

Computational Fluid Dynamics: an important modelling tool for the water sector

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Abstract

Modelling has been used frequently for both system understanding and optimization. However, the challenges put on the models are constantly growing. This entails new regulations for effluent, more accurate energy consumption predictions, predictions of greenhouse gas emissions, enlarging the scale towards urban water systems, to name but a few. Hence, simulations are being pushed into ranges where the models currently in use have greater uncertainty. This is exacerbated by the fact that the submodels in use may lack sufficient detail or may not be in proper balance with the full model when coupled solutions are attempted. In this contribution we want to highlight how computational fluid dynamics models can assist in resolving some of these issues.

Keywords

Computational Fluid Dynamics; Water treatment; Good Modelling Practice; Simplified models

INTRODUCTION

Computational Fluid Dynamics (CFD) models have been extensively and successfully used in a wide range of engineering disciplines including, but not limited to, automotive engineering, chemical engineering, mechanical engineering and aerospace engineering for many decades. In recent years, there has been a steady increase in CFD modelling in the wastewater treatment (WWT) field, both in academia (universities and research institutes) and industry (mainly consultants). This growth is due to increased availability of quality CFD models and dedicated software tools, increasing power and affordability of computing power, and increasing regulations and need for optimization of municipal and industrial WWT unit processes.

To date, CFD models have been primarily used for evaluation of hydraulic problems of WWT unit processes and this is mostly how the wastewater community currently perceives their benefit.

However, a potentially more powerful use of CFD is to simulate integrated physical, chemical and/or biological processes involved in WWTP systems on a spatial scale. On the other hand, CFD models can also be used to gather knowledge that can accelerate improvement in plant models for everyday use. With this increased usage of CFD, it also becomes important to stipulate guidelines for Good Modelling Practice (GMP). This contribution focuses on the aspects of CFD for acquiring detailed system knowledge as well as GMP and is an effort of the IWA Working Group on CFD for wastewater which resides under the specialist group Modelling and Integrated Assessment (MIA) and consists of the authors of this abstract.

RESULTS AND DISCUSSION

CFD for improved system knowledge

A general protocol for use of CFD as a tool for improving/developing simpler models was recently proposed by Laurent et al. (2014). The concept is illustrated in Figure 1 and consists of the following steps:

1. **CFD model formulation:** CFD models representing detailed features of the process tank geometry, as well as physical, chemical and biological components (turbulence, biokinetics, aeration, viscosity, density couples, solids transport...).
2. **Data collection:** lab or field test of appropriate process variables (velocity profiles, species concentration profiles, gas hold-up measurement, residence time distribution, etc.) to validate results of the CFD model.
3. **CFD model validation:** comparison of the CFD model prediction with the data.
4. **Comparison to simpler model predictions:** comparison to the results of simpler models for the same geometry and loading condition should allow shortcomings to be evidenced.
5. **Improved simple model:** the latter shortcomings lead the modeler in developing next generation models that better capture the phenomena needed to reach the modelling goal.

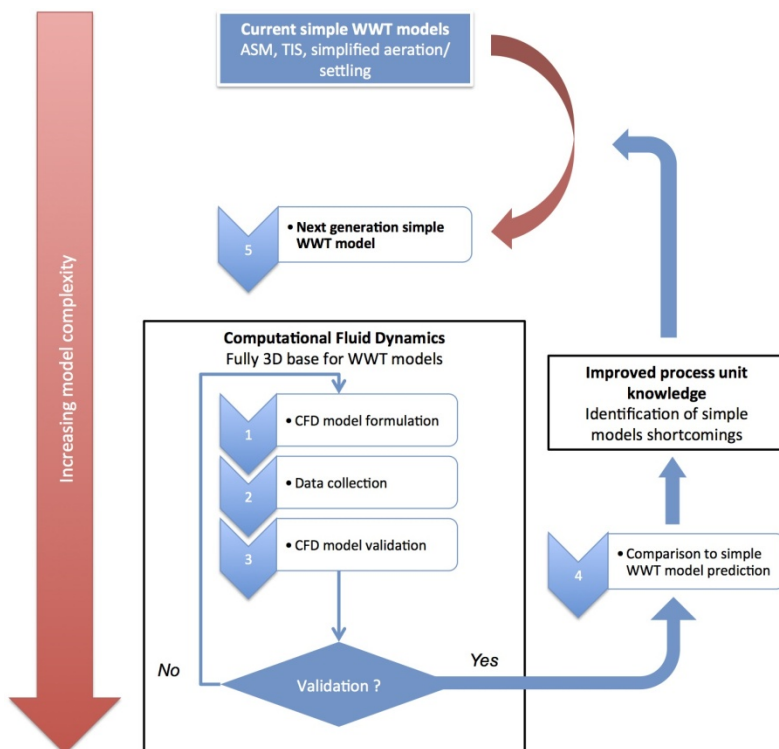


Figure 1. Illustration of the concept of using CFD for creating next generation simple system models (source: Laurent et al., 2014).

