\bar{X}	$3.87 { m kg} { m m}^{-3}$
parameter in hindered settling function $v_{\rm hs}$, cf. (9)	q	3.58[-]
proportion parameter	$f_{ m P}$	0.2 [-]
critical concentration	$X_{ m c}$	$5{ m kg}~{ m m}^{-3}$
parameter in effective stress function $\sigma_{\rm e}$, cf. (10)	α	$0.1 \mathrm{m^2 \ s^{-2}}$
solid density	$ ho_{ m s}$	$1050 { m kg} { m m}^{-3}$
solid-fluid density difference	Δho	$52 \mathrm{kg} \mathrm{m}^{-3}$
acceleration of gravity	g	$9.81 \mathrm{m \ s^{-2}}$
diffusion coefficient	$d_{ m S}$	$1.00 \times 10^{-6} \mathrm{m^2 \ s^{-1}}$
heterotrophic yield	Y	0.67[-]
heterotrophic maximal specific growth rate	$\mu_{ m max}$	$4.8 \mathrm{d^{-1}} = 5.56 \times 10^{-5} \mathrm{s^{-1}}$
heterotropic decay rate	b	$0.6 \mathrm{d}^{-1} = 6.94 \times 10^{-6} \mathrm{s}^{-1}$
half-saturation coefficient (hsc) for heterotrophs	$K_{\rm S}$	$20 \mathrm{g} \mathrm{m}^{-3} = 0.02 \mathrm{kg} \mathrm{m}^{-3}$
hsc for denitrifying heterotrophs	$K_{\rm NO_3}$	$0.5 \mathrm{g \ m^{-3}} = 5.00 \times 10^{-4} \mathrm{kg \ m^{-3}}$

TABLE 1. Parameters employed for the simulation of reactive settling.

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

$$v_{\rm hs}(X) = \frac{v_0}{1 + (X/\bar{X})^q},\tag{9}$$

where the parameters v_0 , \bar{X} and q have the values given in Table 1 (Torfs et al., 2015b), and

$$\sigma_{\rm e}(X) = \begin{cases} 0 & \text{for } X < X_{\rm c}, \\ \alpha(X - X_{\rm c}) & \text{for } X > X_{\rm c}, \end{cases}$$
(10)

where the values of α and the critical concentration $X_{\rm c}$ are indicated in Table 1.

3. Numerical method

3.1. Spatial discretization. We define the batch settling flux function $f_{\rm b}(X) := X v_{\rm hs}(X)$, set

$$d_{\rm comp}(X) := v_{\rm hs}(X) \frac{\rho_{\rm s} \sigma_{\rm e}'(X)}{g \Delta \rho}$$
(11)

and define the primitive

$$D(X) := \int_{X_{\rm c}}^{X} d_{\rm comp}(s) \,\mathrm{d}s.$$
(12)

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

$$\frac{\partial X}{\partial t} = -\frac{\partial}{\partial z} \left(f_{\rm b}(X) - \frac{\partial D(X)}{\partial z} \right) + (\mu(S_{\rm NO_3}, S_{\rm S}) - (1 - f_{\rm P})b) X_{\rm a}, \qquad 0 < z < B, \quad t > 0.$$
(13)

A special feature of (13) is that as a consequence of (10), (11) and (12), this PDE is second-order parabolic wherever the solution X exceeds X_c and first-order hyperbolic for lower concentration values. Thus, the PDE (13) 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).

Note that the total flux within the parenthesis on the right-hand side of (13) is

$$v(X, X_z)X = f_{\rm b}(X) - \frac{\partial D(X)}{\partial z}.$$
(14)

This means that for (13) we can utilize ingredients of the numerical method presented by Bürger et al. (2013) with the addition of the reaction term. To find numerical updates for the two portions $X_{\rm a}$ and $X_{\rm i}$ of X, we use the idea by Diehl (1997) and Jeppsson and Diehl (1996b). To this end, we introduce the percentage $p := X_{\rm a}/X$ when X > 0, so that $X_{\rm a} = pX$ and $X_{\rm i} = (1 - p)X$ hold, and rewrite Equation (1) as

$$\frac{\partial(pX)}{\partial t} = -\frac{\partial}{\partial z} \left(v(X, X_z) pX \right) + \left(\mu(S_{\text{NO}_3}, S_{\text{S}}) - b \right) pX, \qquad 0 < z < B, \quad t > 0.$$
(15)

The idea of the numerical method is the following. In each discrete time step, X is first updated via a discretized version of (13), assuming X_a is known. This means that the flux (14) is known during this time step. Since the flux of (15) is p times the known flux (14), it is only the variable p that needs to be updated, and this can be achieved by a discrete version of (15). Then the concentration of the second particulate component is simply $X_i = (1 - p)X$. The numerical updates of S_{NO_3} , S_S and S_{N_2} are then straightforward for the corresponding equations (3)–(5).

