A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling

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A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling

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ABSTRACT

To date, computational fluid dynamics (CFD) models have been primarily used for evaluation of hydraulic problems at wastewater treatment plants (WWTP). A potentially more powerful use, however, is to simulate integrated physical, chemical and/or biological processes involved in WWTP unit processes on a spatial scale and to use the gathered knowledge to accelerate improvement in plant models for everyday use, that is, design and optimized operation. Evolving improvements in computer speed and memory and improved software for implementing CFD, as well as for integrated processes, has allowed for broader usage of this tool for understanding, troubleshooting, and optimal design of WWTP unit processes. This paper proposes a protocol for an alternative use of CFD in process modelling, that is, as a way to gain insight into complex systems leading to improved modelling approaches used in combination with the IWA activated sludge models and other kinetic models.

Key words | biokinetic models, CFD, complex systems, fluid motion, multi-phase flow, transport models

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INTRODUCTION

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 modelling 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 (Henze *et al.* 2000) as well as the anaerobic digestion model (Batstone *et al.* 2002). 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.

Computational fluid dynamics (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

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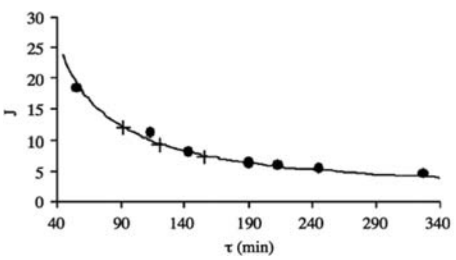
treatment plant process elements since Larsen's pioneering study presented the first CFD model for activated sludge sedimentation incorporating solids transport and settling (Larsen 1977). The use of CFD as a full transport modelling approach for wastewater treatment tanks was already visualized over 20 years ago (Samstag *et al.* 1992), 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 WWTP, notably for outfalls and flow splitting devices, as well as for chemical mixing. With steadily increasing computational power over the past decades, it is no longer 'impractical' to use CFD for unit process analysis involving multiple phases and physical, chemical, and biological processes.

The use of CFD to simulate physical, chemical, and/or biological processes in WWTP tanks where fluid flow characteristics are important has long been hampered by lack of availability and high cost of CFD software (including pre and post-processing), steep learning curves for their use, and limitations in computational power. Now that commercial and open-source software packages with a choice of turbulence models and graphical user interfaces for pre and post processing are available, however, researchers have been able to explore the CFD approach to investigate WWTP unit process performance. These initial results have so increased acceptance of CFD in helping elucidate the impact of the spatial variations in velocity profiles on process outcomes that it can now be used for the prediction of performance of unit processes beyond sedimentation. For example, the insertion of bio-kinetic models into CFD simulations of WWTP processes as well as their validation (e.g. Glover *et al.* 2006; Le Moullec *et al.* 2010a; Gresch *et al.* 2011; Sobremisana *et al.* 2011) provided significant and reliable insights into complex contaminant removal performance in these processes.

As more experience is gained in CFD-based process modelling, researchers and engineers will achieve a better understanding of where and when simpler models are adequate and be able to suggest potential improvements in the TIS models themselves. Indeed, from these insights, simpler representations of these mechanisms can now be developed and used in significantly less computationally intensive unit process models. For example, Alex *et al.* (2002) proposed a method for derivation of simple model structures based on CFD simulations. Also, Potier *et al.* (2005) showed the daily significant change of activated sludge reactor hydrodynamics with liquid flowrate, that is, τ the residence time (Figure 1).

