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Settler dynamic modeling and MATLAB simulation of the activated sludge process

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ABSTRACT

Mathematical modeling of sedimentation has attracted considerable attention in the past decades, and nowadays, one of the most popular models of secondary settler in activated sludge processes is the one proposed by Takács et al. [I. Takács, G.G. Patry, D. Nolasco, A dynamic model of the clarification-thickening process, Water Res. 25 (10) (1991) 1263–1271]. This model is based on a discretization in finite volumes (or layers) of the spatial domain, and in a rather inconsistent way, the number of layers is usually considered as a model parameter chosen so as to fit experimental data. In this study, a simple convection–diffusion partial differential equation (PDE) model is first formulated and solved using a Method of Lines strategy allowing the use of various spatial discretization methods with largely improved accuracy and efficiency. Model parameters are estimated using experimental data collected in batch settling experiments by De Clercq [J. De Clercq, Batch and continuous settling of activated sludge: in-depth monitoring and 1D compression modeling, Ph.D. Thesis, Universiteit Gent, Faculteit Ingenieurswetenschappen, Belgium, 2006], showing the good model predictive capability. Finally, the PDE settler model is coupled with a standard ASM1 representation of the activated sludge process, and implemented in a MATLAB dynamic simulator.

1. Introduction

The secondary settler is an important process unit in a wastewater treatment plant as it allows the separation of the solid and liquid phases. The solid particles accumulate in the lower part of the settler and are partly recirculated to anoxic and aerobic tanks, where they participate in the purification process following the principle of the activated sludge process. On the other hand, clear water flows out of the tank. See Fig. 1.

The design of secondary settlers has long been based on empirical considerations[3]. A first physical model of batch sedimentation was developed by [16], in which the sludge transport is described by a mass balance partial differential equation. Further studies introduced several model extensions in order to reproduce experimental observations: continuous settling [18], limitation of the sedimentation flux from layer to layer [22,26], dispersion [11], and compression [12,17].

In today's practice, Takács' model [22] is by far the most widely used mathematical representation of the secondary settler in published studies and commercial software environments. However, recent studies (e.g. [15,19,25]) highlight several drawbacks of this model, and in particular the fact that the number of discretization layers is used as a model parameter in order to match the experimental observations. Indeed, a typical number of 10 layers is used to introduce (artificial) numerical diffusion and smooth off the concentration profiles. This model is therefore used without selecting a number of layers in agreement with numerical convergence (the number of layers should be selected large enough so that the numerical solution to the mass balance equations is computed with an acceptable accuracy) and without distinguishing model formulation (i.e. the physical model parameters) and numerical solution (i.e. the number of layers or grid points in a numerical algorithm).

With the rapid advances in numerical methods and computational techniques, partial differential equations (PDEs) can nowadays be solved routinely on modest computers. In particular, the Method of Lines [20], which is a straightforward two-step procedure, where the PDEs are first discretized in space, then integrated in time, can be used to solve the convection–diffusion PDE describing material transport in the secondary settler. Based on such a simulation tool, the present study aims at estimating the unknown model parameters, i.e. the parameters related to the settling velocity and dispersion effects, from batch experimental data available from [5,6]. The resulting settler model is then coupled to the Activated Sludge Model 1 (ASM1) [13] to build a

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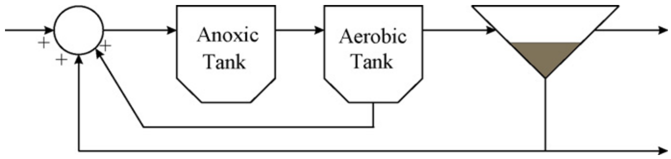

Fig. 1. Activated sludge process.

complete simulator of the wastewater treatment plant. The code is implemented in MATLAB based on a MOL library [23].

This paper is organized as follows. The next section presents a simple convection–diffusion (i.e. parabolic) PDE of batch settling, highlighting the importance of the boundary conditions (i.e. the conditions imposed at the secondary settler inlet and outlets). On this basis, a numerical solution procedure based on the MOL is developed in Section 3. In Section 4, model parameters are inferred from experimental data collected on a pilot plant [5–7]. A continuous settling model is then coupled to an activated sludge model, including anoxic and aerobic tanks, and simulation results are discussed in Section 5. Finally, Section 6 draws some conclusions and perspectives.

2. Modeling of batch sedimentation

Mass balances allow the following partial differential equation and boundary conditions to be derived (more details on the derivation of the model PDE and boundary conditions can be found in several studies, including [5,7,8,16,18]:

$$\frac{\partial C}{\partial t} = -\frac{\partial(\nu_s C)}{\partial z} + D\frac{\partial^2 C}{\partial z^2} \tag{1}$$

$$\begin{cases} \text{At } z = z_0: & \nu_s C - D\dfrac{\partial C}{\partial z} = 0; \\ \text{At } z = z_\mathrm{L}: & \nu_s C - D\dfrac{\partial C}{\partial z} = 0, \end{cases} \tag{2}$$

where C is the concentration in solid particles, ν_s is the settling velocity, and D is the dispersion coefficient. The boundary conditions simply express the fact that the material flux at the system boundaries are equal to zero in batch mode.

Table 1
Parameter estimation based on the three available experiments

Residual cost function	"3670–6120–7290"
J^*	6.184×10^9
Variance and standard deviation	"3670–6120–7290"
σ^2	440520
σ	663
99% confidence interval	"3670–6120–7290"
$y \pm 2.58 \times \sigma$	$y \pm 1712$
Parameters and 99% confidence intervals	"3670–6120–7290"
$\nu_0 \pm 2.58\sigma_{\nu_0}$	16.982 ± 0.0074
$\nu_0' \pm 2.58\sigma_{\nu_0'}$	$195.031 \pm \infty$
$r_\mathrm{p} \pm 2.58\sigma_{r_\mathrm{p}}$	$(16.018 \pm 189.828) \times 10^{-3}$
$r_\mathrm{h} \pm 2.58\sigma_{r_\mathrm{h}}$	$(4.942 \pm 3.992) \times 10^{-4}$
$D \pm 2.58\sigma_\mathrm{D}$	$(10.724 \pm 4.100) \times 10^{-2}$
Correlation coefficients	"3670–6120–7290"
$\rho_{\nu_0, r_\mathrm{p}}$	−0.542
$\rho_{\nu_0, r_\mathrm{h}}$	0.125
$\rho_{\nu_0, D}$	0.519
$\rho_{r_\mathrm{p}, r_\mathrm{h}}$	−0.002
$\rho_{r_\mathrm{p}, D}$	−0.015
$\rho_{r_\mathrm{h}, D}$	−0.033

Different initial conditions can arise, but in laboratory experiments, a (at least approximately) constant initial distribution is usually achieved by mixing, i.e. $C(t = 0) = C_0$.

