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Knowledge-based model and simulations to support decision making in wastewater treatment processes

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Abstract

In this paper, mass and momentum balances are used to model and simulate the most significant phenomena occurring in a continuous urban sludge clarifier. This model is designed to be the core of a digital twin in the future. This has two consequences: the choice of a one-dimensional model only and a numerical scheme for simulation that allows a reasonable runtime. We propose a different way of writing of the dynamic model of the clarifier. Instead of using volume fractions and velocity of solid particles as state variables, we use volume fractions and flux of solid particles. This approach, which is used for conservation law systems, gives more stable simulation results for hyperbolic systems.
This paper focuses on comparative discussions of these two different versions of the model. The numerical simulation scheme is presented. In addition, the simulation is compared with experimental data obtained in a full-scale wastewater treatment plant.

Keywords: Urban sludge continuous settling, Dynamic mass and momentum balances, nonlinear hyperbolic system, Rusanov numerical approximation

1. Introduction

The efficiency of wastewater treatment facilities is a worldwide major problem. Urban wastewater treatment plants are regulated by European directives, such as 91/271/EEC. The biological treatment unit of a treatment plant purifies wastewater before it is released into the natural environment by using a clarifier. The quality of the clarified water strongly depends on the instantaneous hydraulic loads arriving upstream, on the design of the equipment and on the operating conditions. The settling of the sludge in the clarifier enables the separation of more concentrated sludge that is pumped down and clarified water that is released up into the environment in an overflow. Thus, the quality of the plant effluent is highly dependent on the performance of the clarifier. In order to optimise its operation, modelling and simulation are the first steps to perform.

In the literature, the modelling of clarifiers is obtained through mass and momentum balance equations for solid particles. The latter is written as a static or dynamic partial

differential equation (Chauchat (2013), Garrido (2003)) or replaced by a constitutive relation representing the velocity of solid particles (Li (2014)). In the case where the momentum balance is represented by a PDE, the global model is weakly hyperbolic and the position of the so-called sludge blanket corresponds to the front of a shock wave. This shock is related to a discontinuity in the solid particle volume fraction and a peak value in the flux.
In this paper, we present two choices of state variables for the sludge settling modelling in a clarifier (Valentin (2022)) and discuss the simulation results with respect to experimental data.

2. A 1-D schematic representation of the clarifier

Fig. 1 shows a 1-D schematic representation of the clarifier. It is connected to the wastewater treatment process at three points, one inlet and two outlets:
• one inlet where the sludge, consisting of fluid and particles, flows into the clarifier by gravity from the upstream biological aeration tank at the volume flow rate $Q_f(t)$ and with a particle concentration $C_f(t)$. The sludge feed is situated at a depth of $z = z_f$,
• one top outlet for clarified water at $z = 0$, with a volume flow rate $Q_e(t)$ and particle concentration $C_e(t)$,
• one bottom outlet for compressed sludge at $z = z_b$, with a volume flow rate $Q_u(t)$ and particle concentration $C_u(t)$. Some of the compressed sludge is recirculated back into the aeration tank at a volume flow rate $Q_{ur}(t)$ and some is extracted from the clarifier at a volume flow rate $Q_{ue}(t)$ such that $Q_u(t) = Q_{ur}(t) + Q_{ue}(t)$.

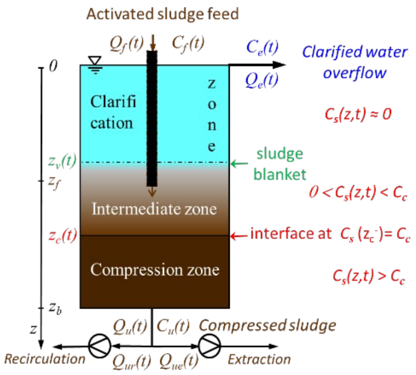

Figure 1: Schematic view of a clarifier

A	***1175 m²***
A_k	*0.02 m/s*
ε_c	*4.1 10⁻²*
n_r	*2*
n_s	*11*
ρ_l	*1000 kg/m³*
ρ_s	*1030 kg/m³*
σ_0	*0.5 kg/ms²*
z_b	*2.8 m*
z_f	*1.8 m*

Table 1: Model parameter values

The open-air settler content can be divided into two moving interfaces separating three zones:
• The upper interface is the sludge blanket, located at depth $z_v(t)$. It separates the clarification zone (which contains no or very few particles) from the intermediate zone,
• The lower interface is defined by the intermediate/compression threshold and is located at depth $z_c(t)$ where a change in the particles behaviour occurs as the particle concentration $C_s(z,t)$ exceeds the critical threshold C_c. Above this threshold, interparticle stress comes into effect. Under $z_c(t)$, the liquid phase flows through a porous network of concentrated particles, Toorman (1996). The model parameter values are given in Table 1.