We introduce the spatial discretization by dividing the interval (0, B) into N cells 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 cell j and likewise $P_j = P_j(t)$ the approximation of p. The numerical fluxes between cells j and j+1 are defined as follows. The convective flux f_b is discretized by the standard Godunov numerical flux, i.e.,

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

If the numerical compressive flux is defined as

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

then the total flux (14) between cells j and j+1 is approximated by $F_{j+1/2} := G_{j+1/2} - J_{j+1/2}$. The corresponding flux of (15) 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 cell j to j+1. Consequently, the value of $P_{j+1/2}$ at the boundary between the cells is the one in

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the left cell, i.e. P_j . If $F_{j+1/2} \leq 0$, then the value is P_{j+1} , i.e.

$$P_{j+1/2} = \begin{cases} P_{j+1}, & \text{if } F_{j+1/2} \le 0, \\ P_j, & \text{if } F_{j+1/2} > 0. \end{cases}$$
(16)

Defining the zero boundary fluxes and percentages $G_{1/2} = G_{N+1/2} = J_{1/2} = J_{N+1/2} = P_{1/2} = P_{N+1/2} = 0$, we obtain the following semi-discretized ODE system for the PDEs, where $j = 1, \ldots, N$:

$$\frac{\mathrm{d}X_j}{\mathrm{d}t} = -\frac{F_{j+1/2} - F_{j-1/2}}{\Delta z} + \left(\mu(S_{\mathrm{NO}_3,j}, S_{\mathrm{S},j}) - (1 - f_{\mathrm{P}})b\right)X_{\mathrm{a},j},\tag{17}$$

$$\frac{\mathrm{d}(P_j X_j)}{\mathrm{d}t} = -\frac{P_{j+1/2} F_{j+1/2} - P_{j-1/2} F_{j-1/2}}{\Delta z} + \left(\mu(S_{\mathrm{NO}_{3},j}, S_{\mathrm{S},j}) - b\right) X_{\mathrm{a},j},\tag{18}$$

$$\frac{\mathrm{d}S_{\mathrm{NO}_{3},j}}{\mathrm{d}t} = d_{\mathrm{S}} \frac{S_{\mathrm{NO}_{3},j+1} - 2S_{\mathrm{NO}_{3},j} + S_{\mathrm{NO}_{3},j-1}}{\Delta z^{2}} - \frac{1 - Y}{2.86Y} \mu(S_{\mathrm{NO}_{3},j}, S_{\mathrm{S},j}) X_{\mathrm{a},j},\tag{19}$$

$$\frac{\mathrm{d}S_{\mathrm{S},j}}{\mathrm{d}t} = d_{\mathrm{S}} \frac{S_{\mathrm{S},j+1} - 2S_{\mathrm{S},j} + S_{\mathrm{S},j-1}}{\Delta z^2} - \left(\frac{\mu(S_{\mathrm{NO}_3,j}, S_{\mathrm{S},j})}{Y} - (1 - f_{\mathrm{P}})b\right) X_{\mathrm{a},j},\qquad(20)$$

$$\frac{\mathrm{d}S_{\mathrm{N}_{2},j}}{\mathrm{d}t} = d_{\mathrm{S}} \frac{S_{\mathrm{N}_{2},j+1} - 2S_{\mathrm{N}_{2},j} + S_{\mathrm{N}_{2},j-1}}{\Delta z^{2}} + \frac{1 - Y}{2.86Y} \mu(S_{\mathrm{NO}_{3},j}, S_{\mathrm{S},j}) X_{\mathrm{a},j}, \tag{21}$$
$$X_{\mathrm{a},j} = P_{j} X_{j},$$

$$X_{i,j} = (1 - P_j)X_j.$$

These equations are thus exact conservation laws for each of the N cells (layers). Note that $X_{i,j}$ can be defined after the entire simulation.