The settling velocity law ν_s can be formulated in several ways (see [10]). In this work, Takács formulation [22] is chosen:

$$\nu_s(C) = \max(0, \min(\nu_0', \nu_0\ (\mathrm{e}^{-r_\mathrm{h}(C - C_\mathrm{min})} - \mathrm{e}^{-r_\mathrm{p}(C - C_\mathrm{min})}))) \tag{3}$$

This double exponential (see Fig. 2) contains five parameters:

- ν_0 is the theoretical maximum velocity $[m/h]$, obtained at the intersection of the ν_s vertical axis and the extension of the right exponential curve;
- ν_0' is the practical maximum velocity $[m/h]$;
- C_min is the minimum concentration below which the settling velocity vanishes $[\mathrm{g/m^3}]$;
- r_h determines the particle behavior for increasing particle density;
- r_p determines the particle behavior at weak concentration values.

These parameters are a priori unknown and have to be estimated from experimental data. In this study, initial parameters values are taken from [4]; see Table 3 and Fig. 2.

3. Method of Lines (MOL) strategy

Consider the PDE problem

$$x_t = f(z, t, x, x_z, x_{zz}), \quad z \in \Omega, t \geq 0 \tag{4}$$

$$0 = b(z, t, x, x_z), \quad z \in \Gamma, t > 0 \tag{5}$$

$$x(t = 0, z) = x_0(z), \quad z \in \Omega \cup \Gamma \tag{6}$$

where $x \in \Re^{n_\mathrm{pde}}$ is the vector of dependent variables (e.g. concentration), z is the spatial coordinate, and t is the time. A subscript notation is used for the several partial derivatives, i.e. $x_t = \partial x/\partial t$, $x_z = \partial x/\partial z$. Eqs. (4)–(6) represent a system of PDEs defined in a spatial domain Ω, their associated boundary conditions (BCs) defined on the boundary surface Γ of Ω, and initial conditions (ICs) defined on the complete spatial domain.

One of the most popular approaches to the numerical solution of PDE models is the Method of Lines [20], which proceeds in two separate steps:

- approximation of the spatial derivatives using finite difference, finite element or finite volume techniques;
- time integration of the resulting semi-discrete (discrete in space, but continuous in time) equations using an appropriate solver.

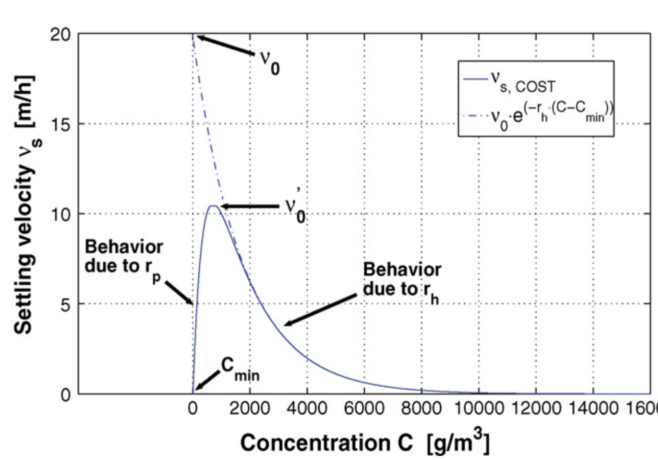

Fig. 2. Settling velocity law.

