CFD for wastewater treatment: an overview

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ABSTRACT

Computational fluid dynamics (CFD) is a rapid emerging field in wastewater treatment (WWT), with application to almost all unit processes. This paper provides an overview of CFD applied to a wide range of unit processes in water and WWT from hydraulic elements like flow splitting to physical, chemical and biological processes like suspended growth nutrient removal and anaerobic digestion. The paper's focus is on articulating the state of practice and research and development needs. The level of CFD's capability varies between different process units, with a high frequency of application in the areas of final sedimentation, activated sludge basin modelling and disinfection, and greater needs in primary sedimentation and anaerobic digestion. While approaches are comprehensive, generally capable of incorporating non-Newtonian fluids, multiphase systems and biokinetics, they are not broad, and further work should be done to address the diversity of process designs. Many units have not been addressed to date. Further needs are identified throughout, but common requirements include improved particle aggregation and breakup (flocculation), and improved coupling of biology and hydraulics.

Key words | biokinetics, computational fluid dynamics, digestion, flow splitting, modelling, sedimentation

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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 2016). However, guidelines are limited and there are very few academic groups which focus on education or research

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into CFD in the wastewater sector. As such, a working group within the IWA Specialist Group Modelling and Integrated Assessment (MIA) was formed with the goal to encourage such a community to form. Laurent *et al.* (2014) described an alternative way of using CFD as a supplement to using simpler models. Wicklein *et al.* (2016) focuses on good modelling practice for CFD modelling of WWT. However, there is also lacking an analysis of unit operations, including historic analysis of work focusing on development of specific unit process approaches. The purpose of the current paper is to provide a review of the state of the art of applying CFD to analyze water and WWT plants, and to provide a critical assessment of future research needs.

The current paper is organized around plant unit processes where CFD has been used and which are particularly promising for future application. While many of the techniques apply to both clean water and WWT processes, the primary focus of the paper is on applications of CFD to analyzse WWT and specifically to water resource recovery facilities (WRRF). The basic principles and function of unit operations are covered in well-known reference texts (Tchobanoglous *et al.* 2003). We limit our consideration to general methods solving for computational domains in either two or three dimensions (2D or 3D).

WHAT IS CFD?

CFD provides a solution to the momentum and continuity equations for fluid mechanics. Numerical schemes for solution of these equations are necessary because these partial differential equations typically have no analytical solution, and hence the fluid domain is generally discretised in a grid or mesh scheme. Formulation of these equations in one dimension generally requires an assumption of homogeneity or symmetry in the other two dimensions, incompatible with geometry, such that CFD problems are almost always multidimensional (2 or 3D) or compartmentalised using a static approximation (Alvarado *et al.* 2012). CFD has been used for analysis of scientific problems and industrial processes since at least the 1940s. Presentation of the fundamentals of CFD theory is beyond the scope of this paper. For a detailed review of the techniques of CFD, refer to standard books on the subject, for example, Roach (1982), Patankar (1980), Fletcher (1991a, 1991b) and Ferziger & Peric (2002). A good introduction to the basic equations of CFD for application to activated sludge processes is included in Karpinska & Bridgeman (2016).

APPLICATION OF CFD TO WATER AND WWT

We discuss application of CFD to processes and problem areas specific to WWT. We proceed through the normal flow stream in a WRRF, but begin with hydraulic elements that are found in almost all WWT facilities, flow splitting and other hydraulic transport facilities.

Flow splitting and evaluation of head losses

Flow splitting is a critical unit operation that enables balanced flow to multiple units across a range of flows. They are generally based on flow over a static weir, and hence hydraulics are fundamental to their function. CFD has been used relatively extensively in engineering practice for analysis of flow splitting between process units and for estimation of complex head losses in hydraulic profiles. Not a great deal of this practical work has been reported in the literature, however. Figure 1 presents a visualization of a 3D CFD flow splitter simulation developed at a recent workshop sponsored by the CFD working group, Marques (2015a).

Hassan *et al.* (2014) present results from CFD analysis on a tapered longitudinal manifold and a uniform longitudinal manifold. Two manifold configurations were tested at different inlet flows, and results suggested that the tapered manifold provided relatively equal flow distribution compared with the uniform longitudinal manifold. Knatz (2005) indicated that the influent direction relative to the channel may impact the results.