3. A 1-D dynamic model of the clarifier

The knowledge-based model includes two dynamic mass and momentum balances of urban sludge added with physical constitutive equations under standard simplifying assumptions, Valentin (2022). As the liquid and solid phase densities ρ_l and ρ_s are constant, the two most natural state variables are the particle volume fraction, ε_s, and the particle flux, $f_s=\varepsilon_s v_s$ with v_s the particle velocity. The corresponding hyperbolic system of conservation laws is then defined, if $\varepsilon_s>0$, by:

$$\partial_t \varepsilon_s+\partial_z f_s = \frac{f_{1s}}{\rho_s}\delta_f \quad (1)$$

$$\partial_t f_s+\partial_z\left(\frac{f_s^2}{\varepsilon_s}\right)=\varepsilon_s g\left(1-\frac{\rho_l}{\rho_s}\right)-\frac{\partial_z\sigma_e(\varepsilon_s)}{\rho_s}+\frac{r(\varepsilon_s)(\varepsilon_s v_m-f_s)}{\rho_s\varepsilon_s(1-\varepsilon_s)}+\frac{f_{2s}}{\rho_s}\delta_f \quad (2)$$

with $\sigma_e(\varepsilon_s)$ the interparticle stress between the particles, $r(\varepsilon_s)$ the liquid/solid drag force and $v_m$the average velocity of the liquid/solid mixture (also the total volume flux of the suspension). f_{1s} and f_{21s} are the source terms representing the sludge feed inlet in the particle mass and momentum balances equations respectively. They depend on Q_f and C_f. δ_f is a Dirac function that represents the location of the sludge feed at $z=z_f$. The two boundary conditions are $v_s(0,t)=\frac{-Q_e}{A}$ and $v_s(z_b,t)=\frac{Q_u}{A}$.

Various kind of constitutive equations that describe the compression and drag phenomena have been proposed in the literature, Li (2014). $r(\varepsilon_s)=\frac{\rho_l g}{A_k}\varepsilon_s^{\frac{2}{(3-n_r)}}$ is proposed in Chauchat (2013) and the following $\sigma_e(\varepsilon_s)$ expression, that depends on the particle volume fraction, in Garrido (2003). If $\varepsilon_s>\varepsilon_c$ (in the compression zone), $\sigma_e(\varepsilon_s)=\sigma_0\frac{\varepsilon_s^{n_s}-\varepsilon_c^{n_s}}{\varepsilon_c^{n_s}}$ else (in the two other zones), $\sigma_e(\varepsilon_s)=0$ (see Table 1). $\sigma_e(\varepsilon_s)$ is a continuous function on [0, z_b] but its disadvantage is that it is zero over the upper part of the spatial domain which makes the system weakly hyperbolic only.

Most of the papers in the literature present a model based on a dynamic particle mass balance with the state variable, ε_s, coupled with a constitutive equation that gives the so-called batch or hindered settling velocity (Garrido, 2003), (Li, 2014). This motivated us and others, Chauchat (2013), Valentin (2022) to use first the state variables (ε_s, v_s¿ according to the following hyperbolic system of two PDEs:

$$\partial_t \varepsilon_s + \partial_z \left(\varepsilon_s v_s \right) = \frac{f_{1s}}{\rho_s} \quad \delta_f(3)$$

$$\partial_t v_s + \partial_z \left(\frac{{v_s}^2}{2} \right) = g \left(1 - \frac{\rho_l}{\rho_s} \right) - \frac{\partial_z \sigma_e(\varepsilon_s)}{\rho_s \varepsilon_s} + \frac{r(\varepsilon_s)(v_m - v_s)}{\rho_s \varepsilon_s (1-\varepsilon_s)} + \frac{f_{21s}}{\rho_s} \quad \delta_f(4)$$

This representation is based on the temporal and spatial derivatives of products such as $\varepsilon_s v_s$. As shock waves appear on the two state variables, such product derivatives may lead to mathematical problems. Moreover, the difficulty of numerically solving the model based on the state variables (ε_s , v_s¿ and the oscillations obtained on the spatial profiles of the velocity $v_s$led us to return to the more "natural" state variables that correspond to those used in the so-called conservative approach, the particle volume fraction, ε_s, and the particle flux, $f_s = \varepsilon_s v_s$ (equations (1) and (2)) and to include the interparticle stress in the flux.

