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Raimund Bürger, Stefan Diehl,
Ingmar Nopens

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Stefan Diehl[1], Ingmar Nopens[2], Raimund Bürger[3]

[1]Centre for Mathematical Sciences, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden; telephone: +46 46 2220920, e-mail: diehl@maths.lth.se; corresponding author
[2]BIOMATH, Department of Applied Mathematics, Biometrics and Process Control, Coupure Links 653, 9000 Gent, Belgium; e-mail: ingmar.nopens@ugent.be
[3]CI^{2}MA and Departamento de Ingeniería Matemática, Facultad de Ciencias Físicas y Matemáticas, Universidad de Concepción, Casilla 160-C, Concepción, Chile; e-mail: rburger@ing-mat.udec.cl

Running title: A consistent modeling methodology

ABSTRACT: The aim of this contribution is to build consensus on a consistent modeling methodology (CMM) of complex real processes in wastewater treatment by utilizing both classical concepts and new results from applied mathematics. The real process should be approximated by a mathematical model (process model; ordinary or partial differential equation (ODE or PDE)), which in turn is approximated by a simulation model (numerical method) implemented on a computer. Although this has been done before, often it has not been carried out in a correct way. The secondary settling tank was chosen as a case since this is one of the most complex processes in a wastewater treatment plant and the simulation models developed decades ago have no guarantee of satisfying fundamental mathematical and physical properties. Nevertheless, such methods are still used in commercial tools to date. This particularly becomes of interest as the state-of-the-art practice is moving towards plant-wide modeling. Then all submodels interact and errors propagate through the model and severely hamper any calibration effort and, hence, the predictive purpose of the model. The CMM is described by applying it first to a simple conversion process in the biological reactor yielding an ODE solver, and then to the solid-liquid separation in the secondary settling tank, yielding a PDE solver. Time has come to incorporate established mathematical techniques into environmental engineering, and wastewater treatment modelling in particular, and to use proven reliable and consistent simulation models.

KEYWORDS: Secondary clarifier, thickener, continuous sedimentation, partial differential equation, simulation model, numerical method

Introduction

Wastewater treatment (WWT) systems are widely studied with the aid of mathematical models (Gujer, 2008; Henze et al., 2000). Detailed models exist for the biological processes occurring in the system. However, a biological WWT system also includes a secondary settling tank (SST) for the separation of the cleaned liquid from the activated sludge. It has also a thickening function to recycle and retain the solids and, hence, the biological activity in the system. A typical WWT model consists of a very complex biological submodel and a rather simplified sedimentation submodel. The reason for the latter is mainly a practical one. Indeed, the biological models typically consist of ordinary differential equations (ODEs), whereas a sedimentation model includes both time and space dependence, turning it into a partial differential equation (PDE). The main commercial simulators, however, do not provide reliable simulation methods for these PDEs; there is no guarantee that the simulations satisfy fundamental mathematical and physical properties. One reason for this has been the lack of established solvers for the particular type of nonlinear PDE that models continuous sedimentation. Therefore, many workarounds have been proposed for the simulation of integrated WWT models in an ODE environment (Abusam and Keesman, 2009; Chatellier and Audic, 2000; David et al., 2009a, 2009b; De Clercq et al., 2003; Dupont and Dahl, 1995; Dupont and Henze, 1992; Giokas et al., 2002; Hamilton et al., 1992; Härtel and Pöpel, 1992; Koehne et al., 1995; Nocoń, 2006; Otterpohl and Freund, 1992; Ozinsky et al.,1994; Plósz et al., 2007; Queinnec and Dochain, 2001; Takács et al.,1991; Vaccari and Uchrin, 1989; Verdickt et al., 2005; Vitasovic, 1989; Watts et al., 1996; Zheng and Bagley, 1998). Although acceptable at the time of their development, these simulation models should be reconsidered as both knowledge and computational power have evolved significantly. In short, the problem is not the ODE environment, rather the heuristic unreliable workarounds in the numerical implementation. De Clercq (2006) and De Clercq et al. (2008) utilize the mathematically proved reliable PDE solver by Bürger et al. (2005) for the secondary settling tank (SST). An example of a combination of PDE and ODE solvers is the simulation model by Diehl and Jeppsson (1998), which utilizes the Activated Sludge Model no 1 (ASM1) by Henze et al. (1987) and a PDE solver for the SST. The PDE solver includes the sedimentation of the flocculated multi-component particles (Jeppsson and Diehl, 1996b).

SSTs often cause problems in the daily operation of wastewater treatment plants (WWTPs). Factors influencing the solid-liquid separation include hindered and compression settling, flocculation-breakup, non-settleable solids fractions, sludge viscosity and density. Furthermore, hydrodynamic impacts (geometry/design of the SST, horizontal density currents, solids influent and removal) have been studied in more detail and resulted in additional knowledge that has not yet been included into integrated WWT models. Hence, the problematic behavior often observed in practice cannot be explained by current state-of-the-art models. Moreover, new pressures on WWT systems have come into the picture. An important one with respect to the SST is the occurrence of extreme hydraulic events most possibly induced by climate change. The development of mitigation strategies calls for improved settler models. When developing the latter, it makes a lot of sense to start from the state of the art in the modelling of continuous sedimentation that has been achieved in different disciplines. Knowledge in applied mathematics, chemical engineering and environmental engineering should be combined and utilized with the aim

of building SST models efficiently, but first of all consistently.

The clarification-thickening process also appears in several other applications, such as the mineral, chemical, food, pulp-and-paper and other industries. Researchers in different disciplines therefore tackled basically the same problem, gained a lot of insight and produced new results during several decades. From our experience there persists a wide gap between different fields, particularly between mathematics and environmental engineering science, which we would like to bridge. New results in mathematical publications require fairly advanced skills to be understood fully, so applied mathematicians need to "translate" and explain how the results can be used in the applications. The specific nonlinearities of the continuous sedimentation process have led to intense mathematical research during the last two decades. The environmental engineering field should now benefit from these results.