Tong *et al.* (2009) used CFD to investigate balancing the flow through a wide range of manifold geometries. Results

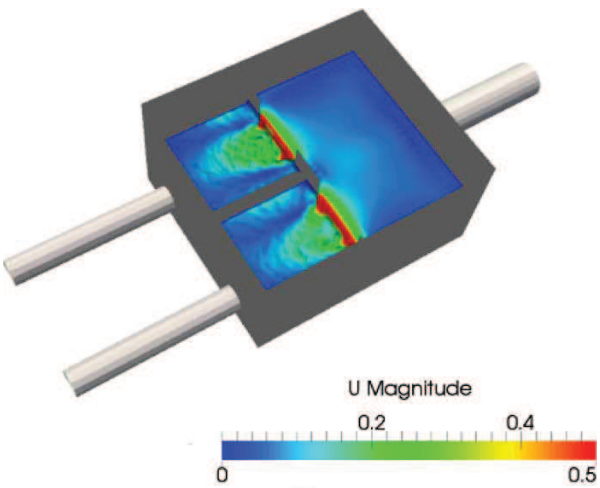

Figure 1 | Surface velocity profile for a flow splitter from open source CFD software (Source: Marques 2015a).

showed that optimal flow uniformity could be achieved by expansion of the cross-sectional area, linear or non-linear tapering of the distribution manifold or varying the cross-sectional area of the outflow channels modifications.

Research needs

Research work has focused on general flow distribution, as fluid flow manifolds are ubiquitous in engineering practice, from fuel cells to chemical reactors. However, there is very little peer-reviewed research that is specific to flow splitting in water and WWT processes. A key limitation that has not been addressed in the literature is the potential impact of solid and gas phases. Solids may impact splitters by differential movement of particulates within the splitter, which may increase viscosity or density and hence induce differential flow (see relevant section in this paper). The gas phase, particularly in aeration, can have a strong impact on fluid density and momentum (where momentum is imparted from an aerator, for example). This is critically important where a splitter has a particularly turbulent inlet cell, or where splitters are used to distribute flows from an aerobic unit to multiple clarifiers, particularly where centrifugal or laterally directed aeration is used.

Grit removal

Grit chambers use gravity or centrifugal sedimentation to separate large, dense particles from raw wastewater. While the principles are relatively simple, the multiphase nature, and multiple mechanisms can make analysis complex. Analytical evaluation of grit removal goes back to the work of Camp (1942) who developed a rational approach for sizing of grit removal channels based on ideal settling behaviour. Much of current practice, however, relies on manufacturer's recommendations without an analytical basis. CFD provides an alternative to reliance on manufacturer's claims, particularly where the hydraulic configuration mixes gravity and centrifugal sedimentation, such as in a vortex separator.

McNamara *et al.* (2012) present a comprehensive evaluation of three different types of grit removal tank geometries: forced vortex, detritor and lamella. Grit particles of nine different diameters were converted to a continuous distribution equation and modelled with specific gravities of 2.65 based on silica sand and 1.5 based on lab samples from field installations and a sphericity ratio of 0.65. Multiphase (water and air) simulations were carried out to steady state prior to injection of grit particles into the inlet stream.

Research needs

Recent work on grit removal has included many desirable elements of good CFD analysis: efforts at calibration or verification, 3D approach and multi-phase analysis. The best work appears to have included analysis of solids transport and discrete settling. It is not so clear that underflow concentrations have been monitored, however. It has generally been assumed that grit settlement is not density-coupled. A particular opportunity is the use of approaches from other unit operations such as population balances (Nopens *et al.* 2002; Nopens 2005) to describe performance under dynamic conditions. While sedimentation in the primary unit is generally unhindered, there may also be links to other sedimentation approaches in primary and secondary units, particularly hindered settling in solids collection zones.

Primary sedimentation

Primary sedimentation exhibits flocculation, discrete, hindered, and compression settling of near neutral buoyancy colloidal mineral and organic particulates. Process performance is highly influenced by flow, including those influenced by multiphase solid-liquid interactions in sludge blankets. These factors make it a clear target for the application of CFD. As such, primary sedimentation was one of the first unit processes to receive attention from CFD researchers.

A number of analytical approximations have been taken to simplify multidimensional clarifier geometries into a single dimensional finite difference problem, mainly by imposing radial homogeneity or symmetry. Takamatsu *et al.* (1974) applied radial symmetry and a floor boundary condition, together with discretisation in the vertical dimension to identify the optimal depth of a clarifier. The boundary condition for the bottom (sludge) boundary identified in this work has been widely used.

One of the first multi-dimensional numerical models of primary sedimentation was introduced by Imam *et al.* (1983). The model was used a finite difference discretization of the governing equations to simulate the settling of several classes of solids in the flow domain. Results were compared to several different theoretical estimates by Camp (1946) and showed a more realistic lower rate of removal. The work assumed neutral density and therefore would not be expected to be effective in adequately predicting the influence of underflow or sludge blanket solids concentrations.