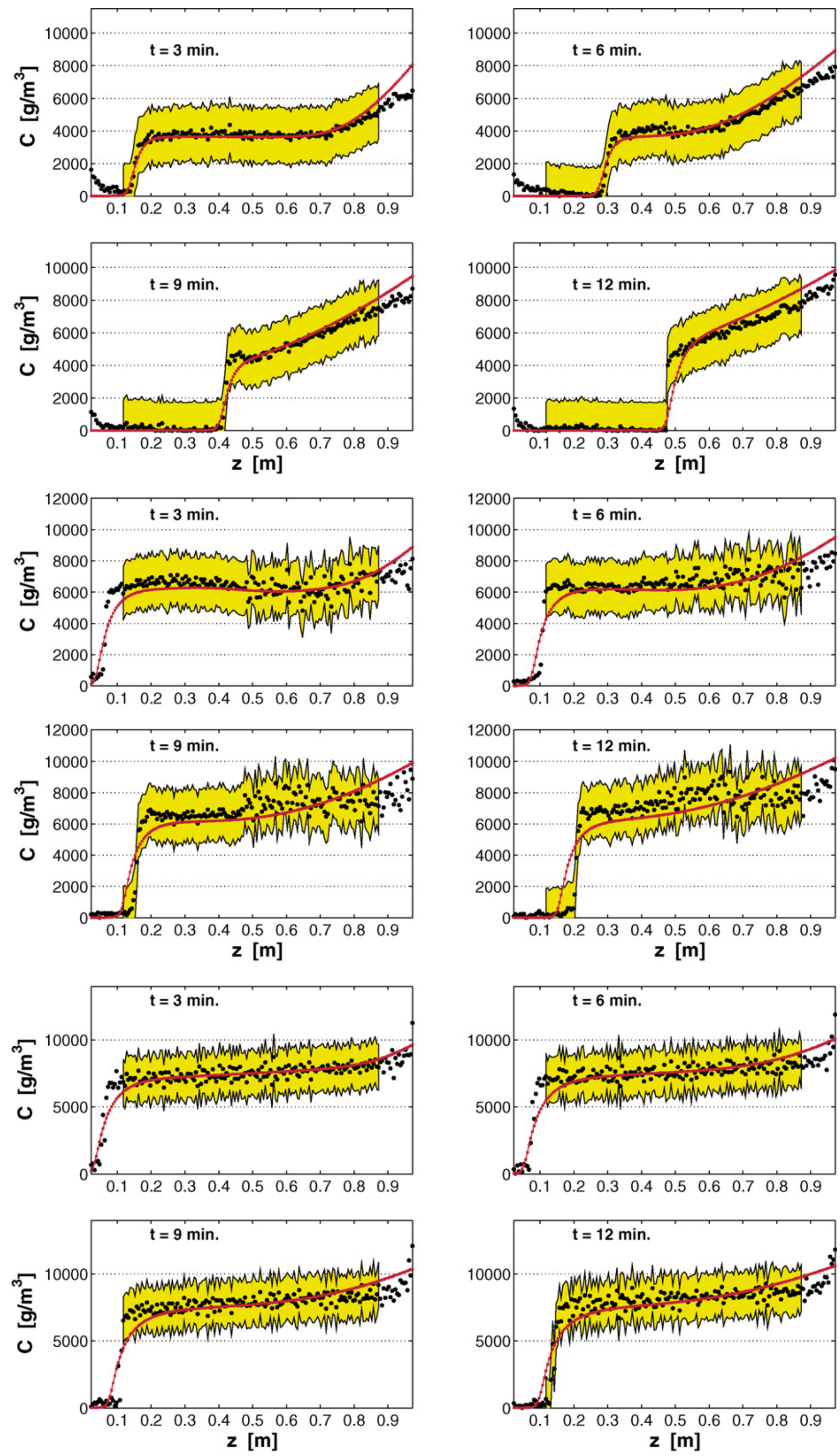

Fig. 3. Direct validation: temporal evolution of the concentration profiles for experiments with $C_0 = 3670$ (top), $C_0 = 6120$ (center) and $C_0 = 7290$ (bottom) g/m^3. Measurement data (black dots), measurement confidence interval (yellow), model prediction (red line). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of the article.)

The success of the MOL stems from its simplicity of implementation and the availability of high-quality time integrators for solving a wide range of problems, including ordinary differential equations (ODEs), and mixed systems of algebraic and ordinary differential equations (AEs and ODEs forming a system of differential-algebraic equations—DAEs).

In particular, the authors Vande Wouwer et al. [23] have recently developed a MATLAB library for the MOL, called MATMOL, in which

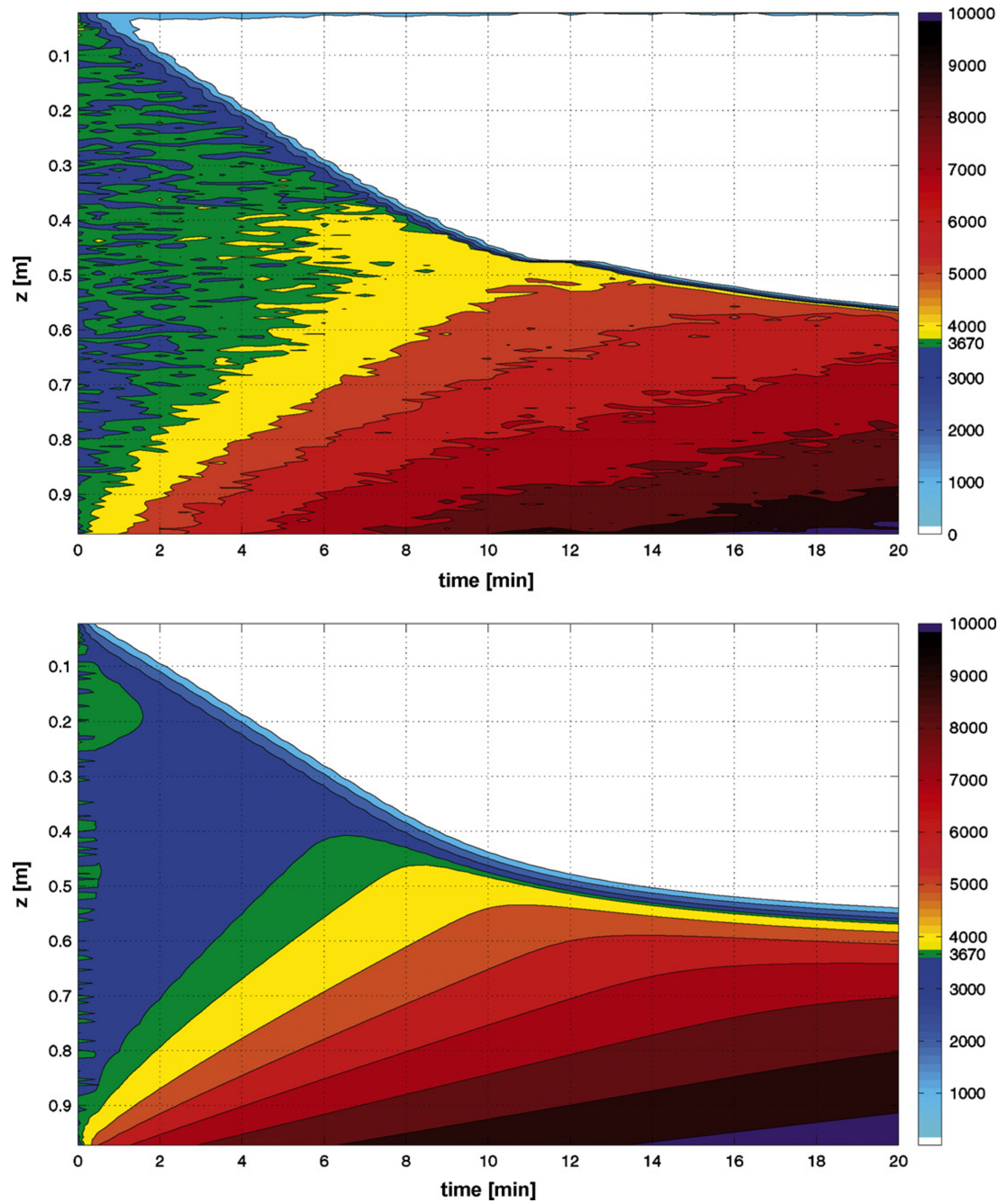

Fig. 4. Iso-concentration curves from the experiment corresponding to $C_0 = 3670\,\mathrm{g/m^3}$, and predicted iso-concentration curves (direct validation).

finite differences (or other techniques such as spectral methods, but in the continuation of this article attention is focused on FDs) are implemented using the concept of a differentiation matrix D, i.e.

$$\tilde{x}_z = D_1\tilde{x} \tag{7}$$

$$\tilde{x}_{zz} = D_2\tilde{x} \tag{8}$$

$$\ldots \tag{9}$$

Substitution of (7)–(9) into (4) and (5) yields a semi-discrete ODE or DAE system

$$\tilde{x}_t = f(z, t, \tilde{x}, \tilde{x}_z, \tilde{x}_{zz}), \quad z \in \Omega, t \geq 0 \tag{10}$$

$$0 = b(z, t, \tilde{x}, \tilde{x}_z), \quad z \in \Gamma, t > 0 \tag{11}$$

$$\tilde{x}(t = 0, z) = x_0(z), \quad z \in \Omega \cup \Gamma \tag{12}$$

where $\tilde{x}$ is the approximate solution. This ODE/DAE system can be integrated in time using one of the solvers available in the MATLAB ODE Suite [21], e.g. ODE15s (which is suitable for stiff ODEs and index 1 DAEs).