3.2. Explicit fully discrete scheme. Let t_n , n = 0, 1, ... denote the discrete time points and Δt 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., P_j^n . The main restriction of the time step (for small Δz) is due to the second-order spatial derivatives in the compression term (Bürger et al., 2005, 2012). The CFL condition for explicit Euler and batch sedimentation is

$$\Delta t \le \frac{1}{k_1/\Delta z + k_2/\Delta z^2},\tag{22}$$

with

$$k_{1} := \max_{0 \le X \le X_{\max}} \left| f_{b}'(X) \right|, \qquad k_{2} := 2 \max_{0 \le X \le X_{\max}} d_{\text{comp}}(X), \tag{23}$$

and where X_{max} is the maximum concentration.

For explicit Euler, the time derivatives on the left-hand side of (17)-(21) are approximated by the standard finite difference ratio and the right-hand side is evaluated at time t_n . First, Equation (17) gives the update X_i^{n+1} according to

$$X_{j}^{n+1} = X_{j}^{n} + \Delta t \left(-\frac{F_{j+1/2}^{n} - F_{j-1/2}^{n}}{\Delta z} + \left(\mu(S_{\text{NO}_{3},j}^{n}, S_{\text{S},j}^{n}) - (1 - f_{\text{P}})b \right) X_{\text{a},j}^{n} \right).$$

The equations for the substrates can be written converted in the same way. For Equation (18), the approximation of the time derivative is

$$\frac{\mathrm{d}(P_j X_j)}{\mathrm{d}t_n} \approx \frac{P_j^{n+1} X_j^{n+1} - P_j^n X_j^n}{\Delta t}.$$

Note that if $X_j^{n+1} = 0$, then there is no particle in cell j, hence the value of P_j^{n+1} is irrelevant, since the product $P_j^{n+1}X_j^{n+1} = 0$. If $X_j^{n+1} > 0$, then we get the following update formula for P_j^{n+1} :

$$P_{j}^{n+1} = \frac{1}{X_{j}^{n+1}} \left[P_{j}^{n} X_{j}^{n} + \Delta t \left(-\frac{P_{j+1/2}^{n} F_{j+1/2}^{n} - P_{j-1/2}^{n} F_{j-1/2}^{n}}{\Delta z} + \left(\mu(S_{\text{NO}_{3},j}^{n}, S_{\text{S},j}^{n}) - b \right) X_{\text{a},j}^{n} \right) \right].$$

3.3. Method-of-lines equations. In order to apply any standard ODE solver for the time discretization, the semi-discretized equation (18) should be rewritten with the variable $X_{a,j} = P_j X_j$. Recall that the total flux F_j depends only on X_j , whereas the formula (16) should be replaced by

$$P_{j+1/2} = \begin{cases} X_{\mathbf{a},j+1}/X_{j+1}, & \text{if } F_{j+1/2} \le 0, \\ X_{\mathbf{a},j}/X_j, & \text{if } F_{j+1/2} > 0. \end{cases}$$

The inert matter can be defined by $X_{i,j} = X_j - X_{a,j}$.

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 (9) and (10), respectively. The heterotrophic maximal specific growth rate μ that we use is given in (7), 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 to 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.

In all numerical examples, we employ the explicit scheme with N = 100 cells 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. The time step Δt is chosen by 98% of the bound given in the right-hand side of (22), with constants k_1 and k_2 defined by (23).

The initial values common to all examples are

$$S_{\rm S}^0 = 9.00 \times 10^{-4} \,\mathrm{kg} \,\mathrm{m}^{-3}$$
 and $S_{\rm NO_3}^0 = 6.00 \times 10^{-3} \,\mathrm{kg} \,\mathrm{m}^{-3}$,

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



FIGURE 1. Example 1 (Kynch test, $d_{\rm S} = 10^{-6} \,\mathrm{m^2 \, s^{-1}}$). Here and in Figures 2 to 6, the visual grid used to display the numerical solution is coarser than the computational grid, and plots of solutions have been rotated for each quantity such that almost all parts are visible.