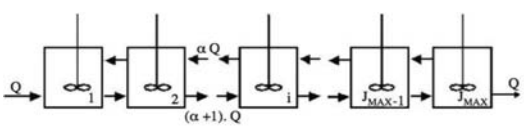
Potier *et al.* proposed a dynamic TIS model with backmixing which is able to simulate variations of the hydrodynamics (J_{app}, the apparent number of CSTR) with the flowrate by incorporating a maximal fixed number of CSTR (J_{max}) and a variable backflow rate (Figure 2). This model was developed from correlations with a large set of lab-scale and full-scale experimental data. In the future, similar approaches could be performed using CFD to determine the appropriate number of tanks in a TIS model depending on the influent dynamics. The issue of biokinetic-hydraulic feedback can also be incorporated (e.g., gas production, changes in fluid properties) through iterative analysis.



$$Pe = \frac{L^2}{\tau . D}$$

with $Pe = 2J$ (precise for $Pe>10$; approximation below)

Figure 1 | Potier *et al.* (2005) model. Change of activated sludge reactor hydrodynamics with the liquid flowrate (*Q*) and the residence time: $\tau = V/Q$; with: *J*, the number of TIS; *Pe*, the Peclet number; *D*, the axial dispersion coefficient.



$$\alpha = \frac{1}{2}\left[(J_{max} - 1) - \left(1 + J_{max}^2\left(1 - \frac{2}{J_{app}}\right)\right)^{1/2}\right]$$

Valid for $J_{app} > 2.5$

Figure 2 | Potier *et al.* (2005) model. Schematic representation and relation between the apparent number of TIS (J_{app}) and the back-mixing coefficient α.

The present paper describes a protocol for this alternative use of CFD modelling to gather more insight into unit process performance and improve conceptualization, calibration, and validation of simpler models. It focuses on how the CFD model can be used to derive next generation simple model structures after it has been built properly following Good Modelling Practice (Wicklein *et al.* in preparation).

PROTOCOL

To date, researchers and engineers may not be clear on the role CFD could potentially play in the field of wastewater treatment modelling particularly if the goal is to understand the interactions in a system of unit processes in a WWTP. It is often perceived as an overly complex modelling tool that uses too much computational time and is therefore not considered. In this contribution we want to share our views on how this simulation tool can be used in the train of thought of wastewater process modelling apart from the current usage as stand-alone tool for unit processes design and troubleshooting. In this way, it can significantly contribute to the further development of wastewater process models to its full extent.

Figure 3 presents a schematic visualization of a protocol for CFD use in improvement of WWTP process modelling. The protocol suggests that CFD be used as a supportive tool for wastewater process modelling rather than as a replacement for simpler modelling approaches, as is often the perception. Indeed, dynamic simulation of a whole WWTP with CFD is still not feasible; and furthermore, its use as a dynamic process model of an entire WWTP would not be cost effective. Hence, this is not what we intend to advocate, but in the meantime, CFD can still greatly serve the community.

The currently used 'simple' WWT models are located at one end of the model spectrum (Figure 3 – top), whereas the

