To Mix, or Not to Mix, That Is the Question

Chapter · May 2017

DOI: 10.1007/978-3-319-58421-8_106

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To mix, or not to mix, that is the question

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Mixing; Computational Fluid Dynamics; Compartmental modelling; reactor design

Summary

The use of Computational Fluid Dynamics (CFD) in the wastewater field has long been limited to troubleshooting of design flaws. Research-wise, this has recently opened up to the potential usage of CFD in the reactor design phase. Another noticeable shift is the one from only considering plain hydrodynamics to the coupling to kinetic models and population balance models (PBM). This vastly assists in design optimisation problems that are either driven by kinetics or physical processes such as flocculation or crystallisation which lead to different optimal solutions as the goal is quite different. This contribution provides some examples of the above and discusses how the know-how should be used to develop new design methods, hereby questioning how ideal mixing should be defined.

Introduction

Computational fluid dynamics (CFD) has become an accepted method for process analysis of fluid flows in many industries. It recently has become widely used for analysis of hydraulic problems in water and wastewater treatment (WWT) but still needs to find wider acceptance for analysis of physical, chemical and biological processes in WWT. There are substantial financial and risk drivers to conduct CFD for better wastewater design (Wicklein et al., 2016).

Recently, a working group was formed under the wings of the IWA Specialist Group “Modelling and Integrated Assessment” (MIA) that brings together the community active in this field. Laurent et al. (2014) described an alternative way of using CFD as a supplement to using simpler models, whereas Wicklein et al. (2016) focused on good modelling practice for CFD modelling of WWT and Samstag et al. (2016) provided an overview of CFD applications in the unit process of a wastewater treatment train. Nowhere (except possibly disinfection) is CFD used in a widespread or routine way as a design or risk-management tool. This offers clear opportunities to further develop the value of CFD in wastewater process evaluation.

This contribution provides some examples of (novel) ways of using CFD and its outcomes to benefit the wastewater sector.

Materials and Methods

Plain CFD examples solve the Navier-Stokes equations either in one or two phase. Mostly, turbulent conditions prevail and a set of turbulence equations are solved alongside.

When coupling to kinetics is required, scalar equations are defined for all species present in the kinetic model. Dissolved species follow the fluid flow and get additional source and sink terms according to the reactions they take part in. These terms can easily be derived from the Gujer matrix of an ASM model. Technically, they are implemented by means of user defined functions (UDF) when the commercial tool Fluent (Ansys) is used.

Results and Discussions

This section is structured as follows: first, a couple of example studies on mixing behaviour of bioreactors are shown, after which a general discussion is provided as to how CFD can aid in cost savings and more cost-effective reactor design.

A fully integrated CFD-kinetic model was developed for the outer ring (partly oxic and partly anoxic) of a concentric plant design (Eindhoven Water and Resource Recovery Plant (WRRF)) as shown in Fig. 1 (Rehman, 2016). It was found that significant deviations from complete mixed conditions prevailed due to the specific design (circular) and placement of inlets, outlets, propellers and recirculation flows. A key issue related to the circular design is the fact that the mixed liquor that is internally recycled is pushed to the outer wall when it hits the wall of air bubbles in the bottom aerated zones. This pushes the air plume to the inner wall and results in a significant heterogeneity of species concentrations and, hence, the local activity of micro-organisms. The heterogeneity can be quantified by introducing cumulative species distributions (CSD) (Fig. 2) which can further be adopted to develop a compartmental model that can be used instead of a tanks-in-series (TIS) approach (Fig. 3). The latter should reduce uncertainty in the mixing model and, hence, unnecessary calibration efforts. Furthermore, this analysis has clearly shown that the design can be improved. In a follow-up study, the obtained knowledge can now be used to test virtual scenarios that cure the major downsides of this process behaviour.