It is noteworthy that this concept, shown here for WWTP unit processes, is also applicable to other processes or systems in the water sector (e.g. unit processes in drinking water systems, more detailed modelling of river stretches,...).

A couple of examples with regard to more accurately modelling the mixing behavior in bioreactors have been reported in the literature (Delafosse, Collignon, et al., 2014; Alvarado, Vedantam, et al., 2012; Le Moullec, Potier, et al., 2011; Potier, Leclerc, et al., 2005). In these contributions it is shown that traditional tanks-in-series models meet their limitations in describing the mixing behavior of a bioreactor and a waste stabilization pond. This often leads to unnecessary calibration efforts in other submodels which contain more detail (e.g. half-saturation indices which lump all kinds of unexplained phenomena).

By means of CFD and tracer tests for validation, a good description of system behavior is retrieved. Based on these models, so-called conceptual compartmental models (CM) can be constructed, which allow an improved description of the system with a limited number of tanks and only accounting for the most important macro-mixing behavior of the system (Figure 2). (Rehman, Vesvikar, et al., 2014) recently demonstrated the impact a more detailed description of mixing with a CM can have on controller development in particular by choosing different sensor locations.

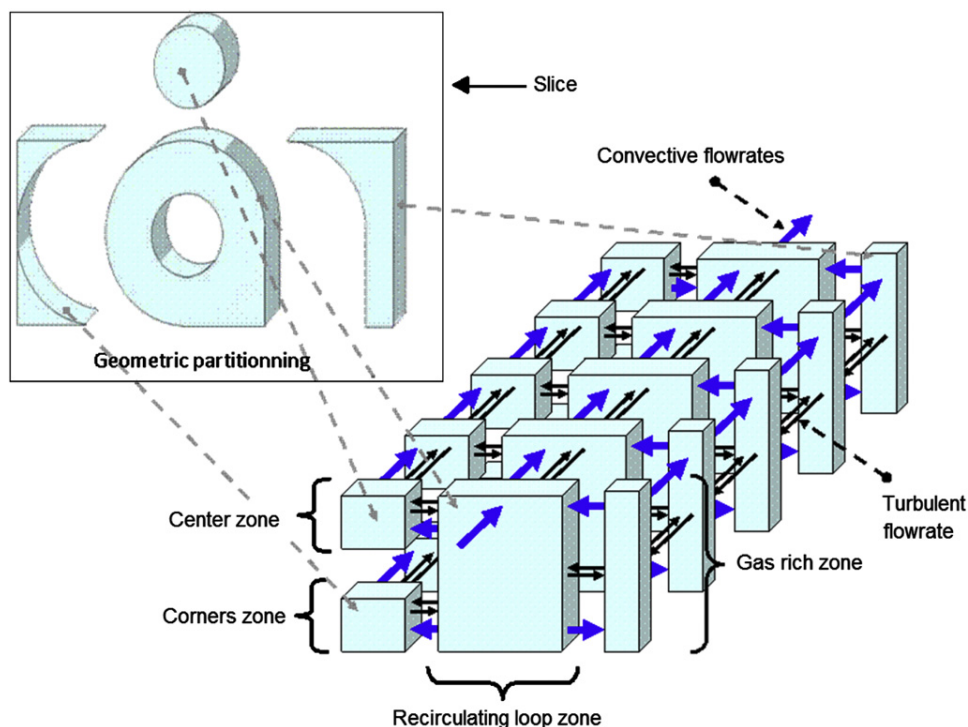


Figure 2. Structure of the compartmental model for a bioreactor based on a validated CFD model (Le Moullec et al., 2011)

Moving towards CMs brings on some challenges though. CMs are more complex and impact the computational load. As usual, a balance between model accuracy and computational load needs to be found in view of the modeling objective. Furthermore, CM structural development is usually based on several steady state (SS) CFD simulations at different conditions of liquid and air flow rate. However, for the cases in between, interpolation is required. This shows that further efforts are

required to further mature the development and usage of CMs. It is noteworthy though that certain types of systems potentially behave in a similar way. Hence, not every system will require a CM development in the future.