Another reason for the gap lies in the traditional modeling approaches. In the WWT field, a "settler model" often means a simulation model implemented on a computer. This has been accomplished by writing down the numerical scheme directly from physical reasoning and experience. There is no analysis provided in what way such a method produces any reliable simulation. On the contrary, such a numerical scheme is often inconsistent in one or another way (e.g. the Takács model). At the same time, there exists a fundamental modeling methodology that is usually not written out but understood among applied mathematicians and utilized in some applied fields, e.g. chemical engineering. This methodology would be beneficial for the SST modeling future and this is the reason for the present paper. Moreover, it is in the interest of the environmental engineering field to use proven reliable models in order to avoid that people loose trust in them. This is especially important when moving to plant-wide modeling.

In this paper, we propose a consistent modeling methodology (CMM), within which future model extensions can be developed and thereby unnecessary pitfalls avoided. We make a clear distinction between a mathematical model and a simulation model. The CMM makes it easier to determine sound and unsound ways of modeling. The paper is organized in the following way. In the next section, the CMM is described by applying it to a principle biological process in the biological reactor. The outcome is an ODE solver. Then the CMM is applied to the continuous sedimentation process and the outcome is a PDE solver. The last section contains some illustrative simulations.

A consistent modeling methodology (CMM)

The CMM is illustrated in Figure 1. The terminology is explained in more detail in the Appendix. After initial observations and experience of the real process, the modeling procedure begins. In this section, we describe the six steps of the CMM by applying it to a biological conversion process occurring in a compartment of the bioreactor within the activated sludge process. *The purpose of the CMM is to create a simulation model that produces reliable simulated data with respect to the input assumptions made and the given physical law.*

FIGURE 1

Step 1: Construction of a mathematical model. The starting point is usually a physical law. Often it is the conservation law of mass (mass balancing) which postulates that the increase of mass per time unit of a substrate in a region equals the net flux into the region ("transport in" minus "transport out") plus the net production within the

region (production minus consumption). Let the region be one of the compartments of the biological reactor. For simplicity, we consider an intermediate compartment of fixed volume V with the in- and outgoing volumetric flow rate Q. If we also make the *idealizing assumption* that the compartment is always completely mixed, then the concentration of a single substance (substrate or biomass) Z is the same in the whole reactor at each time point t. Denoting the incoming concentration of the substance in the compartments by Z^{in}, we can write down the conservation law exactly, namely as the following ODE:

$$V\frac{dZ}{dt} = QZ^{\text{in}} - QZ + rV\,. \qquad (1)$$

Here, r is the reaction rate and the term rV the net production of the substance within the compartment per time unit. The given variables in (1) are V, Q and Z^{in} and the sought variable is Z. To solve the equation, one needs an additional relation between r and Z (and concentrations of other substances). This is called a *constitutive relation*, or a constitutive assumption, and contains the model parameters. A common such is the Monod relation, which for $Z = S_{\text{s}}$ (readily biodegradable soluble COD) can be written as (ignoring for simplicity any dependence on other substances)

$$r = -\frac{\mu_{\max} S_{\text{s}}}{Y_{\text{H}}(K_{\text{s}} + S_{\text{s}})}\,. \qquad (2)$$

The model parameters (in this example $\mu_{\max}, Y_{\text{H}}$ and K_{s}) may have some physical meaning and they can sometimes be determined by laboratory experiments. We may model m substances ($Z_i, i = 1, \ldots, m$) in the compartment by m ODEs of the form (1), which are coupled via the reaction rates similar to (2). We have a nonlinear system of ODEs, which makes up the mathematical model or process model, or just the model of the reactor. A well-known example is the ASM1 by Henze et al. (1987), in which $m = 13$.

Step 2: Establishing well-posedness. In engineering, the system of ODEs of the form (1) would simply be simulated with an ODE solver in a software platform, which many users completely trust and not question its correctness. One may not realise that the solver actually is derived from the mathematical model behind the software platform. The actual solution of the mathematical model, the exact solution, consists of a vector of substance concentrations as function of time, $Z_i(t)$, which satisfy the ODEs at every time point t (given initial data $Z_i(0)$). In many cases it is impossible to write down these functions explicitly in terms of simple expressions like exponentials, power laws, trigonometric functions, etc. This is often referred to as "the equations cannot be solved (explicitly)". Nevertheless, the question whether an exact solution exists or not is still open. If there exists one, it is physically and computationally important that it should be unique for given initial data. Furthermore, small changes in the initial data should only cause small changes in the solution. In other words, a solution should exist, be unique and depend continuously on initial data – the model is then said to be well-posed. Establishing well-posedness is often difficult and requires mathematical tools often originating in physical principles; see e.g. Bürger et al. (2004b). (The existence of a solution can sometimes be proved by utilizing a numerical method, see Step 3 below. The uniqueness of a solution is often proved by starting with two solutions, both satisfying the same initial data, and then one proves that they are actually identical. A similar procedure can often be used to establish of the continuous dependence on initial data.) For our purposes, well-

posedness is of key importance since it ensures that the mathematical model describes the real process in a relevant way. If the mathematical model is not well-posed, then it is meaningless to try to find a numerical method for simulation.

Step 3: Numerical method and simulation program. Fortunately, most ODE models arising from real processes are well-posed and can be solved approximately by efficient and reliable numerical methods, such as Runge-Kutta methods, which are utilized in commercial software packages (e.g. the example in Step 1). The terminology "ODE solver" is well established for such a numerical method, although it only delivers approximate solutions of the unique exact solution of the mathematical model, which is defined at *every* time point t. The numerical approximate solution is only given at *discrete* time points. However, any reliable numerical method should produce numerical solutions that are increasingly better approximations of the exact solution as the resolution of the discrete time points becomes finer. In other words, the numerical solutions *converge* to the exact solution as the time step tends to zero.