4. Numerical discretization scheme

The simulations were carried out using explicit Euler time-discretization and an efficient numerical scheme adapted to hyperbolic and weakly hyperbolic nonlinear PDE systems: a finite volume method spatial-discretization with the Rusanov approximation of the fluxes (Godlewski (1996), LeVeque (2002)).

The state variable vector x and the flux vector $F_s(x)$are defined if $\varepsilon_s > 0$ by $x = \begin{pmatrix} \varepsilon_s \\ f_s \end{pmatrix}$ and $F_s(x) = \begin{pmatrix} f_s \\ \frac{{f_s}^2}{\varepsilon_s} + \frac{\sigma_e(\varepsilon_s)}{\rho_s} \end{pmatrix}$. The state variables are considered as uniform in each volume *i* of the mesh and equal to the average values $\overline{x}_i^k$ at time step *k*.

For time step *k* and volume *i*, the flux at the input interface $i - \frac{1}{2}$ is approximated by:

$$F^k_{i-\frac{1}{2}} = \frac{1}{2} ¿$$

with ${\omega_s}^k = \max_i \left({\rho_i}^k \right)$, ${\rho_i}^k$the spectral radius of the volume *i* which depends on $\overline{x}_i^k$.

Then:

$$\overline{x}_i^{k+1} = \overline{x}_i^k + \frac{\Delta t}{\Delta z} (F ¿¿ i - \frac{1}{2} (\overline{x}_i, t) - F_{i+\frac{1}{2}} (\overline{x}_i, t)) + \Delta t \left(S_1 (\overline{x}_i) \cdot \right.$$

where we assume that $S_1(\overline{x}_i)$ is a good approximation of $\frac{1}{\Delta z} \int_{i-1/2}^{i+1/2} S_1(x)\, dz$

and that the variable time-step Δt respects the CFL (Courant-Friedrichs-Lewy) condition: $\Delta t = \gamma \frac{\Delta z}{\omega_s^k} \, with \, 0 < \gamma < 1$. As $\sigma_e(\varepsilon_s) = 0$ in the clarification and intermediate zones, the system is only weakly hyperbolic.

5. Simulation of a transient state experiment of continuous settling

The model simulation is compared to experimental data obtained in a full-scale settler operated under the following transient state scenario (Fig.3): the sludge feed rate was abruptly increased by a magnitude of two from a value corresponding to a stationary profile at $t = 1.40\,am$ (660 *m3/h*) and abruptly decreased *8 hrs* later (370 *m3/h*). The flow rates and concentrations at the sludge inlet and outlet were measured on-line as well as the sludge blanket position.

Simulations based on this model were performed with various discretization parameters such as spatial mesh size, convergence condition (Courant-Friedrichs-Lewy). They are compared to the experimental data. Measured sludge feed flow rate, $Q_f(t)$, recirculation flow rate, $Q_{ur}(t)$ and extraction flow rate, $Q_{ue}(t)$ as well their mean values are given in Fig.3.

An N-node spatial mesh was used to run the simulations of the discretized model presented in section 4. with the constitutive equations and boundary conditions given in section 3.

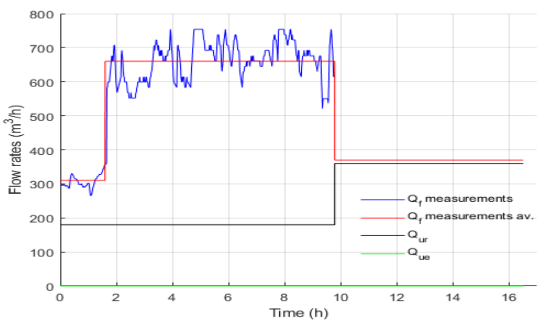

Figure 3: Applied flow rates

The calculated sludge blanket position $z_v(t)$ corresponds to the location where the maximum gradient of the solid concentration is reached. Fig 4.a shows that the simulated and measured sludge blankets positions are very close.