For convective PDE problems, as it is the case in sedimentation modeling, upwind finite difference schemes such as

$$\tilde{x}_z(z_i) = \frac{(-x(z_{i-3}) + 6x(z_{i-2}) - 18x(z_{i-1}) + 10x(z_i) + 3x(z_{i+1}))}{12\,\Delta z} \tag{13}$$

for a flow from left to right, work very effectively and avoid spurious oscillations as generated by centered FDs (which are a standard choice for dispersion terms which have no preferential direction). Upwind schemes with various orders of accuracy have been implemented in MATLAB, either on uniform grids or on nonuniform grids [24]. More details on the use of finite difference schemes for settler simulation can also be found in [2].

Table 2
Parameter estimation based on two experiments

Residual cost function	"3670–6120"	"3670–7290"	"6120–7290"
J^*	4.141×10^9	2.472×10^9	4.051×10^9
Variances and standard deviations	"3670–6120"	"3670–7290"	"6120–7290"
σ^2	442558	264186	434668
σ	665	514	659
99% confidence interval	"3670–6120"	"3670–7290"	"6120–7290"
$y \pm 2.58 \times \sigma$	$y \pm 1716$	$y \pm 1326$	$y \pm 1701$
Parameters and 99% confidence intervals	"3670–6120"	"3670–7290"	"6120–7290"
$\nu_0 \pm 2.58\sigma_{\nu_0}$	16.617 ± 0.00004	19.815 ± 0.023	24.889 ± 0.000009
$\nu'_0 \pm 2.58\sigma_{\nu'_0}$	12.250 ± 0.00004	$16.817 \pm \infty$	11.875 ± 0.000009
$r_p \pm 2.58\sigma_{r_p}$	$(6.149 \pm 0.075) \times 10^{-3}$	$(2.063 \pm 108.873) \times 10^{-3}$	$(5.339 \pm 0.008) \times 10^{-3}$
$r_h \pm 2.58\sigma_{r_h}$	$(4.861 \pm 0.596) \times 10^{-4}$	$(5.459 \pm 99.434) \times 10^{-4}$	$(5.344 \pm 0.048) \times 10^{-4}$
$D \pm 2.58\sigma_D$	$(13.146 \pm 0.010) \times 10^{-2}$	$(8.243 \pm 3.618) \times 10^{-2}$	$(8.058 \pm 0.0008) \times 10^{-2}$
Correlation coefficients	"3670–6120"	"3670–7290"	"6120–7290"
ρ_{ν_0,ν'_0}	−0.497	–	−0.022
ρ_{ν_0,r_p}	−0.287	−0.392	−0.673
ρ_{ν_0,r_h}	−0.373	0.971	0.021
$\rho_{\nu_0,D}$	0.145	−0.231	−0.751
$\rho_{\nu'_0,r_p}$	−0.020	–	−0.117
$\rho_{\nu'_0,r_h}$	−0.306	–	−0.994
$\rho_{\nu'_0,D}$	0.102	–	−0.058
ρ_{r_p,r_h}	0.362	−0.301	0.113
$\rho_{r_p,D}$	−0.197	−0.273	−0.229
$\rho_{r_h,D}$	−0.453	−0.148	−0.063

4. Parameter estimation

Sedimentation can be studied at laboratory scale using a column filled with well mixed suspension. In [5,6], several experiments have been carried out with different sludge types using radioactive tracers and clinical scanner equipment. In the following, three data sets based on sludge coming from a wastewater treatment plant in Deinze, Belgium, are considered. The corresponding initial concentrations are uniform and respectively equal to 3670, 6120 and 7290 g/m^3. The experimental data are used to estimate the numerical values of the main model parameters, i.e, ν_0, ν'_0, r_p, r_h and D (C_{min} is not identifiable as its value is very small compared to the concentration values recorded in the experiments), by minimizing a cost function measuring the deviation between the model prediction and the measured data.

Table 3
Parameters values of Takács settling velocity law [4], settler characteristics from [15] and diffusion coefficient from [11]

ν_s parameters	Values	Units
ν_0	19.75	[m/h]
ν'_0	10.42	[m/h]
r_p	2.86×10^{-3}	[m^3/g]
r_h	5.76×10^{-4}	[m^3/g]
f_{ns} ($C_{min} = f_{ns}\, C_f$)	2.28×10^{-3}	
Settler characteristics	**Values**	**Units**
A	500	[m^2]
Depth z_L	4	[m]
Feed level z_f	1.8	[m]
Q_f	450	[m^3/h]
Q_u	200	[m^3/h]
Q_e	250	[m^3/g]
Diffusion coefficient	**Value**	**Unit**
D	0.542	[m^2/h]

In the construction of this cost function, the data at the column ends are disregarded because of the presence of a stirrer (used to obtain an almost uniform initial concentration) and because of the sludge compression phenomenon at the bottom of the column, which is not described in our simple mass balance model (for more insight in the compression phenomenon, see, e.g. [7]). Despite this precaution, the number of available data remains quite large compared to the number of parameters (the ratio of the number of data points to the number of unknown parameters is about 900 for each experiment). Based on N data points, the parameter estimation problem can be stated as

$$\min_{\theta} J(\theta) = \min_{\theta} \sum_{i=1}^{N} \left(y_i - \hat{y}_i(\theta)\right)^2, \tag{14}$$

under positivity constraints on the n_θ physical parameters θ.

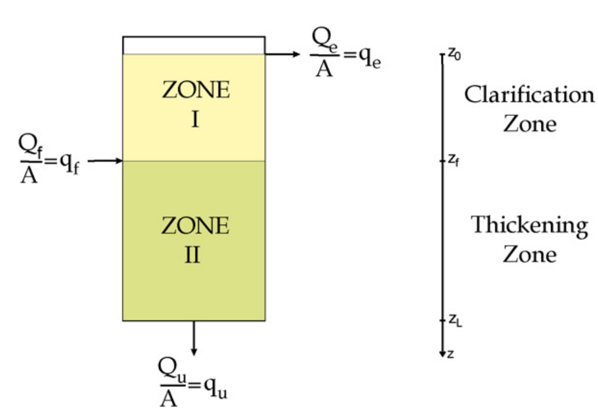

Fig. 5. Secondary settler subdivided in two zones, with the volumetric flow rates corresponding to the feed (Q_f), the clear water outlet (Q_e) and the sludge outlet (Q_u).