Abdel-Gawad & McCorquodale (1984) presented a strip integral numerical model to simulate the performance of primary clarifiers, with emphasis on the prediction of the velocity field and concentration distribution. The hydrodynamic sub-model was calibrated using a measured velocity distribution in a physical model. Solids were modelled as classes of discrete particles with settling velocities based on batch test. The model was calibrated by measurements in full-scale rectangular tanks. The predicted concentration profiles and removal efficiency were in good agreement with the measured values. The sludge blanket and underflow, however, were not modelled.

A 2D, neutral density, turbulent CFD model of rectangular primary sedimentation tanks was developed by Stamou *et al.* (1989) who compared predicted solids profile and residence time distribution (RTD) curves to field measurements. Turbulent flow was modelled using a k-epsilon approach of Rodi (2000). They found that variation in the turbulent Schmidt number from 0.5 to 1.0 resulted in little difference in the flow through curve. Wang & Maxey (1993) explore the problem of discrete settling in a flow field of homogenous turbulence from the perspective of theoretical fluid mechanics. This is sophisticated work with considerable attention to numerical and experimental issues. They produce results for the increase in mean Stokes drag settling speed in uniform turbulence of zero mean velocity (batch conditions).

A generalized settling model (GSM) that includes a model for hindered settling in addition to discrete settling was presented in Mazzolani *et al.* (1998). This was specifically intended to improve upon discrete settling models and 'monodisperse settling models' that do not recognize that typical sedimentation tanks for water and wastewater 'typically treat highly heterodisperse suspensions.' They discuss the difference of their model from the single exponential Vesilind (1968) and double exponential model of Takacs *et al.* (1991). They positively compare results of a 2D numerical simulation of their GSM to discrete and basic hindered models.

Griborio *et al.* (2014) provide a report on a comprehensive evaluation of two primary sedimentation tanks evaluated with 2D and 3D CFD models. The projects included field testing and evaluation of alternative geometries and recommendations on improvement. Notably, the work with the 2D model included full solids transport with density couple, a five-component settling model including a compression model and flocculation using the 2Dc/3Dc model (Griborio 2004). The 3D model did not include these features, but was used to estimate velocity profiles in the inlet and outlet.

Research needs

Primary sedimentation was one of the first areas of water treatment to be addressed using CFD methods. Much of the early work was done in 2D and in relatively coarse grids in custom programs, with a key focus on neutral density hydraulics rather than sedimentation performance. Typically, underflows have been ignored, in spite of the fact that sludge thickening is an important part of the operation of primary sedimentation tanks for WWT. Future work should include analysis of the sludge blanket using appropriate sedimentation models which include hindered and/or compressive settling. There is a need for development of sedimentation models that may include multiple particle distributions for input to the CFD models which would allow for a more accurate representation of effluent quality. Almost all work to date has assumed neutral density conditions. This is certainly not appropriate for sludge blankets, where the presence of solids contributes to fluid density. So density couple should be included in future work including these regions either by a drift flux model or by an active scalar approach. There is a need for future work using high-resolution 3D models calibrated to field solids profile and settling tests. Only the work of Griborio *et al.* (2014) considered here includes effects of flocculation and this is likely a key issue. Emerging alternatives to primary sedimentation such as rotating belt filters may also benefit from application of CFD, as they involve multiple mechanisms, including sedimentation, mechanical-hydraulic coupling, multiphase interactions (Paulsrud *et al.* 2014).

Biological processes (suspended growth)

The focus on suspended growth (flocculent) systems has been in activated sludge basins. Anaerobic digesters are a separate problem addressed below. Activated sludge tanks have a broad range of functionality, including nutrient and carbon removal, pathogen destruction, and removal of micro pollutants. They are also generally compartmentalised, have large recycle streams, and are critically dependent on multiphase contact and effective hydraulics. There are therefore strong potential benefits offered by CFD, including assessing hydraulic behaviour, gas-liquid transfer and biological functionality. At the same time, there are major challenges, including turbulent hydraulics, a multiphase nature (including potentially non-Newtonian fluid behaviour), and biokinetics.

A very comprehensive review is provided by Karpinska & Bridgeman (2016) for CFD of activated sludge reactors. This includes a critical review of (1) Reynolds averaged Navier-Stokes (RANS) simulations, (2) turbulence models, (3) multiphase modelling, with a strong focus and discussion of the need to move to coupled CFD-biokinetic modelling.