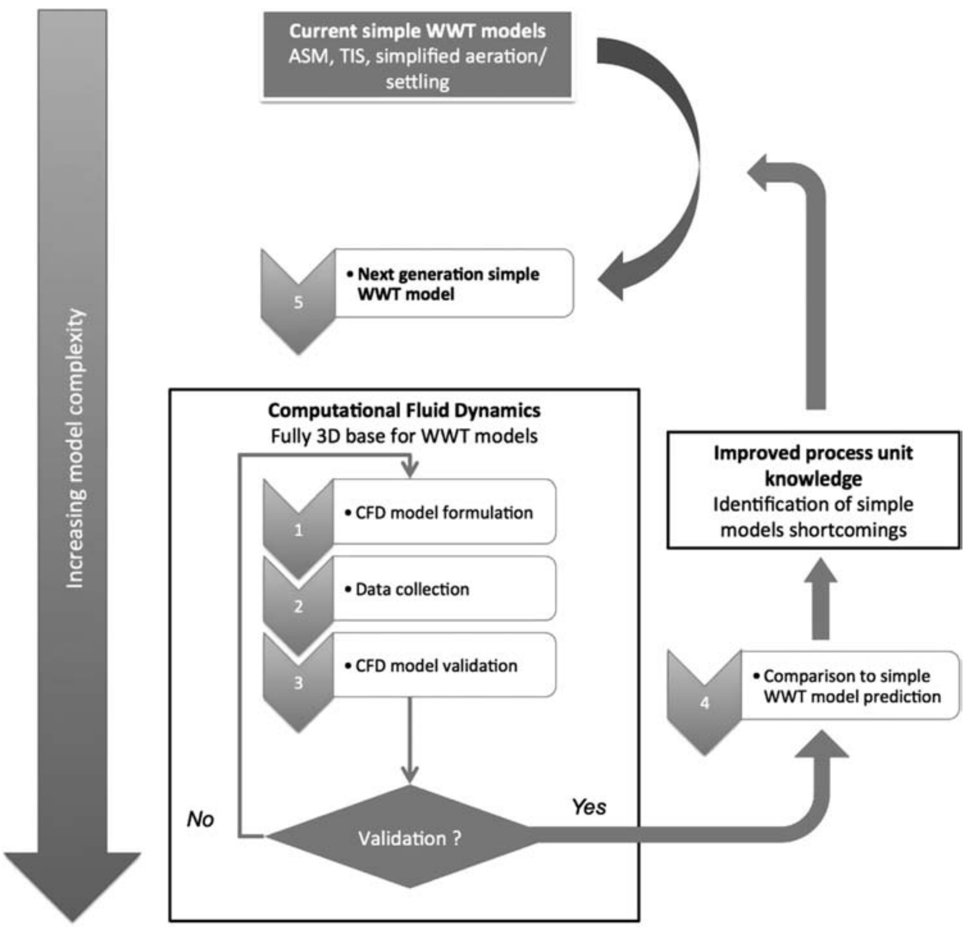


Figure 3 | Conceptual protocol for the potential use of CFD as a supportive tool for WWT process modelling.

complex CFD models are at the other end (Figure 3 – bottom). For certain model objectives, the former models are not adequate and slightly more complex models are required ('next generation simple WWT models'). In order to develop those, one needs improved process knowledge. It is especially in this respect that complex, validated CFD models can serve to provide needed data to help develop improved process mechanistic relationships used in 'next generation simple WWTP models'.

We see this as a 5-step protocol for use of CFD as a tool for improving/developing simpler models

1. CFD model formulation: Development of CFD models representing detailed features of the process tank geometry, as well as physical, chemical and biological components such as turbulence, a coupled ASM biokinetic model, a full-fledged detailed aeration model, viscosity models, density couples, temperature gradients, solids gradients due to settling, etc.
2. Data collection: Lab or field test of appropriate process variables (velocity profiles, species concentration profiles, gas hold-up measurement, residence time distribution [RTD], etc.) to validate results of the CFD model
3. CFD model validation: Compare the CFD model prediction with the data. If correlation and accuracy is insufficient, one should return to steps 1 and 2 and recheck model formulation and data quality/quantity.
4. Comparison to simpler model predictions: Detailed comparison to the results of simpler models for the same geometry and loading condition. Based on this, shortcomings can be pinpointed.
5. Improved simple model: These shortcomings lead the modeller in developing next generation models such as dynamic systemic models, compartmental, or other nonlinear macro-scale mixing models that better capture the phenomena needed to reach the modelling goal.

In the remainder of the paper we illustrate this train of thought through two examples available in the literature that are actually an onset to this protocol, but not originally described in that way.

CASE STUDY: MODELLING A PILOT-SCALE BIOREACTOR

The work in several papers of Le Moullec *et al.* (2008, 2010a, 2010b, 2011) is representative of what could be seen as the application of the protocol introduced above. While it was never presented in the form of a protocol, we feel that the approach is important in illustrating how this protocol could be implemented.