Step 4: Calibration. Identification, calibration or fine tuning of the model is done by adjusting the model parameters in the constitutive relations. Some parameters may be found with specifically designed batch experiments in laboratories (e.g. respirometry). Otherwise real (full-scale) and simulated data are compared. The method of least squares and some suitable optimization algorithm are often used to find the optimal parameters, i.e. to solve the calibration problem. When the process includes biological material that changes over time it is an ultimate goal to develop an on-line calibration method of the full process. If the outcome of the calibration is not satisfactory, one could try new constitutive relations (instead of the Monod expression). The more parameters these have, the more is the freedom of adjustment which adds to the cost of computations, a more ill-conditioned calibration problem (difficult to find unique parameters) and sometimes also an ill-posed calibration problem (some parameters are not identifiable; different values of the parameters may yield the same simulated data; the calibration problem is not uniquely determined, hence not well-posed). More parameters will also induce larger output uncertainty.

Step 5: Validation. As one set of data has been used for calibration, another independent set should be used for validation of the model.

Step 6 and 1: Rebuilding or extension of the model. In the validation step (or already in the calibration step) one often encounters that the real process behaves in a way that cannot be explained sufficiently accurately by the simulation model. Then the only sound way to proceed is to change the mathematical model by changing the idealizing assumptions and restart from Step 1. Note that the simulation model is never changed directly, only indirectly via the mathematical model. This step is often violated in the previous models in the literature.

The CMM applied to the continuous sedimentation process

Step 1: Construction of a mathematical model. The physical law is again the conservation of mass. We want to model the process of solid-liquid separation of activated sludge driven by gravity and it is well known that the particulate concentration depends on both space and time; $C(z,t)$, where the z-axis points downwards, see Figure 2. We thus make the idealizing assumption that the SST is one dimensional. We know that this is

restrictive, but it will lead to a model that can capture the fundamental features of gravity settling and compression, since these phenomena occur in only one dimension. Considering the sludge, we make idealizing assumptions such as: there is no biological activity in the SST; the sludge has flocculated in the preceding reactor and consists of particles of the same size and shape; outside the SST, i.e. in the outlet and effluent pipes, the sludge and water have the same speed.

To capture the processes of gravity settling and compression it is fruitful to consider temporarily batch sedimentation, i.e., sedimentation without bulk flows. Then the conservation of mass can be written as the PDE

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial z}(C v_{\mathrm{s}}) = 0\,, \tag{3}$$

where $v_{\mathrm{s}} \geq 0$ is the downward settling velocity of the particles. This is one equation with two unknowns (C and v_{s}). Hence, a constitutive relation is needed between v_{s} and C. We make the following constitutive assumptions:

1. The *hindered settling velocity* $v_{\mathrm{hs}}(C)$ is a function of the local concentration only (Kynch, 1952). This is the velocity of a layer of constant concentration, i.e., when there is no concentration gradient present. Commonly used formulae for activated sludge are those by Vesilind (1968) and Takács et al. (1991).
2. For high concentrations the sludge may be compressed by its own weight. More specifically, above a critical concentration, denoted by C_{c}, the particles are in constant contact and form a network that can bear a certain stress, the effective solids stress $\sigma_{\mathrm{e}}(C)$, which is assumed to be an increasing function of the concentration above C_{c} and zero below (Aziz et al., 2000; Bürger et al., 2000a; De Kretser et al., 2001).

In accordance with the continuum mechanical derivations by Bürger et al. (2000b), we assume that the downward settling velocity of the particles in batch sedimentation can be written as the following constitutive relation:

$$v_{\mathrm{s}} = \begin{cases} v_{\mathrm{hs}}(C) & \text{for } 0 \leq C \leq C_{\mathrm{c}} \\ v_{\mathrm{hs}}(C)\left(1 - \dfrac{\rho_{\mathrm{s}}\sigma_{\mathrm{e}}'(C)}{Cg\Delta\rho}\dfrac{\partial C}{\partial z}\right) & \text{for } C > C_{\mathrm{c}}\,, \end{cases} \tag{4}$$

where ρ_{s} is the density of the solids, g the gravity of acceleration and $\Delta\rho$ the density difference between the solids and the liquid. Thus, for concentrations greater than C_{c}, the settling velocity is reduced by a compression effect when the concentration increases with depth. This has the same effect on the solution as a nonlinear diffusion phenomenon. Indeed, inserting (4) into (3) yields the following degenerate parabolic PDE with one unknown variable C:

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial z}\big(C v_{\mathrm{hs}}(C)\big) = \frac{\partial}{\partial z}\left(d_{\mathrm{comp}}(C)\frac{\partial C}{\partial z}\right), \tag{5}$$

where the compression function is

$$d_{\mathrm{comp}}(C) = \begin{cases} 0 & \text{for } 0 \leq C \leq C_{\mathrm{c}}\,, \\ \dfrac{\rho_{\mathrm{s}}}{g\Delta\rho} v_{\mathrm{hs}}(C)\sigma_{\mathrm{e}}'(C) & \text{for } C > C_{\mathrm{c}}\,. \end{cases}$$

The flux function in (5), $C v_{\mathrm{hs}}(C)$, is the batch settling flux function originating from Kynch (1952). A consequence of (4) is that hydrodynamic diffusion is a much slower process and need not be modeled.

FIGURE 2

Now we again consider continuous sedimentation in the ideal 1D SST, see Figure 2. The height of the clarification zone is denoted by H and the depth of the thickening zone by B. The volume flows leaving the SST at the effluent and underflow are denoted by Q_{e} and Q_{u}, respectively. We assume that there is either an upward (Q_{e}) or a downward (Q_{u}) volumetric flow at each point of the 1D axis, except for a single point where the feed source is assumed to be situated ($z = 0$). The 1D assumption means several simplifying interpretations of the real process: The concentration is assumed to be the same at each depth z; no horizontal effects are considered; wall effects are neglected; etc. We may assume that the cross-sectional area depends on depth, but for simplicity of presentation we assume here that it is a constant A. A third constitutive assumption is the following:

