COMPUTATIONAL FLUID DYNAMICS IN WASTEWATER TREATMENT

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INTRODUCTION

The purpose of activated sludge systems is to remove the waste from the polluted water by means of microorganisms. Removing the waste appropriately is one aspect; removing the biosolids from the clean water is another challenge. Hence, the settling tank, in which bioflocs are separated from the liquid by gravity, is a crucial operation in biological wastewater treatment systems.
If the settling tank fails, solids will be carried over the weirs into the river. The consequences are significant. Increased turbidity may restrict plant photosynthesis, and the increased oxygen demand may be detrimental for aquatic life.
Mathematical models can be used in many ways to make the settling tanks work efficiently, i.e. they can be applied for control purposes, design, fundamental process understanding, etc… For each aim another model that differs in complexity is most appropriate (Ekama *et al.*, 1997). In this paper only models for settling tank design will be discussed that consist of local elementary balances of mass, momentum and energy. They are referred to as *computational fluid dynamics (CFD)* models and describe the system two- and/or three-dimensionally.
Building a good CFD model is very tedious and a lot of challenges are encountered. In this respect the article will summarize the different steps to be taken when setting up a CFD model.

THE MODELLING PROCESS

The development of a CFD model for settling tanks involves three steps, (i) mathematical modelling and its numerical considerations, (ii) model calibration and (iii) model validation. These issues will be discussed below.

Mathematical modelling & numerical considerations

The first stage of settler modelling always starts with the definition of the process variables to be modeled. A design model to be used for optimizing tank size and internal geometry must have a high spatial resolution and must accurately simulate the physical processes in the tank. For that reason the fundamental Navier-Stokes equations are used to describe the complete flow field in the settling tank. An example of a typical flow field for half of a vertical cross-section of a circular settling tank is given in Figure 1. Additional transport equations are considered for turbulence, solids settling, (de)flocculation of particles and biological reactions. With this set of equations the system can be described three-dimensionally. Unfortunatelly, long computation times are a severe drawback. As a result the model is often simplified by omiting structures such as

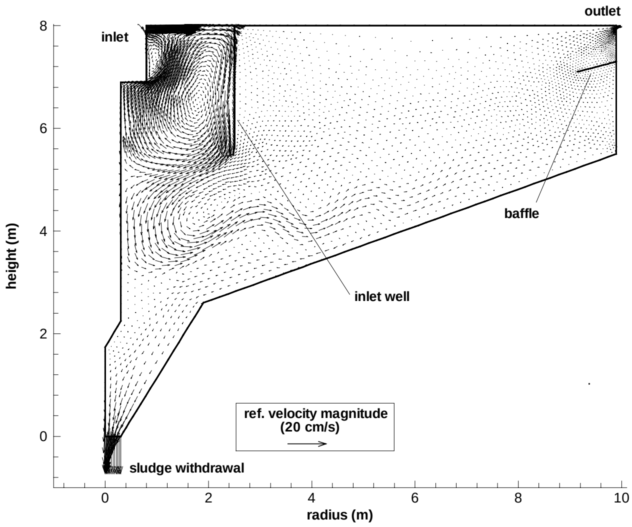

Figure 1 Computed flow field in a cross-section of a circular settling tank

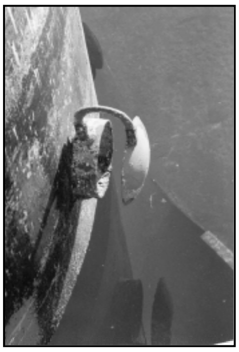

Figure 2 Inlet slot with deflector plate

the sludge removal mechanism and reducing the dimensionality of the model. If the settling tank shows some symmetry it can be modeled along such a plane of symmetry, e.g. a circular settler might be modelled along a radial cross-sectional area. Remark that the condition of axisymmetry for circular settlers does not imply the absence of tangential fluxes in practice. Although not modeled, they can be present as long as the tangential fluxes are locally balanced. This is definitely not always the case. Some designs of inlet slots (e.g. Figure 2), through which the sludge flows into the settler, alter the flow field such that no tangential homogeneity can be assumed. To properly simulate the flow field at such inlet 3D models are needed. Although the inlet is difficult to model in 2D, settlers provided with a so-called baffled inlet well (e.g. Figure 3) allow the simplification however. Turbulence from the inlet structure mainly determines the flow field inside the well (i.e. the inlet zone) and not beyond this region (Lyn & Rodi, 1990; Szalai *et al*., 1994). Hence, the (most interesting) main settler volume beyond the well is properly described.