STEP 1: CFD model formulation

The unit process used for both experiments and modelling purposes was a bench scale channel reactor with a total length of 3.6 m with a rectangular cross section of width and height equal to 0.18 and 0.2 m, respectively. One side of the walls of the reactor was fitted with stainless-steel tubes in which 1 mm holes had been drilled every centimeter for air sparging. Further description is presented in Le Moullec *et al.* (2008).

Development of the CFD model utilizing an Euler–Euler approach is described in detail in Le Moullec *et al.* (2008). CFD simulations were carried out with the CFD software FLUENT. Two turbulence models were tested: a two-phase k-ϵ model and a Reynolds Stress Model (RSM). Boundary conditions were defined as presented in Table 1.

A second order discretization scheme (Quadrative Upwind Interpolation for Convective Kinematics) was selected for the momentum equations, turbulent dissipation rate, and void fraction equations. The Semi-Implicit Method for Pressure-Linked Equations (SIMPLE) pressure–velocity coupling scheme was also used.

STEP 2: data collection

Experiments were carried out to validate the CFD model. Two types of data were gathered. First, laser Doppler velocimetry (LDV) allowed the axial (Ux), lateral (Uy) and vertical

Table 1 | Boundary conditions used for CFD computations

	Inlet	Outlet	Top
Gas	Specified velocity inlet and phase fraction	/	Pressure outlet
Liquid	Specified velocity inlet and phase fraction	Specified velocity outlet and phase fraction	Symmetry boundary condition
Turbulence	Turbulence intensity (10%) and inlet hydraulic diameter	Turbulence intensity (10%) and outlet hydraulic diameter	Turbulence intensity (10%) and outlet hydraulic diameter

(Uz) time-averaged velocity fields to be measured (Le Moullec *et al.* 2008). Second, RTD data was obtained from multiple tracer experiments (Potier *et al.* 2005).

STEP 3: CFD model validation

Mesh sensitivity was examined using different hexahedral cell sizes of 1 cm^3 (130,000 cells), 0.125 cm^3 (1,000,000 cells), and 1 cm^3 with a refinement near the walls (350,000 cells). This last grid offered the best compromise between precision and computational effort.

The results of the CFD model concerning velocity field and RTD simulation (with both passive scalar and particle tracking methods) were compared with the experimental values. The two simulated velocity fields are compared to experimental data (Figure 4). Both models gave similar results and overall agreement was good. The observed discrepancies, respectively near the bubble injection position and near the free surface, were probably due to the simplification made for the gas inlet boundary conditions and the simplified representation of the surface, which was not planar in the experimental setup. In the RTD tests (Figure 5), the RSM turbulence model coupled with the particle tracking method produced a better fit to the experimental results than the k-ϵ model.

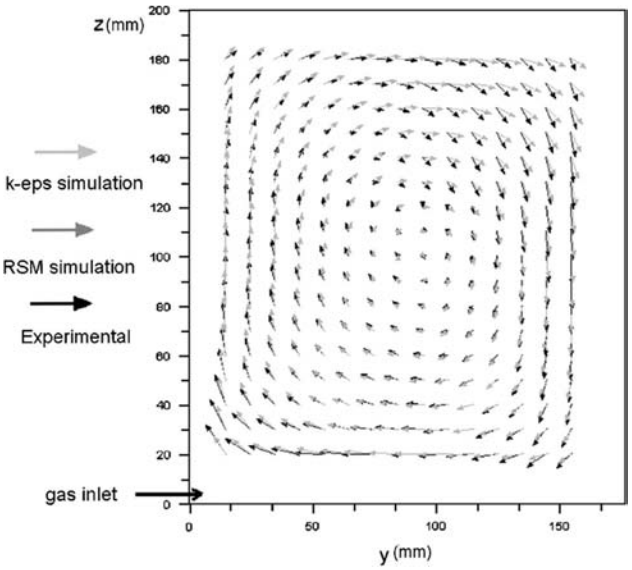


Figure 4 | Overall representation of the experimental and simulated average velocity fields on a vertical plane (*y*, *z*) for both turbulence models (source: Le Moullec *et al.* 2008).