3. Modelling mixing effects: The horizontal flows of an SST, however, are substantial and difficult to capture in a 1D model. The result of currents that mix lower and higher concentrations of sludge could possibly be seen as a result of a large diffusion. According to Fick's constitutive relation, we assume that the corresponding flux is equal to $-\mathrm{d}_{\mathrm{mix}} \frac{\partial \mathrm{C}}{\partial \mathrm{z}}$ with $\mathrm{d}_{\mathrm{mix}} \geq 0$. If mixing currents are expected at certain heights, for example at the feed inlet, we may assume that $\mathrm{d}_{\mathrm{mix}}$ depends on z and let it be larger in a neighborhood of the feed inlet. One of the idealizing assumptions is that the mixture follows the bulk flows in the outlet pipes. This means that as the mixture has left the SST it cannot return, which in turn implies that we must require

$$d_{\mathrm{mix}}(z) = 0 \text{ for } z < -H \text{ and } z > B\,.$$

The resulting term in the PDE is sometimes called a dispersion term and is assumed to be a function of the volumetric flow rates as well (David, 2009a; De Clercq et al., 2003, 2005; Lee et al., 2006; Lev et al., 1986; Plósz et al., 2007; Verdickt et al., 2005; Watts et al., 1996).

With a certain mathematical interpretation in mind called the weak sense, which allows for discontinuous solutions, we can write the conservation law of mass as the following convection-diffusion PDE, defined for $-\infty < z < \infty$:

$$\begin{aligned} &\frac{\partial C}{\partial t} + \frac{\partial}{\partial z} F(C, z, t) \\ &= \frac{\partial}{\partial z}\left(\left(\gamma(z) d_{\mathrm{comp}}(C) + d_{\mathrm{mix}}(z)\right) \frac{\partial C}{\partial z} \right) \\ &\quad + \frac{Q_{\mathrm{f}}(t) C_{\mathrm{f}}(t)}{A} \delta(z)\,. \end{aligned} \tag{6}$$

The last term is a source term containing the feed volumetric flow Q_{f}, the feed concentration C_{f} and the Dirac delta distribution δ. The convective flux function F contains the hindered settling velocity within the SST and the two volumetric upward and downward flows:

$$F(C, z, t) = \begin{cases} -Q_{\mathrm{e}}(t) C / A & \text{for } z < -H\,, \\ v_{\mathrm{hs}}(C) C - Q_{\mathrm{e}}(t) C / A & \text{for } -H < z < 0\,, \\ v_{\mathrm{hs}}(C) C + Q_{\mathrm{u}}(t) C / A & \text{for } 0 < z < B\,, \\ Q_{\mathrm{u}}(t) C / A & \text{for } z > B\,. \end{cases}$$

The depth axis is thus divided into four zones: the effluent zone ($z < -H$), clarification zone ($-H < z < 0$), thickening zone ($0 < z < B$) and underflow zone ($z > B$). The function $\gamma(z)$ is equal to 1 inside the SST, i.e. in the interval $(-H, B)$, and 0 outside. Hence, outside the SST there is neither sedimentation nor compression, only bulk flows. The fundamental features of Equation (6) are the following. If $d_{\mathrm{mix}} > 0$, then the equation has a diffusion term, which

implies that the solution has no discontinuities. In a mathematical model, we would like to be able to handle all special cases, also $d_{\mathrm{mix}} = 0$. Recent analysis shows that even in this case (6) is still well-posed (Bürger et al., 2005). For concentrations below C_{c}, the compression term vanishes ($d_{\mathrm{comp}} = 0$), the equation becomes hyperbolic and the solution may have discontinuities. This happens normally above and at the sludge blanket level. For higher concentrations the compression term smoothes the solution, which is then continuous. This occurs normally below the sludge blanket.

In this first step of the CMM, the mathematical model is Equation (6) together with initial data $C(z,0)$. The sought variable is the concentration $C(z,t)$ for $-\infty < z < \infty, t > 0$. The interesting output concentrations are $C(z,t)$ for $-H < z < B$ and the effluent and underflow concentrations (cf. Figure 2):

$C_{\mathrm{e}}(t) \coloneqq \lim_{\varepsilon \to 0+} C(-H-\varepsilon, t)$,
$C_{\mathrm{u}}(t) \coloneqq \lim_{\varepsilon \to 0+} C(B+\varepsilon, t)$.

Step 2: Establishing well-posedness. The investigations of well-posedness for PDEs of the form (6) and hence the development of a reliable numerical method are particularly complex. For instance, the solution of Equation (6) may contain discontinuities (e.g. the sludge blanket level), the interpretation of the PDE has to be made in a special mathematical sense called the weak sense. Another problem is that (6) does not have a unique solution for given initial data. An additional physical principle has to be added, a so-called entropy condition. Such an entropy condition should account for shock waves not only within each zone, but also at the space discontinuities (the feed inlet and the outlets). We do not go into the details here; see LeVeque (2002) for a general theory for shock waves within each region, and Bürger et al. (2005) and Diehl (2009) for equations of the form (6). In the special case when $d_{\mathrm{comp}} = d_{\mathrm{mix}} = 0$, Equation (6) was first presented and analyzed independently (with different mathematical approaches) by Chancelier et al. (1994) and Diehl (1996). More general results were later presented by Bürger et al. (2004b). A major break-through concerning the well-posedness of a version of (6) was made by Bürger et al. (2005). We also refer to this publication for further details of (6). They consider the case $d_{\mathrm{mix}} = 0$, however, the case $d_{\mathrm{mix}} > 0$ causes no new complication in the analysis. By an exact solution of the mathematical model we mean a solution of (6) that satisfies a suitable entropy condition (Bürger et al., 2005; Diehl, 2009).

Step 3: Numerical scheme (simulation model). Since the concentration depends on two variables, the discretization has to be made along both the z- and t-axis. The z-axis is thus divided into intervals, or layers, that correspond to 1D finite volumes. Without going into details (we refer to text books in numerical analysis, e.g. LeVeque (2002)), the fundamental principles for PDE solvers of (6) include the following:

- there is an upper limit of the time steps in relation to the size of the layer, the so-called CFL condition (Courant-Friedrichs-Lewy);
- the numerical update of the convective flux term F, called the *numerical flux*, is critical and should have a certain form, which in mathematical terminology is called consistent;
- the numerical flux should automatically take the entropy condition (see Step 2) into account.