Good modeling practice for CFD

In the application of CFD as discussed before care must be taken to use the principles of Good Modelling Practice (GMP) which is also highlighted in Figure 1. Model validation forms an important aspect in this. Indeed, CFD models are powerful tools that have become increasingly easy to use with graphical user interfaces (GUI) to assist with model development, operation, and post processing. However, WWT unit processes involve a complex interaction of fluid mechanical, biological, and chemical processes, therefore despite the improved prospects for application of CFD, the models still require significant expertise and experience to produce good quality and, hence, useful results. However, with regards to GMP, no handbook dedicated to wastewater treatment is available. Therefore, steps 1, 2 and 3 of the protocol presented in Figure 1 and published by (Laurent, Samstag, et al., 2014) need to be further detailed. Figure 3 provides an overview of the different important aspects of GMP related to CFD.

After identifying the objective, the key assumptions for the modeling are to be defined. This includes the following aspects:

- Two or three dimensional space,
- Steady state or dynamic problem,
- Single phase, single phase with multi-species, or multiphase simulation,
- Newtonian or non-Newtonian behavior,
- Turbulence modelling,
- Potential need for additional transport equations.

Once the modelling approach is determined, model development includes the steps illustrated in Figure 3. Each of these activities has specific minimum requirements to develop quality results. Some important issues are briefly detailed in the following sections. A more elaborate paper on the topic of GMP for CFD is being prepared by the Working Group (Wicklein, Batstone, et al., Submitted).

Defining the problem geometry. For CFD models, accurate geometric information is required as this can have a significant impact on flow behavior. Furthermore, often the model objective is to assess the impact of geometry on fluid hydraulics. If available, 3D CAD-drawings can be imported into most CFD model development tools. If not, it is advisable to spend ample time collecting this data accurately from sources such as 2D paper design, as-built drawings, photographs, and field measurements and verifications. If older design drawings are used, an effort should be made to validate their accuracy through field measurement or other checks. The model domain should be sufficiently large so that flow conditions at the model boundaries do not create artificial conditions within the region of interest.

Meshing. For solution of the RANS equations it is necessary to discretize the flow domain into a computational mesh to define the actual locations where equations of flow will be solved. There are many approaches to mesh generation and computational cell type available. It is important that the mesh is sufficiently refined in the region of interest, and sufficient quality overall to provide a converged solution. Grid quality analysis is a key issue for successful CFD simulations. A grid independence check statement must be performed to verify whether the grid coarseness has an effect on the solution.

Application of boundary conditions. The flow field computed by the CFD model is a direct function of the flow conditions applied at the domain boundaries, known as boundary conditions. Typical boundaries include inlet boundaries, outlet boundaries, pressure boundaries, symmetry boundaries, and wall boundaries.

Solver setup. Once the mesh is developed, the model solver needs to be setup to calculate the CFD solution. In general, a double precision solver with second order discretization should be used for all wastewater problems. Many of the constituents modeled occur in low concentrations, implying the need for high numerical accuracy.

Calibration and verification. The core CFD model, if setup properly, should not require calibration to accurately solve the fundamental fluid flow equations for a single phase with appropriate boundary conditions. However there are uncertainties in many typical wastewater applications that may require some level of calibration. Submodels for scalar quantities (e.g. solids) often require empirical fits that are subject to many factors that cannot be isolated for a given problem without some local data. For example settling velocities can be measured on site. Solids profiles can be measured under one condition and the model compared to the measured data. Often, modifications in the fit parameters for the empirical models can improve the depiction of local performance.

This validation step may not be needed in the case of design simulations or when other validation studies show reliability of the CFD equations. There, one can also use that “knowledge” to judge whether a model output makes sense or not.

Furthermore, it should be noted that data collection for validation is both time consuming and resource intensive as it typically requires advanced measurement techniques. Velocity measurements such as Acoustic Doppler Velocimetry (ADV) or Laser Doppler Velocimetry (LDV) are typically used which require specific skills and expertise to conduct (Vanrolleghem, Clercq, et al., 2006). Additionally, spatial profiling of certain components within the reactor (e.g. dissolved oxygen) and reactive tracer methods have been reported (Gresch, Braun, et al., 2011). Usually, the validation is performed by visual inspection of 2-3D graphs of experimental data and model predictions. However, caution should be taken as these can be subjective, as it involves pattern recognition rather than the normal comparison of model error using an error evaluation technique. Verification by solids and dye profiling (tracer test) is also a relatively inexpensive and well-documented procedure and can be used for verification of solids transport modelling for many wastewater treatment applications (Bender and Crosby, 1984). However, caution is needed when only variables are measured at in- and outlets as this leaves the internal of the reactor as a “black box”.