STEP 4: comparison to simpler model predictions

TIS model was built from correlation between the number of TIS and both gas and liquid flowrates as well as reactor geometry. Potier *et al.* (2005) model was used for this purpose. Then, TIS and CFD hydrodynamic models were coupled with ASM1 biokinetic equations using standard parameters values to simulate biological reactions occurring in the pilot reactor. Comparison of both models prediction with experimental nitrate concentration profiles along reactor length is shown in Figure 6. Even if biokinetic parameters were not at all calibrated in this study, one can observe that the

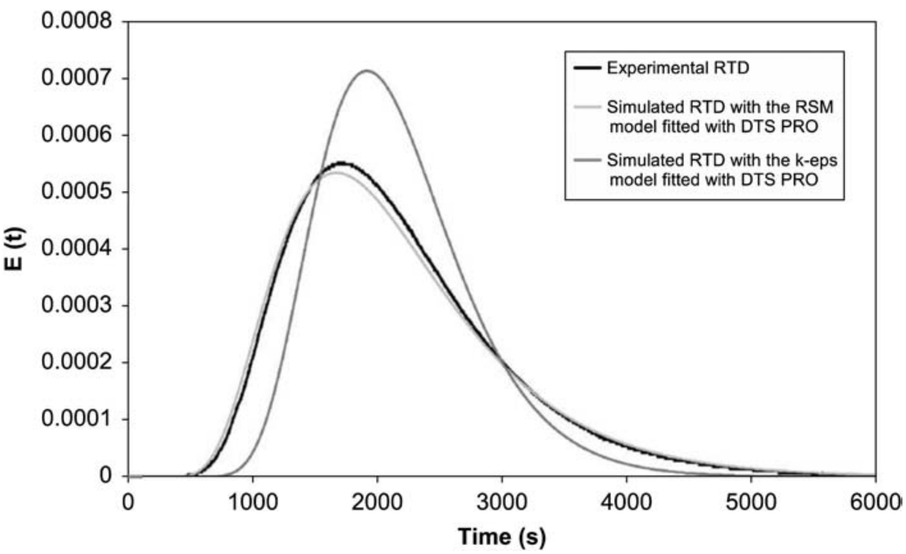


Figure 5 | Comparison between experimental and simulated RTD data obtained with the RSM and the k-ϵ turbulence models and the particle tracking method for a liquid flow rate of 3.6 L min^{-1} and a gas flow rate of 15 L min^{-1} (source: Le Moullec *et al.* 2008).