They conclude, 'The complete CFD simulation of the complex multiphase flow in AS tanks remains a challenge, due to the high CPU and RAM requirements and limited feasibility resulting from the imposed convergence criteria. Although there is still no unequivocal protocol on CFD methodology, the most computationally efficient scenario, RANS/unsteady RANS (URANS) closed by a k-ε turbulence model has been adopted as the standard for the modelling of AS tanks …'

Within the area of mixing modelling, efforts have been made in activated sludge tanks by estimation of velocity and solids profiles. Samstag *et al.* (2012) showed that if density couple was not included, mechanical mixing in an activated sludge reactor was significantly overestimated. They used a 3D commercial CFD model with multiphase simulation of water and air and an active scalar transport model for solids calibrated to field tests. Le Moullec *et al.* (2008) used a multiphase 2D Euler-Euler scheme and simulation of particle tracking in a Lagrangian reference frame using a commercial CFD package to model velocity profiles and RTD in an aerated channel whose characteristics had been previously measured at lab scale (Potier *et al.* 2005). Tracer experiments were simulated using a passive scalar approach. Influence of solids gradients on fluid flow was not modelled.

Flocculation in activated sludge influences a number of factors, including solid phase characteristics, and potential biological activity. Parker *et al.* (1971, 1972) evaluated factors influencing flocculation in activated sludge mixed liquors. The work did not include CFD, but they proposed a simple model for floc breakup and agglomeration which has been used by subsequent researchers in full CFD models of sedimentation. The model (Parker *et al.* 1972) proposed that floc breakup and agglomeration could be related to the root mean velocity gradient, G. In contrast to this, Ducoste & Clark (1998) found in experiments that important parameters were controlled by the turbulence intensity and not by G. Nopens *et al.* (2002) and Nopens (2005) present results from experimental testing and calibration of a population balance model for flocculation in activated sludge. While a promising alternative approach to the Parker *et al.* (1970, 1971) models, the authors conclude that model improvement is needed.

There has been extensive work over the last 10 years on coupled biokinetic-hydraulic models (since computing capabilities made this possible), generally coupling CFD with variants of the IWA ASM series models (Henze *et al.* 2000). This can be divided into statically linked models where CFD is solved and biokinetics overlain or dynamically linked models where both are linked and the biokinetics solved together.

Laursen (2006) completed a very comprehensive study of the hydrodynamic and biokinetic modelling of activated sludge applied to full-scale WWTP case studies. Commercial software was used to develop full 3D CFD simulations of three different full-scale aeration tank geometries. Features included: (1) Biokinetic modelling using the ASM3 model (Henze *et al.* 2000), (2) Active density coupling of solids concentrations, (3) Liquid turbulence simulated by k-epsilon and shear strain transport models with air bubbles and sludge flocs modelled using a zero equation model, (4) Air diffusers modelled as bubbly flow calibrated to detailed laboratory velocity and air fraction measurements, (5) Propeller mixer modelled by both sliding mesh and momentum source models and (6) Calibrated viscosity models. Interesting practical problems were considered in three case studies.

Littleton *et al.* (2007) used a 3D commercial CFD model to simulate fluid flow in a closed loop reactor with aeration and consumption of dissolved oxygen (DO) simulated using a supplemental equation with a goal of identifying zones where simultaneous nitrification-denitrification was likely. The CFD model was validated with field data obtained from a test tank and a full-scale tank. Solids gradient influences on the flow pattern were not simulated.

Le Moullec *et al.* (2010a) compared pilot plant results to three different integrated models including simulation of hydrodynamics and biological reactions using the ASM1 model (Henze *et al.* 2000): (1) continuously stirred tank reactor (CSTR) and axial dispersion models, (2) a full 2D multiphase Euler-Euler CFD model integrated with ASM1 kinetics, and (3) a compartmental model in which coarse grid velocity components were determined by CFD independently of the biological kinetics and then the kinetics applied to the steady state velocity field determined by the CFD model. The compartmental model well predicted measured DO concentrations in the range of 2 to 4 mg/L, better than either the systemic model or the full CFD model. All three models over-predicted measured COD concentrations. The two CFD models did a better job predicting nitrate concentrations (in the range of 30 to 60 mg/L) than the systemic model. All three models under-predicted ammonia concentrations. None of these models incorporated the influence of solids concentration gradients on the velocity profile. Additional results from the full multiphase (air and water) CFD model are reported in Le Moullec *et al.* (2010b).

Sobremisana *et al.* (2011) simulated hydrodynamics, floc dynamics, and biological reaction kinetics for activated sludge. A planar 2D CFD hydrodynamic model was developed for a baffled flow-through reactor using a commercial CFD package. Constant density was assumed. The quadrature method of moments was used to estimate floc aggregation and breakup. This solution was integrated with the hydrodynamics through user-defined subroutines. The ASM1 model was implemented using a convection and diffusion application of the commercial software with rate expressions for species reaction defined by ASM1. Results were not compared to field or pilot scale results or to the results from CSTR models.

