Water Quality Research Journal of Canada | 50.1 | 2015

Editorial

It is no secret that the global freshwater bodies are under large pressure in terms of quality. The main pollution contributors are, among others, water resource recovery facilities (WRRFs) and combined sewer overflows. WRRFs play an important role in urban water management and, hence, good knowledge of their behavior is required. Mathematical models have been excellent tools to elucidate and summarize this knowledge. Traditionally, models have been restricted to macroscale process behavior. However, we have now come to a point where computational power allows investigating the process at meso- and even microscale, depending on the objective. This allows us to: (1) increase system understanding, and (2) optimize the design and operation. The specific modeling tool that has matured to the level where these studies at smaller scale have become possible is called computational fluid dynamics.

This modeling framework has been used for many years in other fields such as aeronautics and more recently chemical and environmental engineering. The time has come to start exploiting this exciting tool which has also attracted attention within the International Water Association through its Working Group on Computational Fluid Dynamics under the umbrella of the Specialist Group on Modeling and Integrated Assessment. The working group wants to provide guidance on good modeling practice for usage of CFD models, but also to compile successful case studies where CFD has led to improved system design and operation. In the latter, all unit processes present in the most general train of a WRRF, including disinfection, are included.

CFD can serve different purposes. In the past, it was mainly used as a tool for troubleshooting, and it was restricted to usage of the plain Navier-Stokes equations in conjunction with a turbulence model. In WRRF applications, significant efforts then followed in secondary settler modeling in an attempt to understand the functioning of settlers, as they are often the limiting factor of a conventional WRRF. For this purpose a solids transport equation needs to be solved simultaneously. Nowadays, the spectrum of CFD models has further evolved and more ingredients are added, such as species transport leading to reactive flows when biokinetic models are incorporated. Also, light transmittance has been incorporated in disinfection and lagoon models, for instance. Validation remains challenging as now, next to computational demand, the availability of sensors becomes limiting, especially given the required spatial resolution. Validated CFD models lead to process knowledge and the models can be used to improve reactor design and operation. Another use can be that the knowledge is translated into the next generation simplified models, or metamodels, which have the potential of being more accurate and thus better tools for system optimization.

Software codes are available both from commercial vendors as well as from open source communities, where the latter is really gaining ground quickly.

In this special issue, we have grouped a number of papers describing successful case studies and research developments of CFD in the water and wastewater field. The bulk of the papers deals with disinfection and advanced oxidation, as a lot of activity is ongoing in this field. The remaining two papers deal with flow splitting and the impact of a jet stream in a bioreactor.

The paper by Ducoste & Alpert (2015) deals with UV-H_2O_2 advanced oxidation. The authors combine CFD with detailed kinetics of the advanced oxidation process and compare a CFD model with a model of plain ODEs not accounting for detailed flow and heterogeneity potentially arising from that. Moreover, next to the Eulerian approach they also tested a Langrangian approach. They found both approaches to agree. The authors also attempted to validate the model during which they found that the liquid matrix and operating conditions are important factors. The CFD model was further used for improved reactor design.

Duran *et al.* (2015) studied ultraviolet (UV)-initiated advanced oxidation processes driven by an immobilized photocatalyst. The reactor was modeled using CFD which allowed for the integration of fluid flow, species transport, chemical reaction kinetics and fluence rate distribution. Furthermore, different turbulence models (laminar, AKN and RSM) were compared. Experimental validation was

doi: 10.2166/wqrjc.2014.101

performed confirming the ability of the integrated CFD model to predict photoreactor performance under different regimes. Finally, new reactor configurations were tested for design optimization, yielding a 50% performance increase. This illustrates that still major process improvements can be achieved by proper analysis.

Crapulli *et al.* (2015) constructed a CFD model to investigate the inaccuracy introduced by mixing-limited devices in accurately quantifying microbial inactivation kinetics for nearly opaque UV transmittance fluids. A Taylor-Couette flow device was adopted and experiments using both passive and reactive tracer were executed to validate the model. The process behavior was further studied by means of sensitivity analysis in which the impact of absorption coefficients and inactivation rates was quantified.