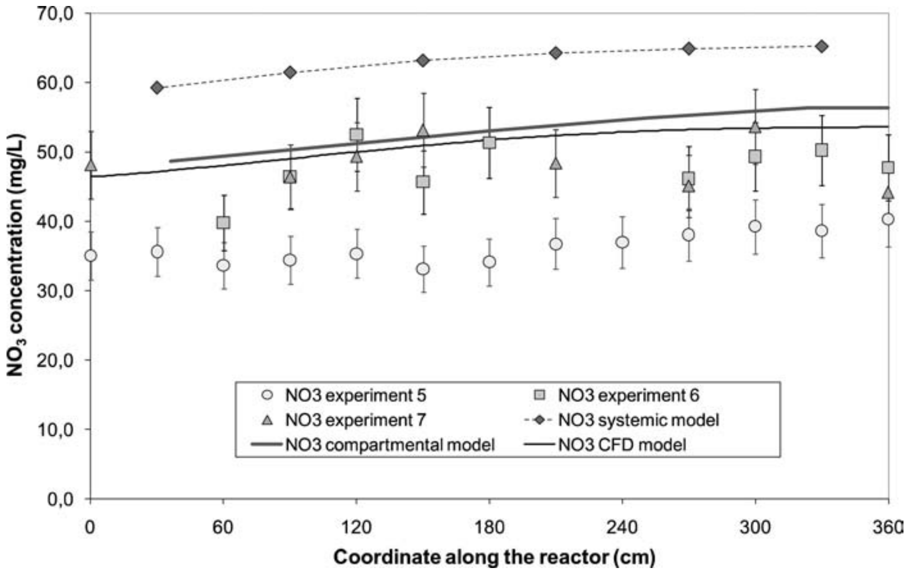


Figure 6 | Nitrate concentration profile along the reactor for two experiments carried out on the pilot-scale bioreactor (source: Le Moullec *et al*. 2011).

CFD model provided a better prediction than the TIS model, probably due to averaging of concentrations in the TIS model. Also, the CFD model describes the reactor in 3 dimensions, allowing the predictions of zones with low oxygen concentration, where denitrification could occur. The TIS model may not capture this. One should also keep in mind that default ASM1 parameter values used in this study were calibrated using TIS models.

STEP 5: improved simple model

In an effort to correct the shortcomings of the TIS model, a compartmental model (CM) was developed (Le Moullec *et al*. 2010a). This latter approach simulates the reactor as a network of spatially distributed functional compartments (Figure 7). Definition of this kind of model relies on the results of the steady-state CFD hydrodynamics model (STEPS 1–3). 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. Figure 5 shows that the fit of this somewhat more complex model is much better than the TIS approach and very close to the CFD-ASM1 model (STEP 4). This work (Le Moullec *et al*. 2011) demonstrated the possibility to accurately predict pollutant concentrations, not only with a detailed CFD-biokinetic model (STEP 4), 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. In the future, derivation of CM based on the combined CFD-biokinetic model results could also be investigated. This approach could give more insight in terms of processes and improve methodology of model derivation. However, it should be limited to research purposes due to its high computational cost.

OTHER APPLICATIONS OF THE PROTOCOL

The work of Alvarado *et al*. (2012) also illustrates what could be seen as the application of the protocol. In this work, the hydrodynamic modelling of a full-scale waste stabilization pond was considered. The methodology followed the different steps of the protocol

1. A 2D CFD model was used with a grid-size of 75,000 elements. A k-ϵ model was used to describe turbulence.
2. A tracer study using Rhodamine WT dye was conducted in order to assess the RTD. Bathymetry of the pond was also investigated.
3. CFD model validation by comparing experimental RTD with the simulated one obtained by coupling CFD model with a scalar transport equation.
4. Results were compared to a TIS model which failed to predict accurately both experimental and CFD RTDs.

5. The following methodology was proposed to build a CM of the pond: (1) determine different zones, (2) determine volumes of different zones, (3) determination of number of compartments per zone and (4) determination of convective and exchange fluxes in and between zones.

Figure 8 shows the comparison between simulated and experimental RTDs as well as the structure of the CM. The three models were coupled to ASM1 kinetics. The results were significantly different between TIS and CM which illustrates the importance of the hydrodynamic model when modelling biochemical processes.

COMPARISON OF THE COMPUTATIONAL REQUIREMENTS OF CFD AND SIMPLER MODELS

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 (Le Moullec *et al.* 2011). CM 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 behaviour of the complex system (Alvarado *et al.* 2012).

However, 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 (Potier *et al.* 2005).

PERSPECTIVES ON FUTURE APPLICATION

The examples illustrate the power of CFD as a supportive tool in developing improved 'next generation' WWTP models. Further application of this protocol may suggest conditions which exclude the necessity to build a new CFD model in certain cases as we gain knowledge on the behaviour of similar systems.