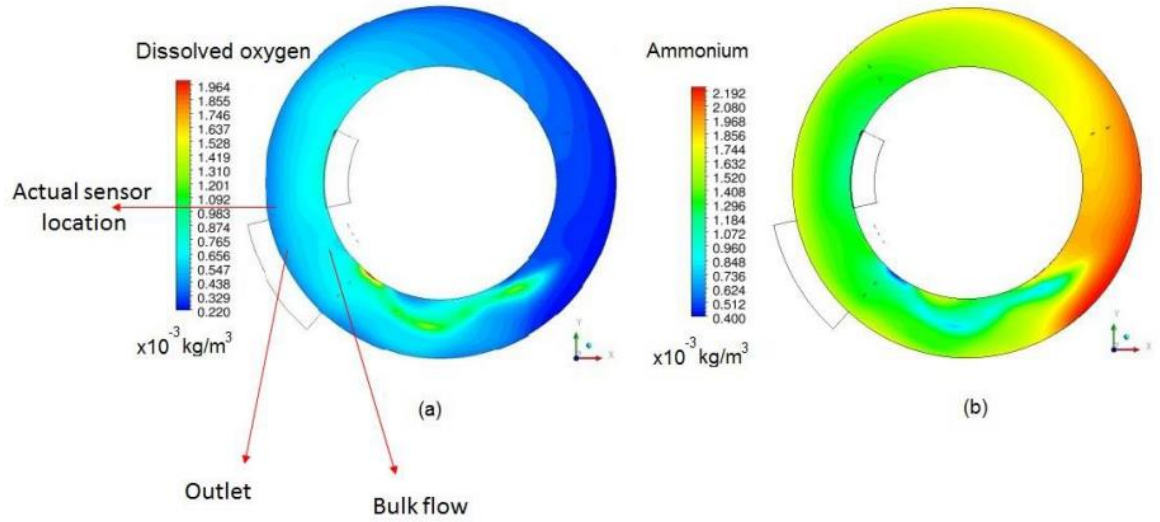

Figure 1 Dissolved oxygen (a) and ammonium (b) concentrations at 3.45m depth in the outer ring of the Eindhoven WRRF

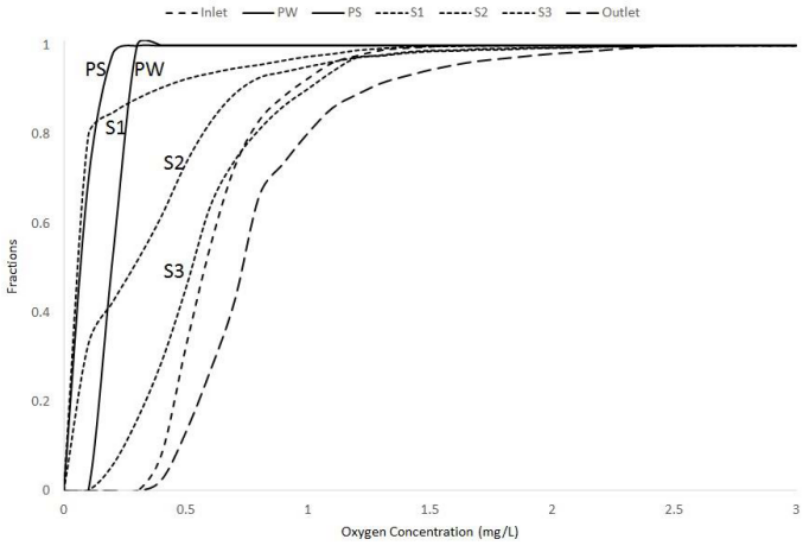

Figure 2 Cumulative species distributions of dissolved oxygen at different locations in the outer ring of the Eindhoven WRRF. Steep curves reveal less heterogeneity and vice versa