One such numerical flux is the Godunov numerical flux. Its formula is derived from the unique exact solution, see Diehl (1996) and Jeppsson and Diehl (1996a). An explicit and a semi-implicit reliable numerical

method for (6) were presented by Bürger et al. (2005), see the simulations in the last section. Both methods utilize the Engquist-Osher numerical flux. This model has also been used for the calibration and simulation of batch and continuous sedimentation of activated sludge by De Clercq et al. (2006, 2008).

Step 4: Calibration. The model parameters for calibration are the critical concentration C_c, those contained in the expressions for $v_{hs}(C), \sigma_e(C)$ and $d_{mix}(z, \dots)$. There are numerous reports on the calibration of different hindered settling formulae. This is sufficient for determining the convective flux F. In the compression function d_{comp}, all model parameters are present. Only a few experiments have been reported on the compressibility properties for activated sludge, see De Clercq et al. (2006, 2008).

Step 5: Validation. The mathematical model consisting of (3) and (4), modeling batch sedimentation of minerals, has been validated, e.g. Bürger et al. (2000a, 2004a), Garrido et al. (2000). For the SST operation, some partial results were presented by De Clercq (2006).

Step 6 and 1: Rebuilding or extension of the model. An inherent problem with our mathematical model is that there are several influential features of the real process that the idealizing assumptions made do not take into account. Some of these are related to the feed and discharge mechanisms. A modification with a distributed feed, still in 1D, has been presented by Nocoń (2006).

Further comments on the CMM

A simple necessary convergence test

It is difficult to prove whether a numerical scheme produces approximate solutions that converge to the exact solution of the model equation as the mesh size tends to zero (the number of layers tend to infinity). However, the scheme should at least pass the following convergence test: For given initial data, feed concentration etc., run the scheme with an increasing number of layers, e.g. 10, 50, 100, 200, ... The numerical solutions obtained should be qualitatively the same, with quantitatively smaller and smaller differences. If a scheme does not pass this test, it should not be used under any circumstances. We emphasize that passing this test is a necessary, however not sufficient, condition for being a reliable simulation model.

The traditional 10-layer-model approach

The traditional layer model could be seen as a simulation model outcome in two ways.

First, it can be fitted into the CMM in the following way. One makes the idealizing assumption that the SST consists of a fixed number of well-mixed compartments, usually 10, and that there are flows between these. Then, the conservation of mass yields 10 ODEs, which are coupled due to the fluxes between the compartments. The problem is how to model these fluxes in a physically correct way. If this were done in a satisfactory way, standard ODE solvers could be used as the simulation model. The first approach that also included the clarification zone was presented by Vitasovic (1989), who suggested a minimum-flux condition for the numerical flux updates with some additional heuristic conditions. The same approach was also used by Takács et al. (1991) in their simulation model, which still today is the most common one in the WWT field, but not in others. However, an inherent problem is that the mass balance is not sufficient to determine the fluxes uniquely between the compartments (this is the reason for the additional entropy condition). Several shortcomings of the traditional layer models have been reported (Jeppsson and Diehl, 1996a, 1996b; David et al., 2009a). From a

modelling point of view, one may question that the SST is subjectively discretized first (idealizing assumption) and then the mass balance is used. Indeed, there are no compartments in the SST.

The second way is the following. In many of the publications where layer models are used or created, one can indeed find a PDE as the mathematical model. This means that the layer model is used as a numerical method (PDE solver), which has been created without a proper connection to the PDE. Such a procedure severe violates the CMM. For example, the Takács model does not pass the necessary convergence test described above. This has been illustrated by Jeppsson and Diehl (1996a), who also showed how the minimum-flux update by Vitasovic should be adjusted to become a consistent numerical flux update, namely the Godunov method. Looking at these two flux updates without having the PDE background, it is not easy to judge which one is correct. The findings by Vitasovic and Takács et al. put forward around 1990 were in the right direction, however, we now strongly recommend that correct numerical fluxes are used instead.

The solids-flux theory and extensions

For more than half a century, the paper by Kynch (1952) has been the origin of a platform often referred to as the solids-flux theory from which many conclusions on the operation and design of SSTs have been drawn, see Ozinsky et al. (1994), Ekama et al. (1997), Diehl (2001) and references therein. With the assumptions by Kynch, the solids-flux theory is in fact based on a PDE which is a special case of the mathematical model (6), namely by setting $d_{\mathrm{comp}} = d_{\mathrm{mix}} = 0$, i.e. only hindered settling is considered. We refer to Diehl (2008) for the classical and extended results interpreted by means of operating charts for both stationary and dynamic situations. Hence, the CMM allows deriving submodels. Another such is provided by the steady-state calculus by Bürger and Narváez (2007), who consider (6) with $d_{\mathrm{mix}} = 0$ but $d_{\mathrm{comp}} > 0$ for concentrations above C_{C}.

Non-flocculated particles

The constitutive relation for the hindered settling velocity can be expressed as any function of the concentration within the CMM. Equation (6) models the concentration of particles that have the same properties (density, size, shape). However, to take into account the non-flocculated particles that do not settle at all and follow the water streams, an appealing approach was put forward by Takács et al. (1991), who suggested that the settling velocity function should be zero for small concentrations.

Varying sludge properties

Some of the properties of the sludge are known to depend slowly on time, such as the sludge density and particle size distribution. Then the settling and compression behaviours are influenced. Such phenomena can be captured by letting the model parameters in the constitutive relations depend slowly on time. The main problem here for the future is to develop on-line calibration methods.

Illustration by simulation

To demonstrate the behavior of the mathematical model (6) for the SST we use the PDE solver by Bürger et al. (2005). We have used the following data: $H = B = 2$ m, $A = 400\ \mathrm{m}^2$, and the hindered settling velocity is described by the Vesilind formula:

$$v_{\mathrm{hs}}(C) = v_0 \mathrm{e}^{-nC}\,, \tag{7}$$

where $v_0 = 9.6 \cdot 10^{-4}$ m/s and $n = 0.37$ l/g, see Figure 3. At time $t = 0$, we assume that the tank is full of sludge at the concentration $C = 2$ g/l. The feed concentration is constant in time $C_{\mathrm{f}} = 4.4$ g/l and so are the volumetric

flow rates $Q_e = 3.9 \cdot 10^{-2}$ m^3/s and $Q_u = 1.7 \cdot 10^{-2}$ m^3/s.