A logical next application for the protocol is in modelling the anaerobic digester process and more specifically, the mixing component of the process. Two-phase gas-liquid models have been performed of anaerobic digesters using CFD to help improve mixing performance. Yet, no CFD transport model of the anaerobic digester had been developed that captured both the biological processes and complete complex three phase fluid characteristics, until quite recently (Gaden 2013). This type of model is needed to completely understand

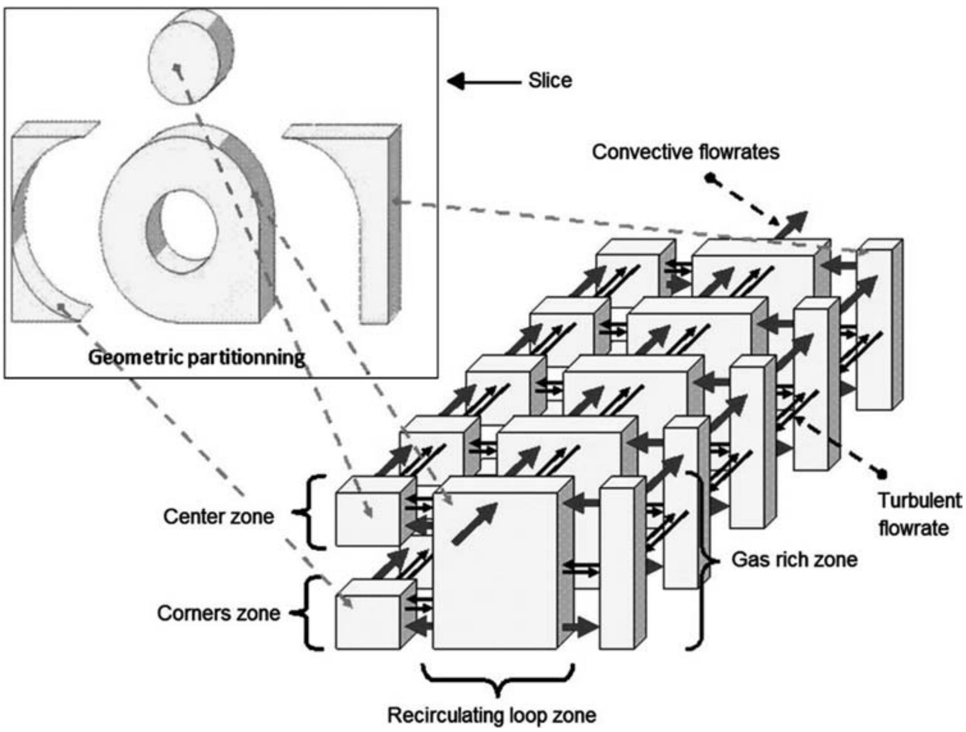


Figure 7 | Structure of the CM (source: Le Moullec *et al.* 2011).