A 3D single phase CFD simulation of an oxidation ditch configuration was implemented by Pereira *et al.* (2011) to determine RTD characteristics. Three different turbulence models were compared: RANS with the standard k-epsilon model; URANS; and Large Eddy Simulation. Once this was accomplished, CSTR and plug flow reactor models incorporating an ASM1 biokinetic models were fitted to the RTD characteristics identified in the CFD simulation.

Rehman *et al.* (2014) presented the results of application of an integrated hydrodynamic and biokinetic model to the distribution of velocity, DO and ammonium in a full-scale closed loop reactor. Tank hydrodynamics were modelled in 3D using an Eulerian two-fluid model for liquid and gas phases with a commercial CFD package. A realizable k-epsilon model was used to model the effects of turbulence and a drift flux model for dispersion of bubbles. The tank was modelled with a free water surface. Mixing propellers were modelled as momentum sources. Biokinetics were modelled using the ASM1 model with addition of an oxygen mass balance to model transfer of oxygen to the liquid phase. Bulk density was calculated based on local suspended solids concentration. Results were compared to field sampling from a full-scale reactor and 15% improvement in results was observed. Results (presented in Figure 2) show significant variation in DO and ammonium concentrations, justifying the greater (1–2 day) simulation time compared to a CSTR model. Impact of different mixing conditions on the system performance was observed.

Laurent *et al.* (2014) present a comparison of the merits of the integrated CFD and biokinetic modelling compared to compartmental models using CFD to establish generalized velocities prior to subsequent biokinetic modelling. Example data from Alvarado *et al.* (2012) and Le Moullec *et al.* (2010a) are discussed. Ratkovich *et al.* (2013) provide a critical review of activated sludge rheology models.

A critical review of the literature relating to hydrodynamic and biokinetic modelling of membrane bioreactors was provided by Naessens *et al.* (2012), with many issues common to activated sludge, but with the additional consideration of membrane-fluid interaction (including fouling management). Experimental and CFD work providing the background to this work is presented in Ratkovich (2010). Saalbach & Hunze (2008) provide a specific example in a multi-compartment system. Apart from hydraulics, CFD has been shown to be an effective tool in membrane fouling prediction, mainly through estimation of membrane shear rate (Boyle-Gotla *et al.* 2014). The latter example also demonstrates application to Anaerobic MBR systems.

Research needs

The work reviewed reveal that activated sludge tank modelling is a well-developed field that showcases application of CFD to wastewater problems. CFD has been generally used to gain insight into the process, not possible through other techniques that have identified significant deviations from mixed or CSTR approaches. Highlights include incorporation of biokinetic, solids and air transport, and rheological models into CFD models for suspended growth biological treatment systems. The most comprehensive work has included: (1) 3D CFD, (2) sedimentation and

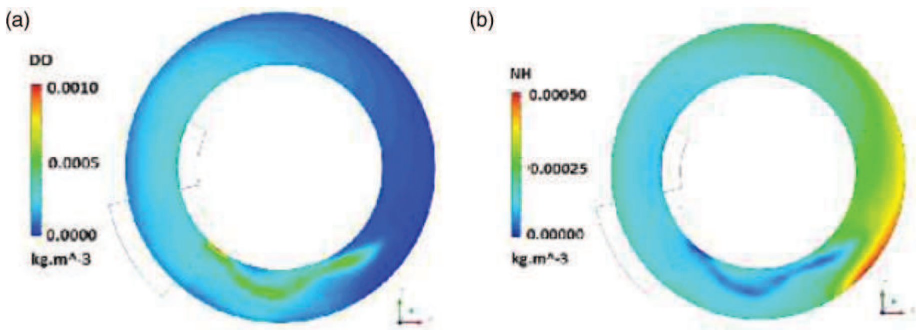

Figure 2 | Oxygen (a) and ammonium (b) concentration plots in a closed-loop reactor (Source: Rehman *et al.* 2014).

solids transport with active density couple, (3) ASM3 biokinetics, (4) calibrated impeller mixing modelling, (5) aeration, and (6) modelling of non-Newtonian viscosity effects. There are still possible extensions to coupling flocculation and CFD, and consideration of interactions at the micro-scale has been limited, but likely the key need is broader application of these techniques, given the diversity of activated sludge process designs, and demonstrated value of CFD done to date. There is also an emerging need to apply CFD techniques to emerging low energy units, such as granular activated sludge, anaerobic mainline treatment units (including anaerobic MBR), suspended carrier systems, and mainline and side stream anaerobic ammonium removal (which is critically dependent on local conditions).

