Compartmental modeling of reactors: impact of turbulence and coupling with reactions kinetics

Keywords: hydrodynamics, water treatment, CFD, biokinetic models, transport models, compartmental model

1. Context

Wastewater treatment plants (WWTP) are complex systems of unit processes with interacting hydraulic, biological, and chemical elements. Optimization of the design and operation of these unit processes can be especially challenging when faced with highly dynamic influent flows with variable pollutant concentrations. Mathematical modeling has proven to be a powerful tool to help environmental engineers understand the impact of these dynamic influent conditions on the overall plant process performance. Past usage of these process models has been to simulate chemical and biokinetic processes using simplified hydraulic assumptions such as the tanks in series (TIS) approach. These simplified process models incorporating TIS have been used in the development of the Activated Sludge Model (ASM) family of models [1] as well as the Anaerobic Digestion Model (ADM) [2]. Although the chemical engineering industry has used macro-scale dispersion-type models (TIS and axial dispersion models) to limit the model's computational complexity while still predict the process performance, simplified dispersion reaction models are not fully equipped to capture complex transport-reaction interactions that occur in a multi-phase, multi-scale WWTP.

CFD has become an accepted method for process analysis in a diverse range of industries from aeronautics to ocean engineering. It has been used for analysis and design of water and wastewater treatment plant process elements since Larsen's pioneering study presented the first CFD model for activated sludge sedimentation incorporating solids transport and settling [3]. The use of CFD as a full transport modeling approach for wastewater treatment tanks was already visualized over 20 years ago [4], but has not been extensively or systematically applied until recently. CFD has evolved into a relatively well-accepted tool by consultants and practitioners for analysis of hydraulic problems in wastewater treatment plants, notably for outfalls and flow splitting devices, as well as for chemical mixing.

However, direct use of CFD approaches that allow substantial expansion to include complex biokinetics or other behavior is currently challenging for practical use due to computing and numerical issues. Nevertheless, CFD studies in the field of wastewater treatment can, along with their current application as design and troubleshooting tool, be used to develop the next generation of more practical, everyday use models.

In an effort to correct the shortcomings of the TIS model, the compartmental model (CM) approach was developed [5]. This latter approach simulates the reactor as a network of spatially distributed functional compartments (Figure 1). The work of [6] demonstrated the possibility to accurately predict pollutant concentrations, not only with a detailed CFD-biokinetic model but also with a simpler hydrodynamic model of which the structure is derived from the results of a single steady-state CFD simulation without biokinetics.

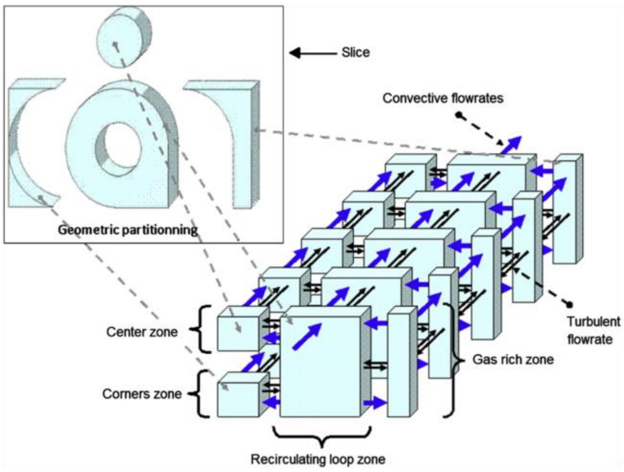

Figure 1. Structure of the CM (source: [6])

The CM allowed the prediction of pollutant concentration within a pilot-scale activated sludge reactor after a few minutes of calculation compared to 1 week of calculation for the CFD-biokinetic approach [6]. Compartmental modeling can be used where the incorporation of biokinetics within a CFD model would be computationally cost prohibitive and where the TIS model is not able to sufficiently describe the macro-scale mixing behavior of the complex system [7].

2. Research objectives

If the CM methodology has already been set up and successfully used in different research works, it is not currently used in industry or consultancy, probably due to lack of dedicated software platform.

The aim of the present project is therefore to continue the development of the compartmental modeling methodology proposed during the PhD of Jeremie HAAG [8]. The idea is to obtain a software able to build and use a compartmental model within the same platform with some automated tasks following the diagram presented on figure 2.

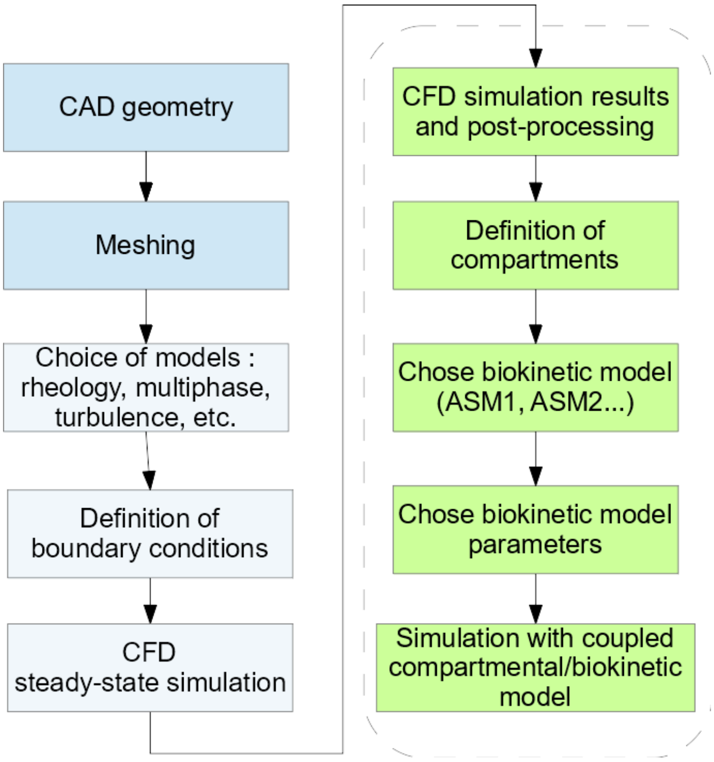

Figure 2. General flow-sheet of the proposed methodology

The following research gaps will be addressed during the PhD:

- Definition of this kind of model relies on the results of a steady-state CFD hydrodynamics model. The number and spatial distribution of compartments are defined according to the homogeneous character of selected parameters with a given tolerance (e.g. gas fraction), as well as the exchange between them (convective flow rates and turbulent backflow rates). The framework of the CM is a discretization of CFD results (with no reaction). Thus, the number of cells and the flowrates between them are calculated from the turbulence and velocity fields. This step need to be integrated within CFD simulation post-processing possibilities in a fully or at least semi-automatized way.
- The present methodology is based on a single CFD steady-state simulation. Influent dynamics effect on model structure is not considered. In the future, this issue could be solved by setting up dynamic CMs as it was already done for TIS [9].

3. Researchers involved

This research project comes within the framework of International Water Association (IWA) Working Group (WG) on Computational Fluid Dynamics. The main aims of the WG are to:

1. promote the exchange of ideas and experiences regarding the use of Computational Fluid Dynamics in the field of water and wastewater treatment;
2. build a network of experts in the field.

Members of the management team (MT) of the WG are from several academic or non-academic institutions (Ghent faculty, Hazen & Sawyer, Carollo Engineers, University of Queensland...). Both Julien LAURENT and Olivier POTIER belong to it. WG MT members.

4. Candidate required skills

- CFD modeling
- Programmation
- Skills in wastewater treatment kinetics modeling would be appreciated

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