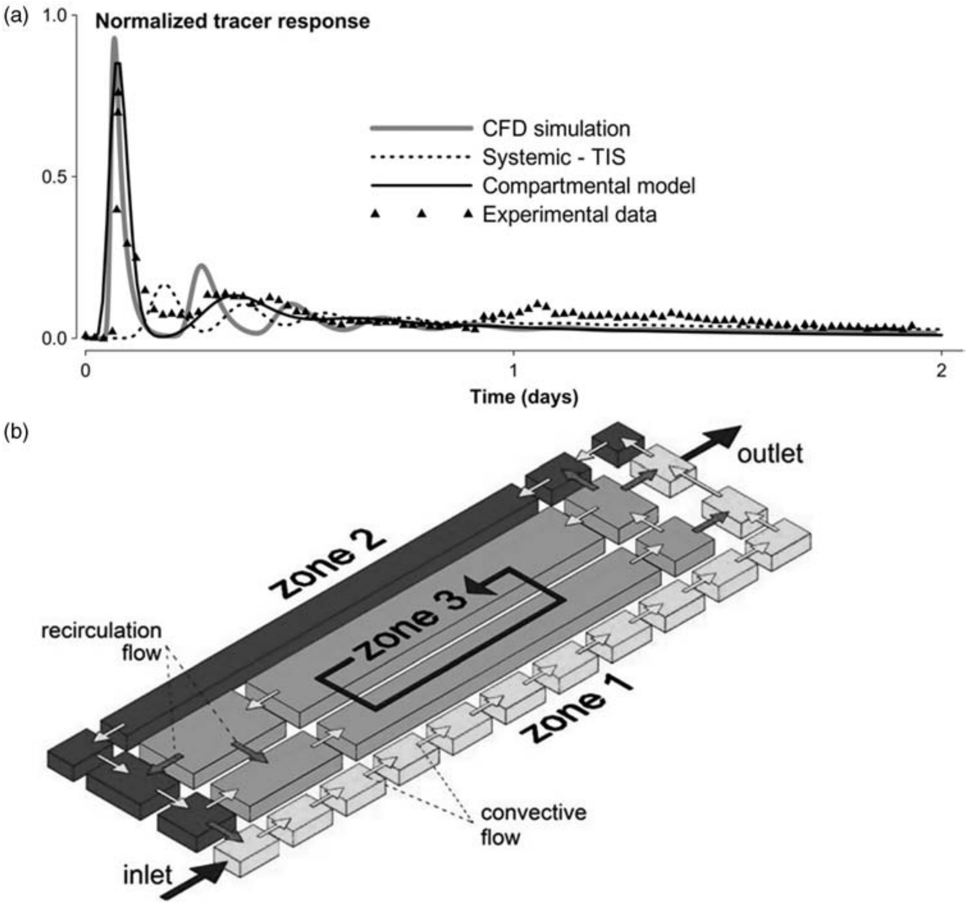


Figure 8 | (a) Comparison of RTD curves obtained in CM versus TIS and tracer experiment. (b) CM layout of the studied maturation pond. (source: Alvarado *et al*. 2012).

the impact of digester mixing systems and changes in digester influent characteristics on biogas production, or to assess the potential upgrades of digester capacity. TIS modelling is widely used to simulate tracer testing (Batstone *et al.* 2005), which may include feedback and bypass links. These multi-parameter TIS models could be validated using CFD to implement improved biokinetics for an assessment of how the hydraulic regime influences process stability. There is every reason to believe that this approach will also prove fruitful for the evaluation of suspended growth treatment tanks.

One question that remains is when exactly one considers the CFD model to be sufficiently validated. What deviations are acceptable? Tools for evaluating this question need to be developed. Where the validation is determined to be inadequate, one needs to reiterate protocol STEPS 1 and 2. With regard to model formulation, recent work on process tank mixing (Samstag *et al.* 2012) has suggested an explanation for past failures to adequately size mixing devices resulting from ignoring density effects in the CFD analysis. In the future, this approach should be incorporated where appropriate into CFD models and will, hence, be included in the evaluation of simpler models.

Another major challenge that exists in biologically-driven wastewater unit processes is due to the complex intersection between potential macro- and micro-scale reactions that occur outside and inside biological floc particles. These two-scale processes can be difficult to model and computationally expensive. Yet, the lack of modelling these two-scale processes can reduce the effectiveness of CFD in simulating specific phenomena in activated sludge systems such as the occurrence of simultaneous nitrification-denitrification processes. Next to these examples, several other submodels can be added to transport based CFD models for further validation and improved process knowledge. This further knowledge development runs in parallel with the application of already gathered knowledge to build the next generation of improved system of unit process models.

CONCLUSION

Direct use of CFD approaches that allow substantial expansion to include complex biokinetics or other behaviour is currently challenging for practical use due to computing and numerical issues. However, 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. A 5-step protocol was outlined describing how this can be done and was illustrated using two examples from the literature. This shows the power of this approach and how it can lead to more reliable everyday models. Further perspectives were given as well as how current CFD model development fits into this train of thought.

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Q1 Please provide all the authors name in Batstone et al. (2002).

Q2 Please provide all the authors name in Henze et al. (2000).

Q3 Levenspiel (1972) is not cited in the text. Please cite else delete from the list.