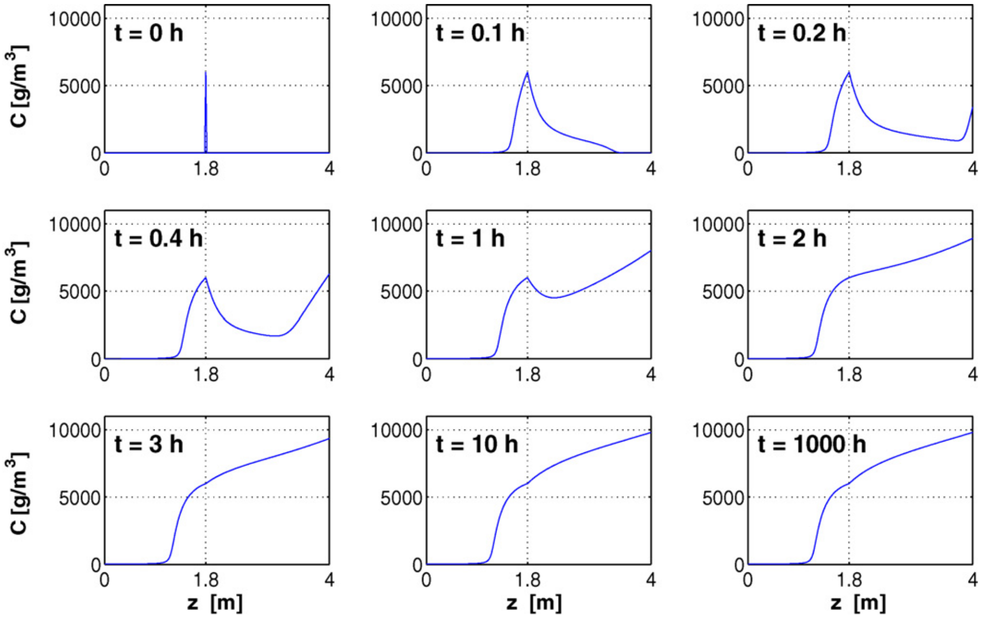

Fig. 6. Dynamic evolution of the concentration profile using a MOL strategy with $n_{\mathrm{I}} = 95$ and $n_{\mathrm{II}} = 116$ (parameters from [4] and $C_f = 6000\,\mathrm{g/m^3}$).

In this expression, y_i denotes the measured data and $\hat{y}_i(\theta)$ the model prediction, which depends on the set of unknown parameters θ (via the solution of the model equations).

As the minimization problem is nonlinear and therefore prone to local minima, two artifices are used:

- a multistart strategy is used in which the parameter estimation procedure is started from randomly chosen initial parameter guesses so as to explore the parameter space and recognize the existence of local minima;
- the minimization of the cost function is initially carried out using a gradient-free optimization method, e.g. Nelder–Mead method as implemented in the MATLAB function FMINSEARCH, followed by a minimization using a gradient-based method such as Levenberg–Marquardt method as implemented in the MATLAB function LSQNONLIN. The gradient-free method is usually less sensitive to the presence of local minima and allows a more "global" approach.

In order to analyse the information content of the data, different data combinations are used: (a) the three available experiments are used for parameter estimation or (b) two experiments out of three are used for parameter estimation, whereas the third one is used for model cross-validation.

In all these cases, the quality of the parameter estimates is evaluated by examining the value of the cost function at the optimum $J(\theta^*)$, by graphical inspection of direct and cross-validation results (when some experiments are left for this purpose as in case (b) above), and by the evaluation of Fisher Information Matrix

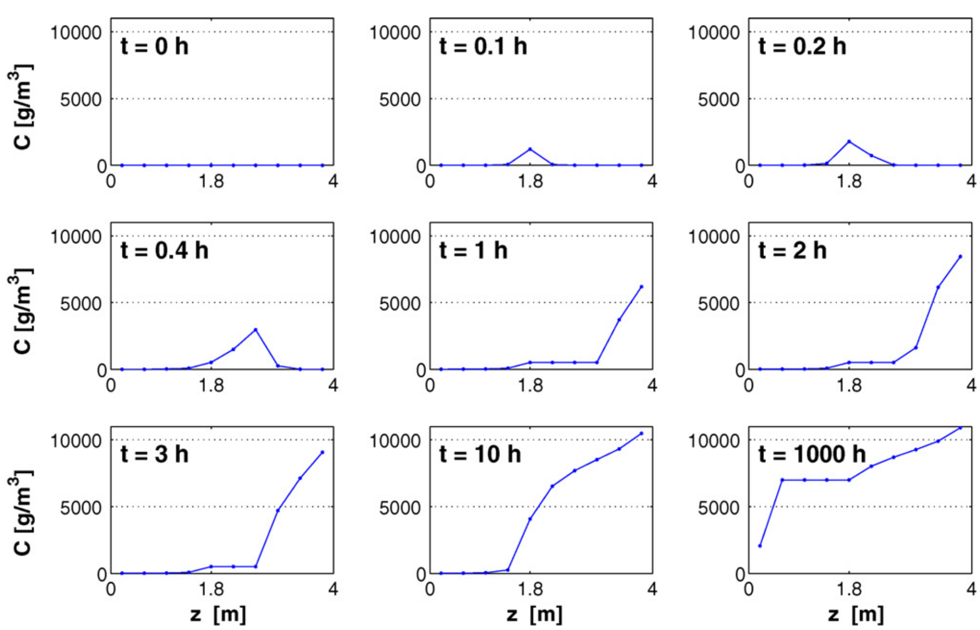

Fig. 7. Dynamic evolution of the concentration profile using the model of Takács with $n = 10$ (parameters from [4] and $C_f = 6000\,\mathrm{g/m^3}$).