4.2. Examples 1 to 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 active biomass and inert matter by $p_0 = 5/7 \approx 0.7143$, so that

$$X_{\rm a}(z,0) = 2.5 \,\mathrm{kg} \,\mathrm{m}^{-3}, \quad X_{\rm i}(z,0) = 1.0 \,\mathrm{kg} \,\mathrm{m}^{-3} \quad \mathrm{for} \ 0 < z < B.$$

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 $d_{\rm S} = 10^{-6} \,\mathrm{m}^2 \,\mathrm{s}^{-1}$ informed in Table 1. Figure 1 and 2 show the numerical results for all unknowns for $T = 2 \,\mathrm{h}$ and $T = 100 \,\mathrm{h}$, respectively. We observe that the solids settle downwards rapidly and form a sludge blanket with a sharp interface at $X_{\rm c} = 5 \,\mathrm{kg} \,\mathrm{m}^{-3}$. Moreover, the concentration increases downwards gradually until reaching about 20 kg m⁻³ at the bottom. Here, and in Examples 2 to 7, the solutions for all quantities are bounded and non-negative. The $S_{\rm NO_3}$ 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



FIGURE 2. Example 1 (Kynch test, $d_{\rm S} = 10^{-6} \,\mathrm{m^2 \ s^{-1}}$): long-time simulation $(T = 100 \,\mathrm{h})$.

formation of readily biodegradable substrate (of concentration $S_{\rm S}$) at the bottom of the column. Furthermore, the solution for $S_{\rm N_2}$ has a plateau at 6×10^{-3} kg m⁻³, which is the initial value of $S_{\rm NO_3}$. This suggests that within the sludge blanket, almost all soluble nitrate degrades into nitrogen.

For this particular case we also present a simulation until T = 100 h to study the longtime behaviour of the model. The results shown in Figure 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 inert matter increases in time (as expected). The substrates slowly approach an equilibrium concentration as a consequence of their slow diffusive movement.

Figures 3 and 4 show the corresponding results for the same scenario but with increased values of the substrate diffusion parameter, namely $d_{\rm S} = 9 \times 10^{-6} \,\mathrm{m^2 \, s^{-1}}$ (Figure 3) and $d_{\rm S} = 1.3 \times 10^{-5} \,\mathrm{m^2 \, s^{-1}}$ (Figure 4). We observe that the changes in this parameter practically do not affect the solids settling behaviour; the solutions for X, $X_{\rm a}$ and $X_{\rm i}$ are virtually the same as in Example 1. However, difference in the solution behaviour of the substrates are appreciable, especially for $S_{\rm NO_3}$. Roughly speaking, since increasing $d_{\rm S}$ means increasing the diffusive flux of each substrate, that is, the flow rate from regions of high concentration to



FIGURE 3. Example 2 (Kynch test, $d_{\rm S} = 9 \times 10^{-6} \,\mathrm{m^2 \, s^{-1}}$).

those of low concentration, we observe that the flux of nitrate into the sludge zone consistently increases comparing the results of Examples 1, 2, and 3. Since the degradation of nitrate takes place due to reactions in that zone, we obtain that for this test, increasing $d_{\rm S}$ produces an overall more rapid denitrification. Corresponding differences 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:

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

for Example 4, and

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

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 Figures 5 and 6. We observe in both examples that the initial



FIGURE 4. Example 3 (Kynch test, $d_{\rm S} = 1.3 \times 10^{-5} \,{\rm m}^2 \,{\rm s}^{-1}$).

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 suspensions-supernate 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 in the present context to evaluate the effect of the initial configuration on the denitrification process. We see that the solution for S_{NO_3} is non-monotone (as a function of z for fixed t), which is also reflected in the solution for S_{N_2} , and comparing the S_{NO_3} plot of Figure 6 with that of Figure 1 shows that the total amount of nitrate at T = 2 h is significantly smaller in Examples 4 and 5 than in Example 1.

In light of the latter observation we measure the time-dependent normalized total mass of nitrate, the so-called normalized inventory, defined by

$$I_{\rm NO_3}(t) := \frac{1}{S_{\rm NO_3}^0 B} \int_0^B S_{\rm NO_3}(z,t) \, \mathrm{d} z.$$



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

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

$$I_{\rm NO_3}^{\Delta}(t) := \frac{1}{S_{\rm NO_3}^0 B} \sum_{j=1}^N S_{\rm NO_3, j}^n \Delta z = \frac{1}{S_{\rm NO_3}^0 N} \sum_{j=1}^N S_{\rm NO_3, j}^n.$$

Note that $I_{\text{NO}3}(0) = I_{\text{NO}3}^{\Delta}(0) = 1$. Figure 7 displays the evolution of $I_{\text{NO}3}^{\Delta}(t)$ for Examples 1 to 5. Comparing the curves for Examples 1, 2 and 3, we find confirmed that an increased value of the substrate diffusion coefficient d_{S} accelerates the denitrification process in the setup of the Kynch test. However, d_{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, but is maintained over a longer period of time in case of the DT, with the effect that the portions of the curve corresponding to slow rates of denitrification (produced in the consolidation stage) lie about 10% and 15%, in the respective cases of the DT Examples 4 and 5, below that of the KT Example 1. This result illustrates how the initial placement of solids mass may influence the rate of denitrification.