Fernandes *et al.* (2015) used CFD modeling to study a process that is an important pretreatment step for efficient disinfection, i.e. the breakup of particles. Indeed, reduction in particle size distribution improves the disinfection process. Particle breakup is usually governed by shear, which is yet another predicted variable by a CFD model predicting the velocity field. Indeed, shear rates or strain rates are actually velocity gradients. In their model, particles were prone to breakup when the strain rate exceeds a critical value predicted by CFD. Experimental validation was performed and the model was found in line with observations. Subsequently, different orifice systems were tested to optimize their design depending on whether weak or strong particles are to be treated.

Saha *et al.* (2015) studied the UV disinfection of microbial cells by tracking them individually, hereby applying a Langrangian particle tracking method. Since it concerned an open channel flow, the water-liquid interface was modeled explicitly using the volume of fluid method. Experimental data validation was performed and the model was subsequently used for scenario and sensitivity analysis to study the impact of several system parameters.

Knatz *et al.* (2015) tackle an important issue in many plants that include parallel lanes and where an incoming flow has to be split. Often, the flow is not at all distributed evenly leading to lanes that are overloaded and others that are underloaded. In this particular paper, the flow inlet distribution to a dissolved air flotation plant is studied. A CFD model was used to optimize the design of the inlet works which led to a reduction of imperfect distribution from a relative difference above 60% between the loads of the different lanes to a relative difference lower than 10%. An important outcome of this study is that the proposed improved design was effectively implemented and the model predictions were confirmed after construction.

A final paper by Karpinska *et al.* (2015) studies hydrojets in WRRFs. In this modeling exercise, the turbulent flow behavior is of importance. Different turbulence models (RANS, URANS and LES) were tested which is tedious and time consuming due to the massive computational load, in particular when using large Eddy simulation techniques. The translation of the acquired knowledge to the macromixing in a simple ASM model is discussed.

From the brief overview of these papers, one can already observe the versatility and the huge potential of CFD models for the WRRF community. One should no longer perceive these models as overly complex, computationally inefficient and only needed for troubleshooting. Successful case studies are contributing to the increased acceptance of CFD models and their advancement of the field. The only warning that is still to be put out is that the use of CFD requires: (1) skilled people to operate them, and (2) thorough model verification and validation. Any model, even a CFD model, always remains a simplification of reality!

We hope this editorial had triggered your interest to read all the papers in detail and see the merit of CFD for yourself. Enjoy the CFD journey!

Guest Editors

Ingmar Nopens
BIOMATH – Ghent University,
Belgium

Domenico Santoro
Trojan Technologies,
ON, Canada

Charles N. Haas
Drexel University,
PA, USA

Peter Vanrolleghem
modelEAU – Université Laval,
QC, Canada

REFERENCES

Crapulli, F., Santoro, D., Sasges, M. R., Ray, S., Mahmoud, H. & Ray, A. K. 2015 Quantifying ultraviolet inactivation kinetics in nearly opaque fluids. *Water Quality Research Journal of Canada* **50** (1), 34–46.

Ducoste, J. J. & Alpert, S. M. 2015 Computational fluid dynamics modeling alternatives for UV-initiated advanced oxidation processes. *Water Quality Research Journal of Canada* **50** (1), 4–20.

Duran, J. E., Mohseni, M. & Taghipour, F. 2015 Computational modeling of UV photocatalytic reactors: model development, evaluation, and application. *Water Quality Research Journal of Canada* **50** (1), 21–33.

Fernandes, A., Lawryshyn, Y., Gibson, J. & Farnood, R. 2015 Experimental and numerical investigation of the breakage of wastewater flocs in orifice flow. *Water Quality Research Journal of Canada* **50** (1), 47–57.

Karpinska, A. M., Dias, M. M., Boaventura, R. A. & Santos, R. J. 2015 Modeling of the hydrodynamics and energy expenditure of oxidation ditch aerated with hydrojets using CFD codes. *Water Quality Research Journal of Canada* **50** (1), 83–94.

Knatz, C., Rafferty, S. & Delescinskis, A. 2015 Optimization of water treatment plant flow distribution with CFD modeling of an influent channel. *Water Quality Research Journal of Canada* **50** (1), 72–82.

Saha, R. K., Ray, M. & Zhang, C. 2015 Computational fluid dynamics simulation and parametric study of an open channel ultra-violet wastewater disinfection reactor. *Water Quality Research Journal of Canada* **50** (1), 58–71.