Secondary sedimentation

Secondary sedimentation would appear to have similar challenges to primary sedimentation, but is actually governed by some different mechanisms, including near neutral solids density, prominent hindered and compressive settling behaviour and higher underflow rates. Modelling goals are also directed by the multiple functions of final effluent clarification, activated sludge thickening, sludge storage and flocculation. Secondary sedimentation was one of the first unit processes to receive attention from CFD researchers. Summary descriptions of some of the most important research follow. This section may be considered as an update to Ekama *et al.* (1997), which contains a comprehensive summary of earlier work in analysis of secondary settling tanks.

McCorquodale and his students and associates at the University of Windsor and the University of New Orleans have been leaders in application of CFD to sedimentation, using customized computer codes based either on the vorticity/stream function method of Roache (1982) or the methods of Patankar (1980). Zhou & McCorquodale (1992a) investigated 2D flow in a radial flow (circular) clarifier. They performed simulations using their Patankar (1980) CFD code incorporating turbulent flow (k-epsilon turbulence model), solids transport, and settling by a double exponential function (Takacs *et al.* 1991). The model also included coupling of the concentration profile with the fluid flow through fluid density. They compared the resulting velocity profile in their model for the cases with and without solids input and underflow pumping. Their results demonstrated the 'density waterfall' that occurs in radial flow clarifiers as a result of solids settling immediately after introduction at the tank inlet. Their comparisons in CFD and physical model tests showed that with no solids present, the velocity pattern in the tank is completely different from when solids are included. They investigated sedimentation in a tank with three different feed well diameters. Results showed that performance was best for the tank with the smallest feed well. Results from the larger feed well were very similar to results from simulations of the case with no feed well at all. More general applications of this CFD technique were presented by these authors for rectangular clarifiers in Zhou & McCorquodale (1992b) and for circular clarifiers in Zhou & McCorquodale (1992c). Other research by McCorquodale and his associates has been crucial to development of the state of the art of clarifier modelling, including McCorquodale *et al.* (1991) and McCorquodale & Zhou (1993). Griborio (2004) covers development and validation of a five-component settling model, flocculation models, and details for quasi 3D CFD for activated sludge clarifiers. This CFD model uses a vorticity/stream function approach to eliminate pressure from the fluid equations and a simple mixing length turbulence model. This work also contains an extensive reference list.

Flocculation (see activated sludge section) is also linked to clarifier performance. The impact of flocculation processes on secondary clarifier performance via simulation was extensively assessed within McCorquodale's group and is detailed in Griborio (2004). Griborio & McCorquodale (2006) used this model to investigate the influence of center-well geometry on flocculation and clarifier performance. They found that the major benefit of optimum center well geometry is in improving hydrodynamic performance and that flocculation had less influence. The same model was used by Gong *et al.* (2009) in analysis of sedimentation in a rectangular sedimentation tank using a 3D turbulent commercial CFD model.

Armbruster *et al.* (2001) present results from use of the mathematical model presented in Lakehal *et al.* (1999). Results were compared to experiments by Krebs *et al.* (1998). Concentration profiles from simulation of dynamic loading over 24 hours of flow based on data from a treatment plant in Germany were presented. De Clercq (2003) developed a 2D CFD model in commercial package incorporating solids transport, density couple, and flocculation. The model was applied to a radial flow (circular) activated sludge clarifier. A Herschel Bulkley rheological model was incorporated by user-defined functions.

A 2D finite element analysis of flows in secondary settling tanks was presented in Kleine & Reddy (2005). They incorporated solids settling using a double exponential function (Takacs *et al.* 1991) and included the influence of density on the momentum equations. The k-epsilon equation was used to simulate turbulence and compared to a constant turbulent viscosity approach. The model was compared to field tests for radial flow circular activated sludge settling tanks and to results from the commercial sedimentation program, SettlerCAD. In comparison to field results the best fit of CFD results was with a Schmidt number greater than 1.

Burt (2010) developed 2D CFD models calibrated by field and laboratory tests. The CFD models were constructed in the commercial software using an algebraic slip model with user-defined functions for definition of density, settling velocity and rheology. An extended drift flux model was compared to a multiple drift flux model which tracked 10 different size groups. A solids profile developed in a recent CFD workshop by the drift flux method of Brennan (2001) is shown in Figure 3.