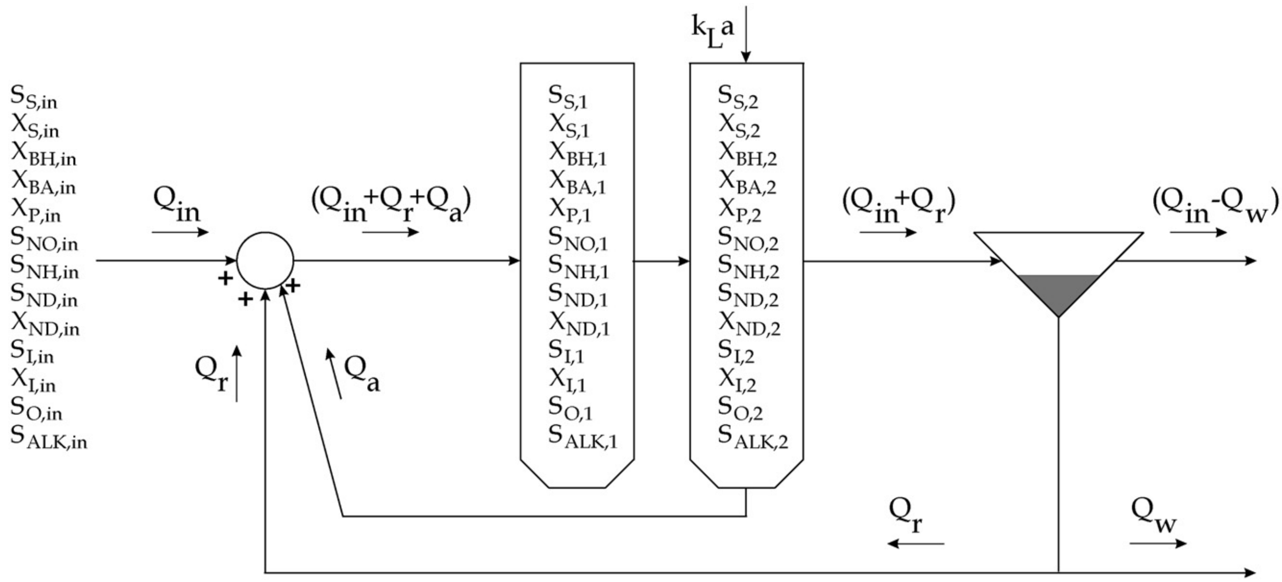

Fig. 8. State and input variables of the activated sludge process.

(FIM) at the optimum:

$$F(\theta^*) = \left(\frac{\partial \hat{y}(\theta)}{\partial \theta}\right)^{\mathrm{T}}_{\theta=\theta^*} \cdot \Sigma^{-1} \cdot \left(\frac{\partial \hat{y}(\theta)}{\partial \theta}\right)_{\theta=\theta^*}, \tag{15}$$

where $(\partial \hat{y}(\theta)/\partial \theta)$ is the sensitivity matrix of the model outputs at each sampling instant with respect to the model parameters θ (this sensitivity matrix is therefore a $N \times n_\theta$ matrix). Often this matrix is a by-product of gradient-based optimization methods, such as the ones implemented in the MATLAB function LSQNONLIN. Σ is the covariance matrix of the measurement errors (which is a $N \times N$ matrix), which is a priori unknown. If it is assumed that the concentration measurements along the column are independent, and have constant absolute errors, then this matrix can be simplified to a diagonal matrix whose diagonal elements are given by [1]:

$$\hat{\sigma}^2 = \frac{J(\theta^*)}{N - n_\theta}, \tag{16}$$

The FIM provides a lower bound of the variance-covariance matrix of the parameter errors

$$Q_\theta(\theta) \geq F^{-1}(\theta) \tag{17}$$

From the FIM, the standard deviations of the parameter errors and correlation coefficients can be deduced as

$$\sigma_{i,\theta} = \sqrt{\sigma^2_{ii,\theta}} \tag{18}$$

$$\rho_{ij,\theta} = \frac{\sigma_{ij,\theta}}{\sigma_{i,\theta} \cdot \sigma_{j,\theta}} \tag{19}$$

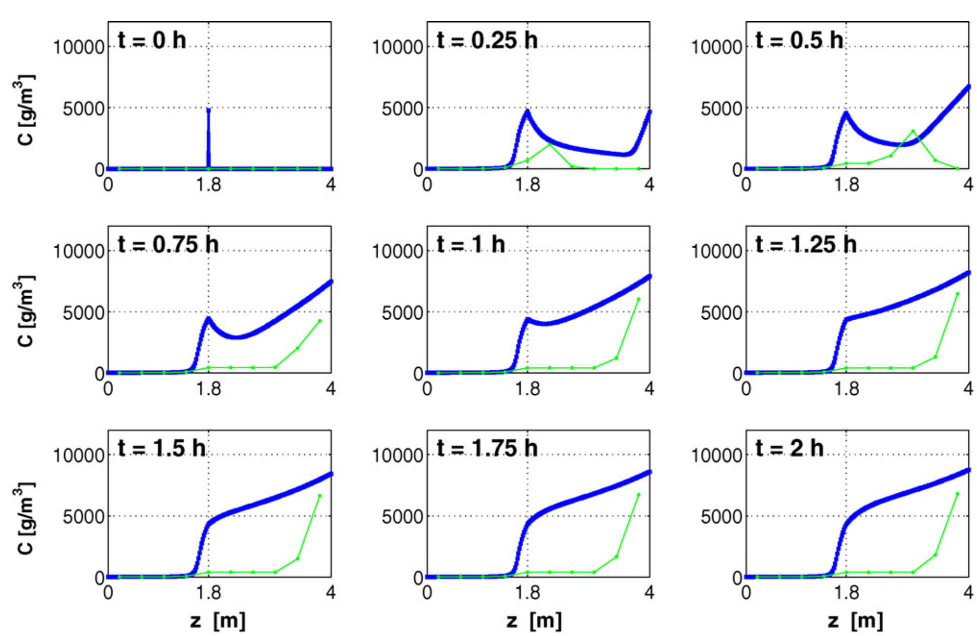

Fig. 9. Concentration profile evolution during the first instants (every 15 min) of simulation with constant inputs. Settler "MOL" with dark line ($n_{\mathrm{I}} = 91$ and $n_{\mathrm{II}} = 111$), settler "Takács" with grey line ($n = 10$).