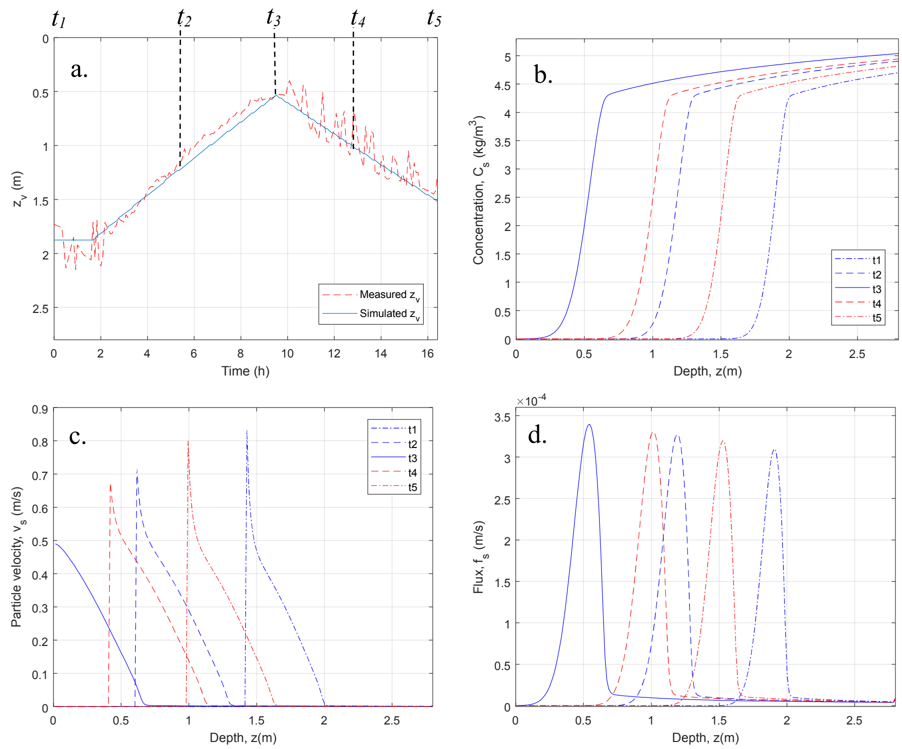

Figure 4: Simulated $z_v(t)$ and $C_s(z)$, $v_s(z)$, $f_s(z)$ spatial profiles (N=200)

Five spatial profiles at t_1, t_2, t_3, t_4 and t_5 are shown in Fig 4.b to Fig 4.d. Fig 4.b presents particle concentration spatial profiles. The particle concentration at the top of the clarifier (z=0) is close to zero. It increases sharply at the depth of the sludge blanket and then increases more moderately to the bottom as soon as the critical threshold is exceeded. The effect of the interparticle stress below the critical threshold is also well highlighted. Spatial profiles $v_s(z)$ and $f_s(z)$ are shown in Fig. 4.c and Fig. 4.d. The shock wave is also clearly visible at the "peak" location. The particle velocity at the bottom of the settler $v_s(z_b)$ is very low compared to the velocity at the sludge blanket position, $5.3\ 10^{-4}\ m/s$, and is set by the Q_u flow rate.

Good results are obtained with this numerical scheme for a mesh size of up to 800 volumes and $\gamma = 0.99$ in the CFL condition. Choosing a lower γ value gives the same results but with a longer runtime due to a smaller Δt. The runtime of a simulation with 200 volumes on a workstation equipped with an Intel Xeon at 3.8GHz is 8 *min* 15 *s*. According to the nature of the numerical scheme, the runtime with N = 800 is 16 times longer that makes 2 *hrs* 12 *min*. Although the simulation gives good results with N = 800 with less numerical diffusion, as this model will be the core of a decision support system and then a digital twin, a compromise must be decided. A spatial discretization of N = 200 seems suitable.

6. Conclusions

As a conclusion, the well-suited conservative state variables are the volume fraction and the volume flux of the solid particles. The expression of the momentum balance includes the compression stress between the particles based on a nonlinear constitutive law taken from Garrido (2003). A numerical scheme with explicit Euler time-discretization and a finite volume method spatial-discretization with the Rusanov approximation of the fluxes works well. The simulation results are close to experimental results by using a set of well-chosen parameter values. It can be used for prediction and decision support for other scenarios of operation. The runtime with a spatial mesh of 100 volumes is still about 2 min 4 s on a workstation equipped with Intel Xeon at 3.8GHz, which may be a limitation of this approach.

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