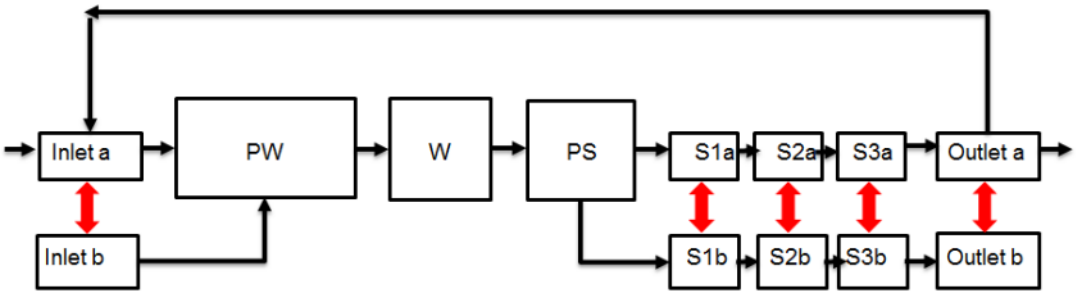

Figure 3 Compartmental model of the outer ring of the Eindhoven WRRF

There are many other examples where the behaviour of a system cannot be described by a systemic model combined with a kinetic model. Some designs seem to behave better than expected, whereas others are underperforming. Kimura et al. (2008) found better performance behaviour of a baffled membrane bioreactor (BMBR) that could not be explained by a CSTR combined with an activated sludge (ASM) model. The unexpected appearance of bio-P removal in systems not designed for it is another example (Barnard et al. 2012; Verrecht et al. 2010). However, ~~little~~ few authors link this to the specific mixing behaviour in a reactor and try to explain it through other complex theories or calibrating kinetics. Surface aerated oxidation ditch plants are yet another example of this as demonstrated by Rehman (2016). Recently, a lot of attention is going to the mixing behaviour of anaerobic digesters which is pretty much still a black box at full-scale mainly due to the difficulty to measure inside the system. Given the elevated viscosity and the typical limited amount of energy input for mixing, it cannot be expected to behave as completely mixed. Gas bubble production will only locally contribute to mixing, but not to a large extent. But it might as well be that this way of operation (i.e. not complete mix) is the key to make the process work. However, it becomes cumbersome to optimise the process without understanding the specifics as to why this is the case. In a sense it seems that reactor

design in general is pretty much either business as usual (based on rules of thumb) or trial and error. Time has come to introduce model-based design. It is noteworthy that this in now common practice in e.g. chemical engineering where reactor design is a very hot topic at the moment.

Even at a small scale one can demonstrate that complete mixing can be problematic. Fig. 4 shows a CFD-ASM simulation of unaerated 2L continuous flow-through respirometer at different flow rates. As can be seen, a high flow rate is needed to achieve almost complete mixed conditions. Compared to an ASM-CSTR model, affinity indices had to be recalibrated significantly. This emphasises that operating reactors under complete mixed conditions is something we might not want to pursue as this will come at a significant cost. It might be wiser to understand the consequences of incomplete mixing and turn this into a benefit of the system operation.

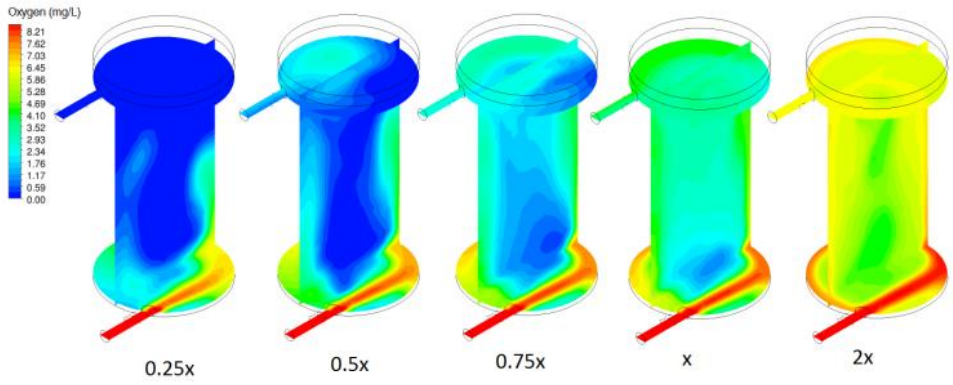

Figure 4 Distribution of dissolved oxygen concentration in an unaerated continuous flow-through respiromter.