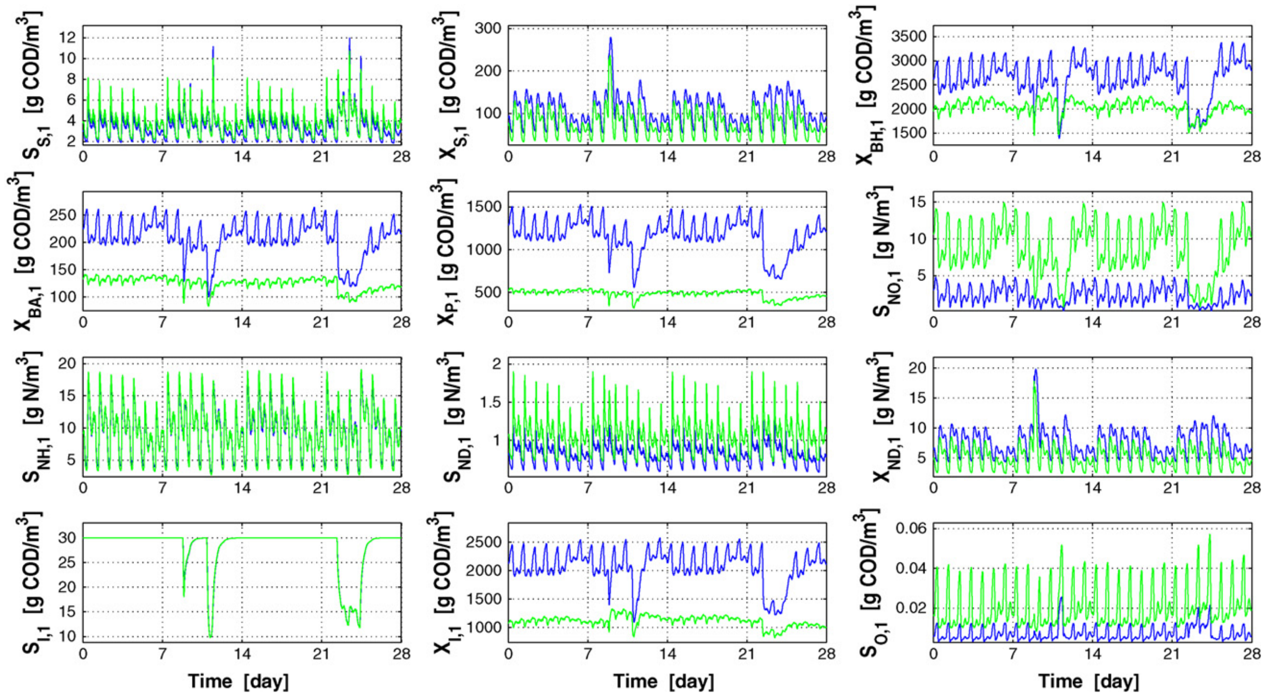

Fig. 10. State variable evolution in the anoxic tank for the weather sequence “Storm–Rain”. Black line: Settler “PDE + MOL”, Grey line: Settler “Takács”.

Table 1 shows the estimation results based on the three available experiments. It is apparent that ν_0' is not identifiable (the parameter sensitivity at the optimum vanishes and therefore the associated uncertainty is high) and that the estimated confidence interval on r_p is quite large. Nevertheless, the direct validation results are acceptable, as shown in Fig. 3 and 4. Fig. 3 shows the temporal evolution of the concentration profiles and compares the experimental data with the model prediction, highlighting the confidence intervals of the data points that have been used for parameter estimation (i.e. excluding the two end regions where unmodelled perturbations occur). Fig. 4 compares the evolution of the isoconcentration curves for the experiments corresponding to $C_0 = 3670\,\mathrm{g/m^3}$.

Table 2 shows the estimation results based on two experiments, keeping the other for cross-validation. Even though the use of experiments corresponding to $C_0 = 3670$ and $C_0 = 7290\,\mathrm{g/m^3}$ leads to a smaller value of the cost function at the optimum, again ν_0' is not identifiable and the confidence interval on r_p, and more embarrassingly on r_h, are very large, which is not

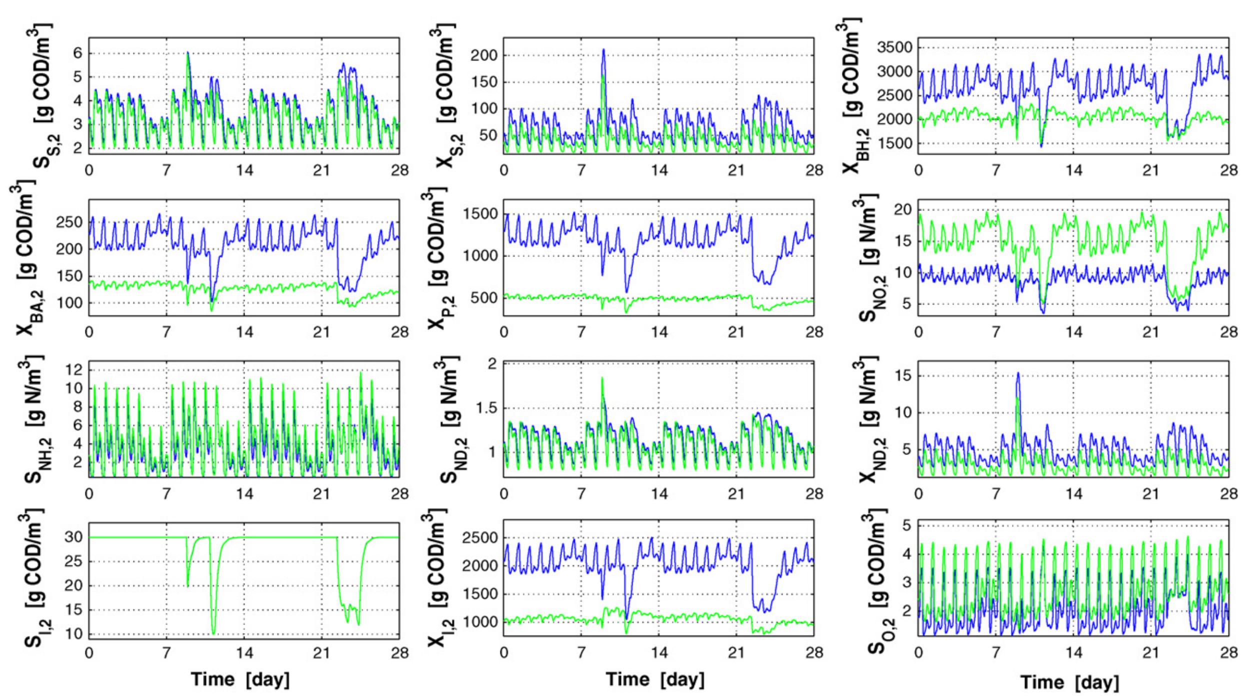

Fig. 11. State variable evolution in the aerobic tank for the weather sequence “Storm–Rain”. Black line: Settler “PDE + MOL”, Grey line: Settler “Takács”.

acceptable. The best combination of experiments is therefore given by $C_0 = 3670 - C_0 = 6120$ or $C_0 = 6120 - C_0 = 7290$. Obviously, it is difficult to find a unique set of parameters describing the three experiments, due to the large difference in initial concentration and the presence of relatively large measurement errors (noisy data) for experiments carried out at larger concentrations (where it is difficult to achieve good mixing conditions and a uniform concentration at the initial time).