CONCLUSION

The potential for CFD in WWT applications is tremendous. However, to date, this potential has not been fully exploited. Indeed, CFD is more than just a tool to study hydrodynamics. We demonstrated how it can be a useful tool to build our next generation simple models for process optimization. This is needed as computational effort still forms a limitation for using CFD in true scenario analysis. Further development of these methods is needed and some challenges remain.

Now that CFD is more frequently used, another challenge surfaces: is the lack of a good guidance with respect to Good Modelling Practice for CFD. The GMP procedure briefly presented in this paper should allow people novel to the CFD related wastewater field to properly conduct a CFD study or to evaluate conducted studies for correctness. This will increase trust in these models and allow exploiting their full potential in the future.

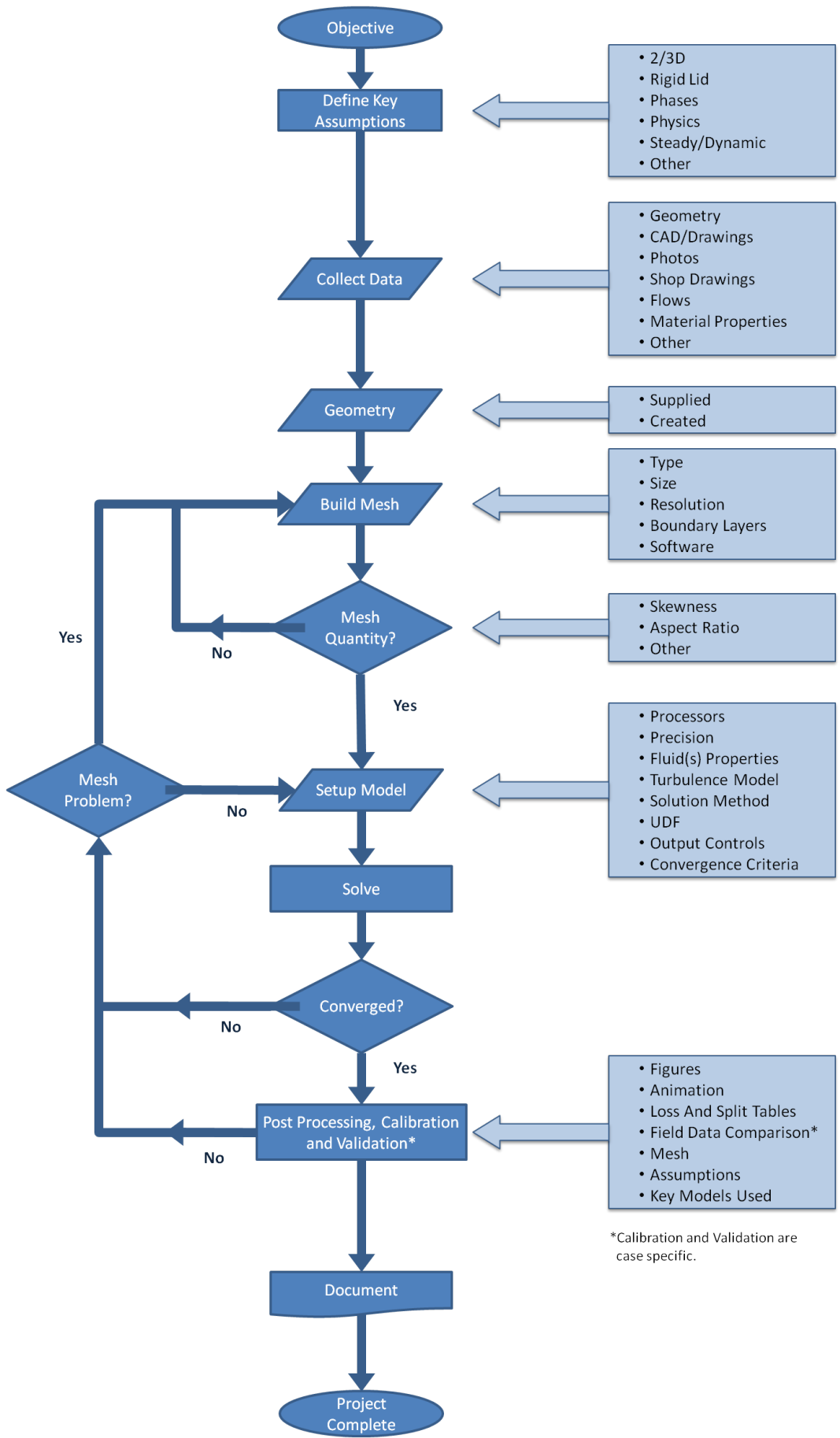


Figure 3. Good modeling practice flow of a CFD study

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