Research needs

Activated sludge secondary sedimentation tank simulation is the most well-developed area of application for CFD in WWT. Initial models were only 2D, but almost all included solids transport and settling with coupling of the solids concentration field to tank fluid flow. A significant improvement has been made with incorporation of GSM including discrete, hindered, and compressive settling regimes and flocculation. The work of Ducoste & Clark (1998) suggests that the relatively widely used Parker *et al.* (1970, 1971) model (for activated sludge flocculation) may not be adequate to capture the influence of flocculation on behaviour of sedimentation tanks, and flocculation and particle interaction has not been included in detail (but is empirically included through scalar compression settling models). Future work should incorporate higher resolution 3D geometric models including GSM and models for flocculation, preferably verified by field tests for solids profile and sludge settling velocity. Hindered settling is typically represented by empirical equations such as the Vesilind or Takacs exponential equations; future work should attempt to further validate physically-based compression models such those of Kinnear (2002) and Bürger *et al.* (2011). Additionally, models should incorporate the entire settling domain from the inlet pipe to the effluent and underflow outlets. Knowledge gained from CFD should also be used to improve 1D models for plant-wide simulation as developed in Guyonvarch *et al.* (2015).

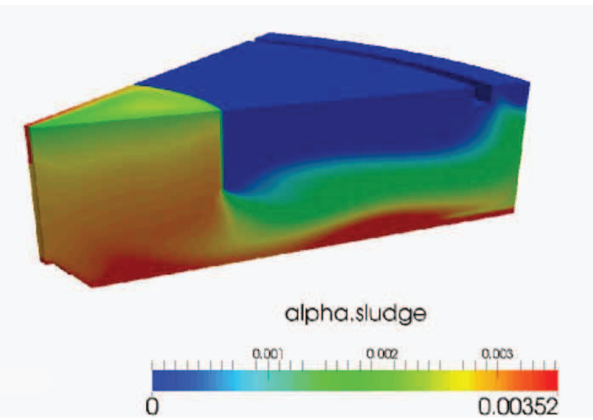

Figure 3 | Solids profile for a secondary sedimentation CFD simulation developed in open source software (Source: Marques 2015b).

Solids handling

Dissolved air flotation

Dissolved air flotation (DAF) is used in water and WWT for solids separation in lieu of gravity sedimentation and for sludge thickening. Amato & Wicks (2009) presented the results of a CFD study of DAF for separation of solids from a pre-coagulated surface water supply. A multiphase Euler-Euler model was used to simulate liquid and air hydrodynamics. A k-epsilon turbulence model was used in commercial CFD software (ANSYS Fluent v.6.3.26). The volume weighted average vorticity was extracted from the CFD model as a measure of floc-bubble agglomeration disturbance, with an average floc-bubble agglomerate diameter of 148 μm in the clarification zone. Floc characteristics were inferred from bubble concentration. These assumptions were used to calculate the location of the 'white water level' which previous work had correlated with good solids removal (See Figure 4).

Anaerobic processes

Anaerobic digesters in a wastewater context are relatively high solids (in-reactor 1–3%), with performance highly dependent on hydraulics. Operating cost of the digester, as well as its overall functionality is critically linked to digester mixing (Verhoff *et al.* 1974). Given that capital costs of digester can be very high (due to large volumes), it is critical that the geometry and mixing systems are appropriately designed. Key issues around poor mixing include short circuiting (critical), dead volume (should be minimised), and plug-flow behaviour (important to note, but not critical to performance). There has been limited work on anaerobic digester systems compared with activated sludge and

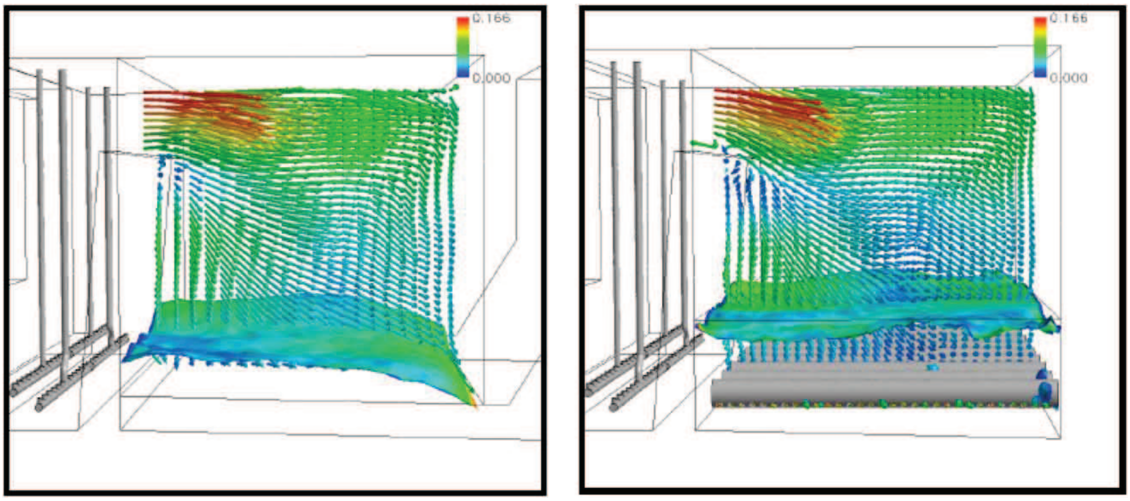

Figure 4 | CFD Predicted white water level and velocity vector plots in a DAF tank, (left) without and (right) with subnatant tubes (Source: Amato & Wicks 2009).

clarifiers and hydraulics and CFD has been noted as a key research need in anaerobic digestion modelling as a whole in a recent review (Batstone *et al.* 2015).