FIGURE 3

In Figure 4a, the case when $d_{comp} = d_{mix} = 0$ m^2/s is shown. Then Equation (6) models hindered settling and bulk flow transport only. It is clearly seen that the solution has several discontinuities among which the sludge blanket is the most distinct one propagating from the bottom. The high concentration in the underflow pipe is shown in the small interval below $z = B = 2$ m. The concentration increases discontinuously across the bottom of the tank. This is a result of the mass conservation when there is no diffusion term in the PDE. The initial amount of sludge in the clarification zone, together with the feed load, implies that some amount of sludge is built up in the clarification zone during approximately the first hour. Then all sludge in the clarification zone settles.

To illustrate the effect of compression, we let $d_{mix} = 0$ while d_{comp} is determined by the constant $\rho_s/(g\Delta\rho) = 2.1$ s^2/m and the effective solids stress function by De Clercq et al. (2008):

$$\sigma_e(C) = \alpha \ln\left(\frac{C - C_c + \beta}{\beta}\right), \qquad (8)$$

where we have chosen $\alpha = 4$ Pa, $\beta = 4$ g/l and $C_c = 6$ g/l, see Figure 3. Thus, $d_{comp} > 0$ for concentrations higher than $C_c = 6$ g/l. In the solution shown in Figure 4b, it is seen that C_c is reached below the sludge blanket. For higher concentrations, which occur below the sludge blanket, the concentration increases continuously all the way into the underflow pipe. For concentration below $C_c = 6$ g/l, there are discontinuities as in Figure 4a. In particular, the temporary build-up of sludge in the clarification zone is the same as in Figure 4a (note the scales on the z-axes).

Finally, in addition to the values above, we now introduce a mixing effect limited to a region around the inlet by using

$$d_{mix}(z) = \begin{cases} 0 \text{ for } |z| \geq b, \\ a\cos\left(\frac{\pi z}{2b}\right) \text{ for } |z| < b, \end{cases} \qquad (9)$$

with $a = 1.4 \cdot 10^{-4}$ m^2/s and in two cases with $b = 0.5$ m and $b = 1$ m, respectively, see Figure 3. The smoothening in a neighborhood of the inlet is clearly shown in Figures 4c and 4d.

FIGURE 4

Conclusions

We describe a consistent modeling methodology (CMM), which can be used to construct models for all processes in wastewater treatment systems. We demonstrate how it can be used to obtain a 1D platform model for the SST.

- A key principle of the CMM is that for a real process that occurs in continuous time and space, the modeling should be done in continuous time and space. The resulting mathematical model is then a PDE. It is then the outcome of mathematics to derive a simulation model (numerical scheme) defined at discrete time and space points (or layers).
- The model parameters are introduced only in the first step of the CMM and turns up in the simulation model automatically. Usually, they are contained in the constitutive relations. Parameters should never be introduced directly in the simulation model. If calibration of the model parameters is not satisfactory, then the mathematical model should be rebuilt. A simulation model (ODE or PDE solver) should never be changed as a result of a poor fitting of simulated data to real.

- Modeling the SST with: (i) the idealized assumption of 1D, (ii) three constitutive assumptions; hindered settling, compression at high concentrations and mixing hydrodynamic effects due to e.g. the feed inlet, (iii) the conservation of mass; then the outcome is the mathematical model (6). The output of the CMM is one of the proven consistent and reliable numerical schemes (PDE solvers) presented by Bürger et al. (2005). Different types of implementations of such schemes, e.g. in an ODE environment, will be presented in a subsequent publication.
- Simulations have been shown demonstrating the impact of the three constitutive assumptions.
- As a consequence of the CMM, together with the fact that there are proven reliable PDE solvers available now, the traditional layer models should be replaced by reliable ones.

Appendix: The terminology of the CMM

Real process: The physical/biological/chemical process to be modeled.

Idealizing assumptions: Simplifying assumptions made in order to define a mathematical model that is not too complicated but still captures the main features of the real process. Examples: 1D, neglecting wall effects, particles are spherical, instantaneously well-mixed compartment.

Constitutive assumption = constitutive relation: an assumed relation between physical (biological/chemical) variables needed to obtain a mathematical model that is not underdetermined. Examples: the Monod relation, the Vesilind expression for the settling velocity as a function of the concentration, Fick's law of diffusion. The constitutive relations contain the model parameters, both kinetic and stoichometric.

Mathematical model = model = model equation = process model: The system of equations that describes the physical law(s). It is a simplification of the real process, taking into account only some of the features in reality, but it models these exactly (and at every time point).

Model parameters: Parameters introduced in the first step of the CMM, usually contained in the constitutive relations. Exactly the same set of parameters is present in the mathematical model and the simulation model.

Numerical scheme = numerical algorithm = numerical method = simulation method = simulation program = simulation model = computer model (the prefixes 'numerical' and 'simulation' can often be used as synonyms): A sequence of instructions for computing real numbers. It can be defined explicitly or implicitly. Examples are Runge-Kutta methods for ODEs, finite-element methods for PDEs. It is often seen as a discretized version of the (continuous-in-time) mathematical model. Therefore, the terminology 'simulation model' is common although it is really not a model (unless the real process is discrete in time).

Entropy condition: An admissibility criterion related to physical principles. It is needed for nonlinear PDEs in conservation law form to obtain the physically relevant unique solution.

Well-posedness: A mathematical model, defined by an ODE or PDE (or system of such) together with initial data at time zero, is well-posed if there exists precisely one solution (existence and uniqueness), and this solution depends continuously on the initial data, i.e. a small change in the initial data will only cause a small change in the solution.

Solution = exact solution: This refers to the solution of the mathematical model subject to the condition that the model is well-posed, defined for all time points. In the case of (6), the solution is $C(z,t)$.