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

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

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

for Example 6 and

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

for Example 7. The respective numerical results are shown in Figures 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 compresibility by a nonlinear diffusion term $\partial^2 D(\phi)/\partial z^2$. This approach corresponds to elastic and in a sense reversible material behaviour which is usually not observed with activated sludge in reality. While this behaviour in an anomalous situation calls for an improvement of the constitutive assumptions concerning sediment compressibility, we emphasize that this test produces an upward movement of



FIGURE 7. Examples 1 to 5: evolution of the approximate normalized nitrate inventory $I^{\Delta}_{NO_3}(t)$. 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 Ex. 1.

solid partices, which is associated with negative values of the velocity v defined in (8). The case discrimination in (16), which goes back to the method by Diehl (1997), has precisely been devised to handle this situation. Thus, Figures 8 and 9 demonstrate that the model is sound, and the numerical scheme works properly, even for settling velocities of variable sign.

4.5. Accuracy and efficiency. To illustrate the accuracy of the method, we plot in Figures 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, we calculated the approximate relative error, defined at a fixed time point,

$$\begin{split} e_N^{\text{rel}} &:= \frac{\|X_{\text{a}} - X_{\text{a}}^{\text{ref}}\|_{L^1}}{\|X_{\text{a}}^0\|_{L^1}} + \frac{\|X_{\text{i}} - X_{\text{i}}^{\text{ref}}\|_{L^1}}{\|X_{\text{i}}^0\|_{L^1}} + \frac{\|S_{\text{NO}_3} - S_{\text{NO}_3}^{\text{ref}}\|_{L^1}}{\|S_{\text{NO}_3}^{\text{end}}\|_{L^1}} \\ &+ \frac{\|S_{\text{N}_2} - S_{\text{N}_2}^{\text{ref}}\|_{L^1}}{\|S_{\text{N}_2}^0\|_{L^1}} + \frac{\|S_{\text{S}} - S_{\text{S}}^{\text{ref}}\|_{L^1}}{\|S_{\text{S}}^0\|_{L^1}}, \end{split}$$

and the observed convergence rates between two discretizations $N = N_1$ and $N = N_2$ given by

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

apart from measuring the CPU time for each run; see Table 2. Our results are consistent with the fact that the scheme is formally first-order accurate in space and time, and moreover the approximated solutions exhibit discontinuities. Of course, while these results suggest that the scheme converges to a definite limit function, a rigorous convergence proof is still



FIGURE 8. Example 6 (overcompressed test, $X(z, 0) = 20 \text{ kg m}^{-3}$ below z = 0.7 m)

under preparation. Furthermore, CPU times indicate that the CFL condition (22) essentially imposes $\Delta t \sim \Delta z^2$, with the effect that halving the spatial discretization Δz (to increase accuracy) and choosing Δt according to (22) causes roughly an eightfold increase in CPU time.

5. Conclusions

A reduced model of simultaneous biological reactions and sedimentation of flocculated particles in batch operation has been written as a system of convection-diffusion-reaction PDEs, and a numerical scheme for its numerical simulation has been 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 reduced model here, 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 numerical ingredients presented by Bürger



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

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 dells are known, which is utilized in the update of the percentage vector.

Numerical examples for the modelling of the last stage of an SBR sequence, where denitrification occurs, indicate that the suggested numerical scheme works well and the expected denitrification process is simulated. Furthermore, these simulations show that the initial distribution of the sludge has a certain implication in the efficiency of reducing nitrate. Turning up the aeration from below so that a layer of sludge appears at the top of the vessel as the aeration is turned off (Diehl test) means a more efficient reduction of the inventory of nitrate than the initially homogeneous concentration of suspension (Kynch test); see Figure 9.

There are obvious continuations of this initial work on reactive settling, which include: a more accurate modelling of the movement of the liquid, in which the substrates are dissolved; the extension to include a full ASM model for the biological reactions; analysis of the convergence properties of the numerical scheme; and development of more efficient time discretizations.



FIGURE 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} and S_S (right).

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FIGURE 11. Example 4 (Diehl test): comparison between a reference solution (N = 3200) and two fastly 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).