These results demonstrate the predictive capability of the model, and the challenge associated to an accurate estimation of the model parameters based on experimental data. Even though the simple mass balance model does not take account of the sludge accumulation at the bottom of the tank and the compression effects, it seems appropriate for a macroscopic view of the secondary settler. A more detailed study of sludge accumulation and compression requires the consideration of a momentum balance as introduced in [5].

5. Dynamic simulation of the activated sludge process

Based on the batch sedimentation model developed in the previous sections, a simple partial differential equation model of continuous settling and its associated MOL solution are presented, using the parameter set from Table 3[4]. Simulation results are compared with those produced by a standard layer representation, together with a flux limiting approach as recommended in [22]. Finally, our PDE model is coupled with the ASM1 representation of the activated sludge process, so as to produce a complete dynamic simulator. The code is developed using MATLAB and is available on request from the authors.

5.1. A simple secondary settler model and simulation code

In order to study continuous settling (Fig. 5), the settler is divided in two zones I and II, corresponding respectively to the zone between the clear water outlet (z_0) and the feed level (z_f) and to the zone between the feed level and the sludge outlet (z_L).

The mathematical model and boundary conditions then become

$$\frac{\partial C_I}{\partial t} = -\frac{\partial(v_{s,I} C_I - q_e C_I)}{\partial z_I} + D_I \frac{\partial^2 C_I}{\partial z_I^2} \tag{20}$$

$$\frac{\partial C_{II}}{\partial t} = -\frac{\partial(v_{s,II} C_{II} + q_u C_{II})}{\partial z_{II}} + D_{II} \frac{\partial^2 C_{II}}{\partial z_{II}^2} \tag{21}$$

$$\begin{cases} \text{At } z_0: & v_{s,I} C_I - D_I \dfrac{\partial C_I}{\partial z_I} = 0; \\ \text{At } z_f: & \begin{cases} C_I = \dfrac{q_f C_f}{q_u + q_e}; \\ C_{II} = C_I; \end{cases} \\ \text{At } z_L: & v_{s,II} C_{II} - D_{II} \dfrac{\partial C_{II}}{\partial z_{II}} = 0. \end{cases} \tag{22}$$

The boundary conditions now express the fact that the sedimentation and dispersion fluxes at the clear water outlet and at the sludge outlet vanish. The boundary condition at the feed level is simply a balance of material fluxes and a continuity condition for the particle concentration.

Consider an initially empty settler (process start-up phase). The initial conditions are then given by :

$$C_I(t = 0, z_I) = 0 \quad \text{and} \quad C_{II}(t = 0, z_{II}) = 0. \tag{23}$$

For numerical simulation, zones I and II are spatially discretized using n_I and n_{II} grid points. Finite difference schemes and a MOL approach are used to produce the results displayed in Fig. 6, which shows space-time evolutions corresponding to a feed concentration $C_f = 6000\,\mathrm{g/m^3}$. The computational load on a standard PC is very modest (for instance, with a PC Intel Centrino 1.73 GHz and 1 GB RAM, a simulation of 1000 h of the settlers discretized using a total of 213 nodes takes about 20 s). For comparison purposes, Fig. 7 shows dynamic simulation results obtained with Takács' model using the same parameter values for the settling velocity law and under the same operating conditions. Classically, the settler is subdivided in 10 layers and a flux limitation from layer to layer is used as detailed in [22]. These simulation results differ significantly. Whereas the PDE model represents a properly working settler, Takács' model predicts overload (saturation) conditions. There are several reasons for these discrepancies, including the crude discretization in a few layers only (10 layers is the typical number recommended in the literature), the flux limitation scheme, and the incorrect formulation of the boundary conditions in Takács' model (an analysis of the pitfalls of Takács' model can be found in [14,15]). As a consequence, it would be necessary to re-estimate the parameters of the settling velocity law in Takács' model and maybe adapt the number of layers so as to have a better agreement. However, this would be only a partial, ad-hoc, solution.

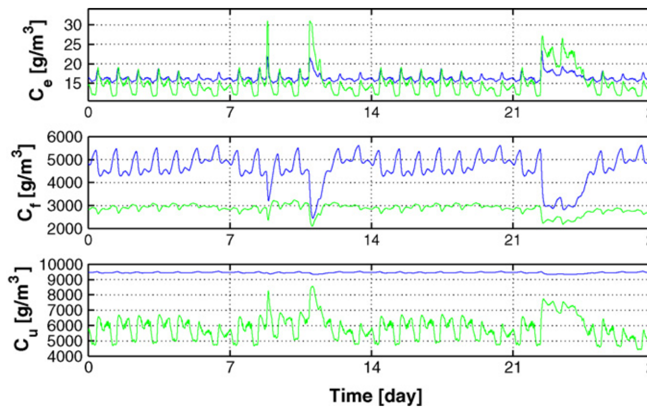

Fig. 12. Concentration evolution at the clear water outlet (C_e), at the feed level (C_f) and at the sludge outlet (C_u) for the weather sequence "Storm–Rain". Black line: Settler "PDE + MOL", Grey line: Settler "Takács".

5.2. The resulting simulator

In a way similar to [9], the PDE settler model can be coupled to the ASM1 representation [13] of the actiated sludge process as illustrated in Fig. 8. Figs. 9–12 show simulation results over a period of 28 days with a sequence of stormy–rainy weather (as suggested in [4]) and highlight the deviation between the prediction of the simulator based on the PDE settler model (with MOL solution) and the one based on Takács' model. The model of Takács predicts smaller concentration values C_u at the sludge outlet, so that the particulate components achieve smaller concentrations in the activated sludge process. The sludge concentration C_u is also more variable in Takács' model, and somewhat unexpectedly, these variations seem to be in opposition with the variations of the feed concentration.

As mentioned in the previous section, these deviations could be reduced by retuning the settler model parameters (in the simulation runs considered here, the parameter set is the same for both models). Again, this is an artificial procedure, and it is important to stress the lack of coherence of Takács' model (crude discretization used as an artificial numerical dispersion, flux limitation from layer to layer, incorrect boundary conditions).

The simulation time of the complete simulator is very modest (about 6 min on a standard PC).

6. Conclusions

In this study, a simple mass balance PDE model of continuous settling is described, and the unknown model parameters (associated to dispersion effects and settling velocity) are estimated by minimizing the deviation between model prediction and experimental data borrowed from [5,6]. The PDE model is very efficiently solved using a Method of Lines strategy and produces realistic concentration evolutions. Finally, the PDE settler model is coupled to a standard ASM1 representation of the activated sludge process and implemented in a MATLAB simulator, which is available on request from the authors.

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