Numerical solution = simulation output = approximate solution: The output data from a simulation program constitute an approximate discrete-in-time solution of the exact one.

Reliable numerical scheme: The word reliable means that the simulated data are consistent with the idealizing assumptions made at the beginning of the CMM (whether simulated data agree with experimental observations is a completely different issue; see Steps 4 and 5 in the CMM). A reliable numerical scheme is robust (consistently handles any physically reasonable input data), conservative (no loss of mass), has no overshoots (the concentration is never negative or above a prescribed maximum value), convergent (approximate solutions converge to the exact solution as the time step (and layer thickness) tends to zero). For a PDE that models continuous sedimentation, an additional requirement is that the approximate solutions should converge to the unique physically admissible solution (which satisfies an entropy condition).

Nomenclature

A	cross-sectional area of SST [m^2]
B	depth of thickening zone [m]
C	concentration in SST [kg/m^3]
C_C	critical concentration [kg/m^3]
F	flux function in (6) [$kg/(m^2h)$]
H	height of clarification zone [m]
K_S	model parameter in (2) [kg/m^3]
Q	volumetric flow rate [m^3/h]
S_S	readily biodegradable soluble concentration [kg/m^3]
V	volume of bioreactor [m^3]
Y_H	model parameter in (2) [–]
Z	substance concentration (substrate or biomass) [kg/m^3]
a	model parameter in (9) [m^2/h]
b	model parameter in (9) [m]
d	diffusion coefficient in (6) [m^2/h]
g	gravity of acceleration [m/h^2]
m	number of substances in bioreactor
n	model parameter in (7) [m^3/kg]
r	reaction rate [$kg/(m^3h)$]
t	time [h]
v_0	model parameter in (7) [m/h]
v_{hs}	hindered settling velocity [m/h]
v_s	settling velocity [m/h]
z	depth from feed level in SST [m]
Greek letters	
α	model parameter in (8) [Pa]
β	model parameter in (8) [kg/m^3]
$\delta(z)$	Dirac delta distribution [1/m]
$\gamma(z)$	characteristic function in (6), equals 1 inside and 0 outside SST
μ_{max}	model parameter in (2) [$kg/(m^3h)$]
ρ_s	density of solids
σ_e	effective solids stress [Pa]
Subscripts	
comp	compression
e	effluent
f	feed
mix	mixing
u	underflow
Superscript	
in	incoming

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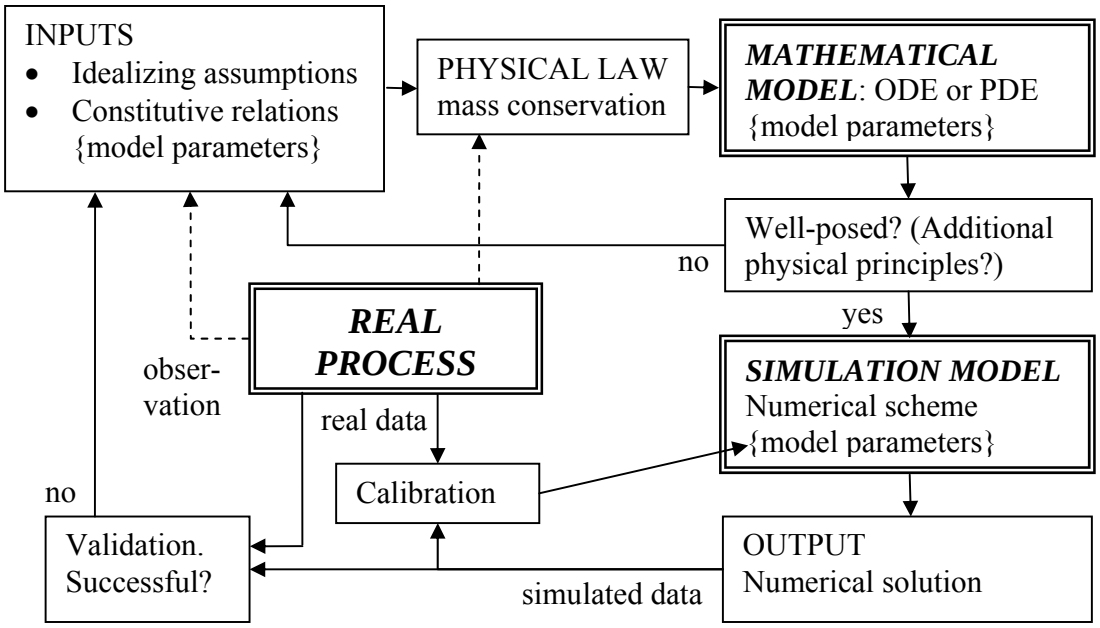

Figure 1: Schematic overview of the consistent modeling methodology (CMM). The dashed arrows indicate the initial observations of the real process. Note that {model parameters} refers to the same set of parameters defined in the constitutive relations.

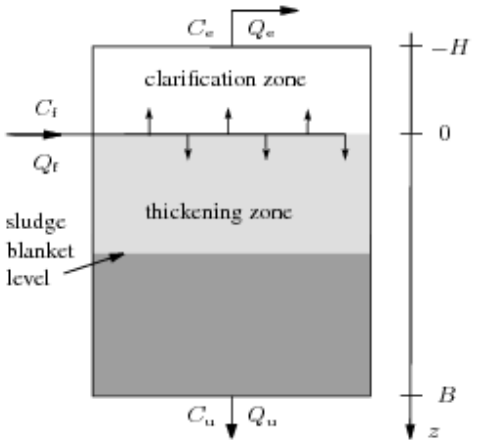

Figure 2: Schematic overview of an ideal 1D SST.