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Example 1, $t = 4 \min$				Example 1, $t = 30 \min$		
\overline{N}	e_N^{rel}	θ	cpu [s]	e_N^{rel}	θ	cpu[s]
20	0.097		0.0016	0.740		0.0108
50	0.033	1.176	0.0120	0.302	0.978	0.0784
100	0.018	0.853	0.0820	0.148	1.026	0.6224
200	0.008	1.194	0.4992	0.072	1.045	4.7687
400	0.004	1.141	4.5871	0.034	1.092	28.0518
800	0.002	0.878	25.9932	0.014	1.224	222.1103
Example 4, $t = 6 \min$						
	Exam	ple 4, t	$= 6 \min$	Exam	ple 4, t	$= 30 \min$
N	$\frac{\text{Exam}}{e_N^{\text{rel}}}$	$\frac{\text{ple } 4, t}{\theta}$	$= 6 \min $ cpu [s]	Exam $e_N^{\rm rel}$	ple 4, t θ	$= 30 \min \\ \operatorname{cpu}[s]$
$\frac{N}{20}$	$\frac{\text{Exam}}{e_N^{\text{rel}}}$ 0.204	ple 4, t θ	$= 6 \min$ cpu [s] 0.0016	$\frac{\text{Exam}}{e_N^{\text{rel}}}$ 0.224	ple 4, t θ	= 30 min cpu [s] 0.0064
	$\frac{\text{Exam}}{e_N^{\text{rel}}}$ $\frac{0.204}{0.110}$	$\frac{\text{ple } 4, t}{\theta} \\ - \\ 0.674$	$= 6 \min$ cpu [s] 0.0016 0.0116	$\begin{array}{c} \text{Exam} \\ e_N^{\text{rel}} \\ 0.224 \\ 0.069 \end{array}$	$\frac{\text{ple } 4, t}{\theta} \\ -1.285$	$= 30 \min \\ cpu [s] \\ 0.0064 \\ 0.0500$
	$\begin{array}{c} {\rm Exam} \\ e_N^{\rm rel} \\ 0.204 \\ 0.110 \\ 0.066 \end{array}$	$\frac{\text{ple } 4, t}{\theta}$ $-$ 0.674 0.745	$= 6 \min \\ cpu [s] \\ 0.0016 \\ 0.0116 \\ 0.0848$	Exam $e_N^{\rm rel}$ 0.224 0.069 0.029	$ \begin{array}{r} \text{ple 4, } t \\ \hline \theta \\ \hline - \\ 1.285 \\ 1.231 \end{array} $	$= 30 \min \\ cpu [s] \\ 0.0064 \\ 0.0500 \\ 0.3952$
$ \frac{N}{20} 50 100 200 $	$\begin{array}{c} {\rm Exam} \\ e_N^{\rm rel} \\ 0.204 \\ 0.110 \\ 0.066 \\ 0.038 \end{array}$	$ \frac{\text{ple } 4, t}{\theta} \\ \hline $	$= 6 \min \\ cpu [s] \\ 0.0016 \\ 0.0116 \\ 0.0848 \\ 0.6108 \\ \end{bmatrix}$	$\begin{array}{c} {\rm Exam} \\ e_N^{\rm rel} \\ 0.224 \\ 0.069 \\ 0.029 \\ 0.016 \end{array}$	$ \frac{\text{ple } 4, t}{\theta} \\ \hline $	$= 30 \min \\ cpu [s] \\ 0.0064 \\ 0.0500 \\ 0.3952 \\ 3.2098$
$ \frac{N}{20} \\ 50 \\ 100 \\ 200 \\ 400 $	$\begin{array}{c} {\rm Exam} \\ e_N^{\rm rel} \\ 0.204 \\ 0.110 \\ 0.066 \\ 0.038 \\ 0.021 \end{array}$	$ \begin{array}{r} $	$= 6 \min cpu [s] 0.0016 0.0116 0.0848 0.6108 4.6543 $	$\begin{array}{c} {\rm Exam} \\ e_N^{\rm rel} \\ 0.224 \\ 0.069 \\ 0.029 \\ 0.016 \\ 0.010 \end{array}$	$ \begin{array}{r} $	$= 30 \min \\ cpu [s] \\ 0.0064 \\ 0.0500 \\ 0.3952 \\ 3.2098 \\ 24.8136$

TABLE 2. Examples 1 and 4: approximate relative errors e_N^{rel} , convergence rates θ (calculated between neighboring values of N) and CPU times cpu for two different simulated times (cf. Figures 10 and 11).

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