Thus far focus was on process kinetics. However, all the above also holds for physical process behaviour. Let us take the example of shear-induced coagulation or flocculation. Here, often the assumption of an average shear (G) is adopted in reactor design. However, pursuing this behaviour is similar to pursuing complete mix in terms of concentrations. It will be very costly to achieve and the question is whether it is really needed. Coagulation systems are actually designed as merely scaled up jar tests by means of some rules of thumb based on energy input. However, the energy dissipation will be different on different scales and one actually needs to think again in terms of distributions. Similar to the CSD discussed before, reactors will exhibit a shear distribution. Depending on the location of a floc or granule it will either be exposed to low shear or high shear. The former will promote flocculation, whereas the latter will promote breakage (depending on floc strength). Obviously, the pattern at which a floc is exposed to different shear environments will be of key importance. This pattern is entirely governed by the mixing pattern and, hence, location of inlet, outlet, inlet flow rate and position and speed of stirring devices. Hence, when scaling up, one should try to achieve a similar shear distribution and recirculation pattern in the reactor. The latter is, however, not straightforward. Again, many studies try to understand why a certain system is not behaving similar as their small scale counterparts. The issue is the scale-up rules that are not accounting for the important aspects of mixing. Also here, model-based design based on CFD models coupled with flocculation models is the way to go. Another observable trend is the scale-down of such processes (e.g. tube flocculators) which makes sense as they have a much better controllability. Hence, it might be smarter to

design smaller reactors and use numbering-up instead of scaling up. Again, in chemical engineering this is an observable trend in order to enhance reactor performance.

A system that actually combines both impact of kinetics and a physical precipitation process is crystallisation. Indeed, local concentrations are important with respect to supersaturation to promote crystal growth. On the other hand, shear levels promote aggregation and breakage phenomena which drive the crystal size distribution. The latter is important when thinking in a Quality-by-Design (QbD) fashion with respect to reuse of the product. Current reactor designs are definitely not optimal in this respect. Tarrago et al. (2016) demonstrated that the CSD could be altered by simply changing the upflow velocity in struvite crystalliser. However, building knowledge is still required to improve the design in a targeted way. Hence, this is another field where advanced CFD modelling can lead to a large leap in process understanding and optimisation.

Discussion

It is clear from the above that mixing behaviour of bioreactors is vastly overlooked and needs more attention. This is important in terms of troubleshooting, which is the classical application of CFD in the wastewater field nowadays. However, the know-how that is built should also be adopted in model-based design. We need to build in the performance of a reactor in its design. We should leave the “era of averaging” as we have the tools at hand to do a much better job in engineering reactors.

When using models for reactor design, there are two new research problems that arise: (1) which method should we use and (2) how do we define optimal mixing.

The former is actually not so straightforward. One would immediately have the reflex of using CFD for this purpose. However, there are a myriad of different design subtleties that one can think of and, hence, the degrees of freedom are enormous. Given the vast computational load of CFD, especially when combined with kinetic and physical models, it is likely not the way to go, at least not in the decades to come. An alternative is to further develop the powerful concept of compartmental models as they are more computationally tractable and, hence, allow to simulate many more scenarios. A strategy could be to use CMs for optimisation and then link this optimal behaviour to reactor design. Obviously, this is a process that will take time. But is for sure the most promising route at this point.

The latter is another interesting point of discussion. Currently, ideal mixing patterns are either CSTR or plug flow. However, mostly we are somewhere in between. But that does not mean that these conditions cannot be “ideal” or optimal. We should probably adapt our terminology here and connect optimal mixing behaviour to the goal of the system. Optimal mixing can then be very different for different technologies. Striving for complete mixing is most likely not even what is required in many cases. We should use advanced models combining CFD, kinetics and physical processes to pinpoint what degree of mixing is optimal for a certain process and design reactors accordingly.

Finally, a question that often arises: Do all reactor operational and design optimisation projects need a CFD study? Well, at first it will be required for a certain amount of cases in order to build up knowledge. However, once sufficient know-how has been acquired, it can be turned into new and better design rules, not requiring a separate CFD study for every case.

Conclusions

This contribution clearly indicates that there is much more beyond the traditional way of using CFD for troubleshooting design flaws in wastewater treatment systems. When used in a smart way, it can lead to significant cost savings for existing plants and a higher level of cost-effectiveness for plants to be designed, hereby justifying the minor cost of a CFD modelling study in the overall project cost. The methodologies shown are generic and can be extended to different unit processes.

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