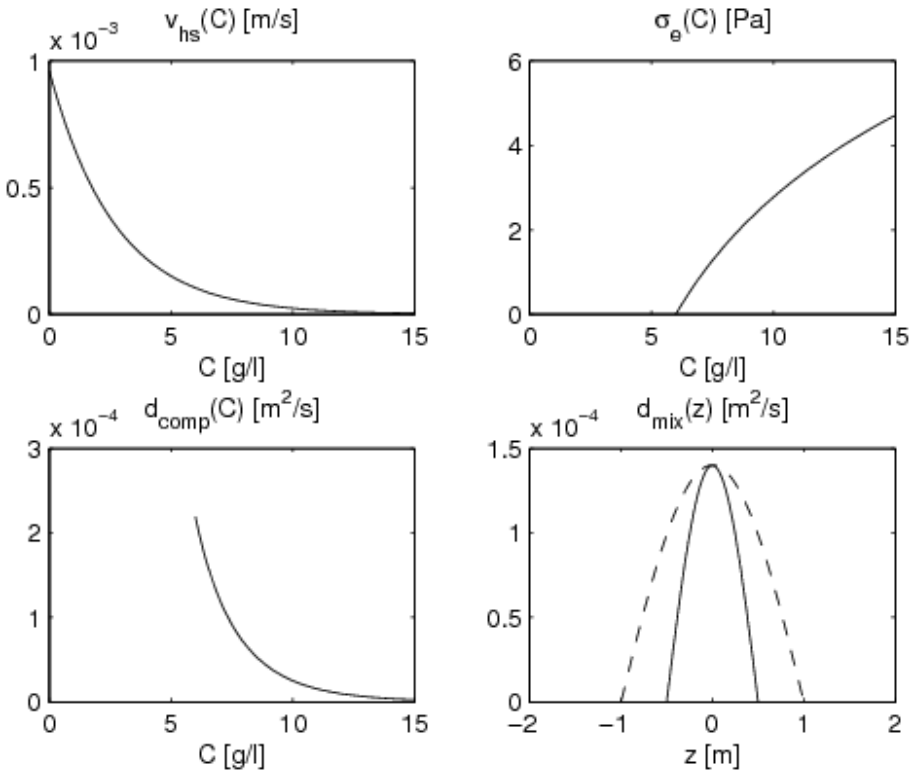

Figure 3: Graphs of the constitutive relations. Note that the critical concentration is $C_c = 6$ g/l.

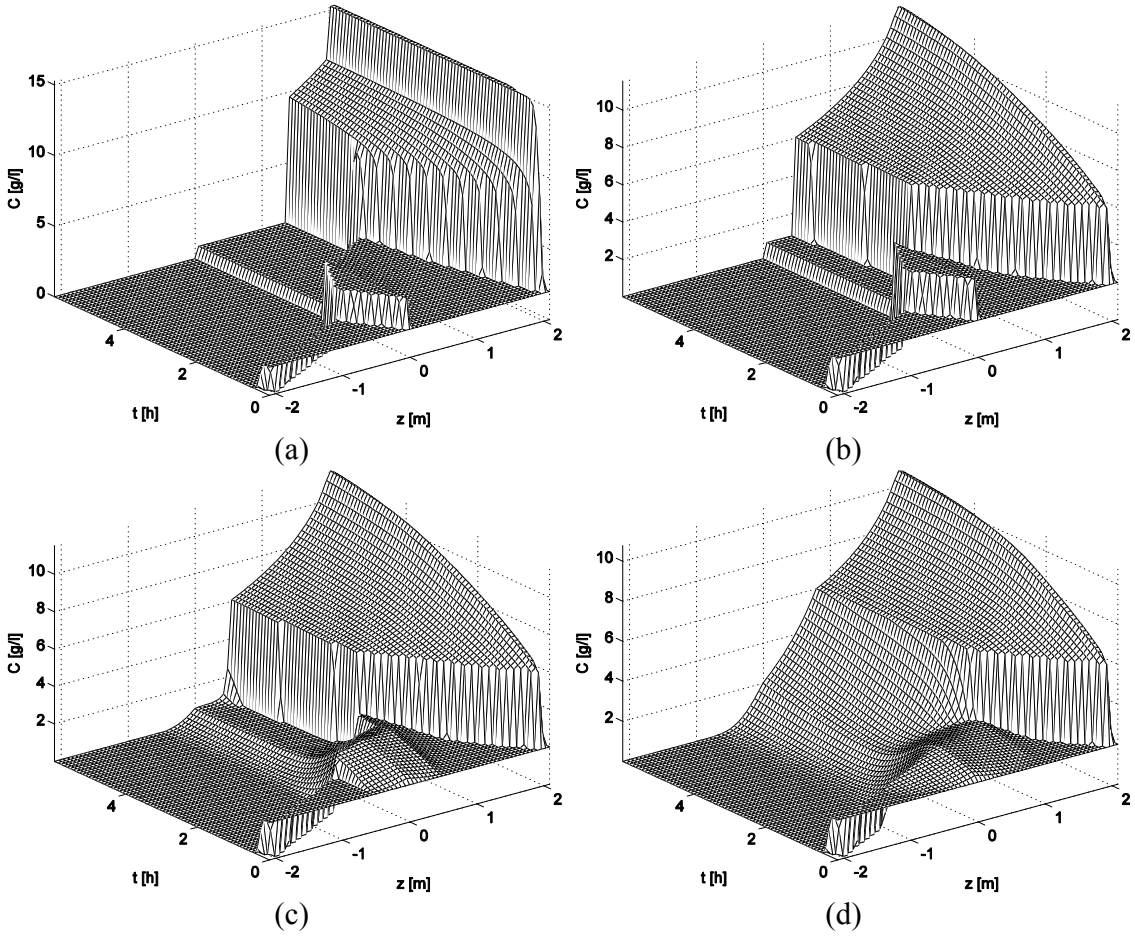

Figure 4: Numerical solutions of Equation (6). (a) The hindered settling and bulk flow transport is considered only ($d_{\text{mix}} = d_{\text{comp}} = 0$). (b) Compression is turned on at high concentrations ($d_{\text{mix}} = 0, d_{\text{comp}} > 0$ for $C > 6$ g/l). (c) Mixing around the inlet and ($d_{\text{mix}} > 0$ for $|z| < 0.5$ m) and with compression as in b. (d) As in c but with the mixing in the larger region $|z| < 1$ m.

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