Figure 3 Empty settler with baffled centre well

After making the choice of the modelled system, the settler geometry has to be implemented in some software (commercial or home-made). The computational domain has to be split in cells over which the mass balances are calculated. This procedure is called *meshing*. How meshing is performed, e.g. the shape of the control volumes, has a pronounced effect on the numerical accuracy and convergence time (Bern & Plassmann, 1999). For that reason it is essential to check the mesh quality. The aspect ratio and the equiangle skew of a cell are the most important parameters to consider. Further, the solution should be independent of the mesh size, i.e. no numerical errors occur due to a too coarse mesh. Proper meshing is also crucial for the solution to converge; even a single badly designed cell can result in divergences. Hence, if divergence occurs the local residual error between consecutive interations should be investigated. Large residual values indicate where the problem originates and if it is related to some badly designed cells. If this is not the case other numerical discretization schemes should be looked for.

The last crucial issue to consider when modelling are boundary and initial conditions. Different boundary conditions might lead to completely different solutions, hence they should be applied with care. On the other hand, initial conditions for the computational domain do not alter the final solution. Instead, they may largely influence the speed at which convergence is obtained. If an initial guess of the flow field is not known, the best solution is to perform unsteady simulations with an empty tank that is gradually filled with sludge.

Model calibration

Before the model can be solved, different types of data are needed. Firstly, to set up the computational mesh the mechanical drawings are essential for correct system dimensions. Secondly, sludge-specific knowledge has to be collected. In this respect, settling velocities are very important since gravitation is the main mechanism to separate the solids from the water. Also related to this issue is the determination of the solids dry density; it is needed for a proper calculation of bulk density and buoyancy. This bulk buoyancy is the dominating term in the vertical momentum equation and, as a consequence, will influence the flow field considerably. Flocculating agents such as polymers and sand are sometimes used in practice to increase the floc density and thus the settling velocity (Vanderhasselt *et al.*, 1999) . They can dramatically alter the solids distribution in the settler. Further, sludge rheology too is influenced by the use of flocculants (Abu-Orf & Dentel, 1997). Here, a correct rheological model is needed since viscous stresses are important for momentum transport.
Note that model parameters are not estimated by fitting model predictions to data; CFD models clearly belong to the class of models that can rely on *a priori* knowledge alone (Dochain & Vanrolleghem, 2001).

Model validation

To check the accuracy of the CFD model simulation results have to be confronted with measurement data. Depending on which part of the model to validate different data sets can be used. Firstly, the simulated solids concentration profile should be validated with measured profiles. Secondly, to validate the velocity profiles many techniques are available. They range from simple flow-through curves (NCASI, 1983) to *in situ* 3D velocity measurements (Kinnear & Deines, 2001). A flow-through curve is an easy way to check the overall hydraulics of the settler. The technique consists of the introduction of some inert material, i.e. tracer, at the inlet. At different locations the tracer concentration is measured in time; the more sampling points are considered, the better the internal flow pattern is validated. More sophistigated techniques are based on accoustic Doppler technology where 3D velocities can be measured (Kinnear & Deines, 2001). With these techniques even complete velocity profiles can be measured at high sampling frequencies. Unfortunately, the particle and not the fluid velocity is measured; the extent of particle entrainment determines the uncertainty on the fluid velocity measurement. To avoid this uncertainty other techniques such as electromagnetic velocity meters can be used. In general, both techniques allow the determination of shear stresses and turbulence properties.

As already mentioned validations can be performed under steady and unsteady conditions. This is very important to consider since a steady state is hard to impose on a full-scale wastewater treatment plant. Unsteady simulations are inherently more difficult and impose more stringent test conditions. Also the quality of the solver becomes important and not only the model.

CONCLUSIONS

Computational fluid dynamics becomes more important in bio-engineering, and more specifically in wastewater treatment technology. Design and optimization of process units can be done in a customized way without any heuristic approach. These sophisticated computational techniques introduce some issues to be taken into account, i.e. mathematical modelling, model calibration and validation. The paper discussed the different steps in the modelling process.

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