A critical issue in CFD of digesters is non-Newtonian behaviour of the solids, which is generally shear thinning, and is influenced by temperature and solids concentration. This behaviour is generally modelled by Bingham or Hershel Bulkley models (or a combination of the two) and sludge rheology in detail is reviewed in Eshtiaghi *et al.* (2013). Sludge rheology can cause digesters to exhibit unexpected and dynamic behaviour (see needs below), due to formation of unmixed 'thick' zones.

The majority of commercial and academic work has been non-reactive hydraulic analysis. Wu & Chen (2008) discuss a general mathematical model that predicts the flow fields in a mined-flow anaerobic digester. In this model liquid manure was assumed to be a non-Newtonian fluid and the flow governed by the continuity, momentum, and k-ε turbulence equations and a non-Newtonian power law model. Commercial CFD software was applied to simulate the flow fields of lab-scale, scale up, and pilot-scale anaerobic digesters. The simulation results were validated against experimental data from literature. The flow patterns were qualitatively compared for Newtonian and non-Newtonian fluids flow in a lab-scale digester. Numerical simulations were performed to predict the flow fields in scale-up and pilot-scale anaerobic digesters with different water pump power inputs and different total solids (TS) concentration in the liquid manure. The optimal power inputs were determined for the pilot-scale anaerobic digester. Some measures for reducing dead and low velocity zones were proposed based upon the CFD simulation results. This was extended in Wu (2009a) with application of a 3D commercial CFD model to anaerobic digestion. The model incorporated the k-epsilon turbulence model, and predictions of pseudo-plastic fluid behaviour based on equations for viscosity and density. The density calculation included the influence of solids concentration, but solids transport and settling was not included, so density effects of solids concentrations gradients were ignored. The model included a multiple reference frame (MRF) approach to model impeller rotation within a MRF zone inside a stationary reference frame. The model was applied to the simulation of mixing with four different mixing systems: mechanical mixing through propellers in external draft tubes, mechanical stirring by side-entry propellers, mechanical pumping by a propeller in an internal draft tube and mechanical stirring by a top-entry propeller. Wu (2009b) presents a CFD simulation of an egg-shaped digester with mechanical draft tube mixing. CFD techniques were similar to those of Wu (2009a).

Wu (2010) presents an Eulerian multiphase flow model that characterizes gas mixing in anaerobic digesters. Liquid manure was assumed to be a non-Newtonian pseudo-plastic fluid that is dependent on TS concentration. Twelve turbulence models were evaluated by comparing the frictional pressure drops of gas and non-Newtonian fluid two-phase flow in a horizontal pipe obtained from CFD with those from a correlation analysis. Commercial CFD software was used for the work. The simulation results in a small-sized digester were validated against experimental data from literature. Comparison of two gas mixing designs in a medium-sized digester indicated that mixing intensity is insensitive to the TS in confined gas mixing, whereas there are significant decreases with increases of TS in unconfined gas mixing.

Moreover, comparison of three mixing methods indicated that gas mixing is more efficient than mixing by pumped circulation while it is less efficient than mechanical mixing. This work did not, however, include solids transport and sedimentation nor did it include simulation of the effects of solids concentration gradients on density and fluid flow.

Results of development of a CFD model to simulate mechanical mixing of sewage sludge at laboratory scale were presented in Bridgeman (2012). The work used the commercial meshing and CFD software. Five different turbulence models were compared. Meshes with 280,000 to 1,600,000 cells were used. A MRF model was used to generate velocity fields around rotating impellers. Velocity profiles in tanks with different solids concentrations were developed, but solids transport and settling was not modelled, so that the influence of solids concentration gradients on the flow was not simulated.

Gaden (2013) presents work resulting in development of a CFD model for anaerobic digestion implemented in the open source CFD platform, OpenFOAM. The model implements a version of the Anaerobic Digestion Model No. 1 (ADM1) in a 10 by 10 2D square grid. The model is two phase (gas and liquid). Buoyancy effects from temperature gradients are included but density impacts from solids concentration gradients are not.

Research needs. Digestion studies to date have treated high solids concentrations as affecting bulk density but spatial distribution of solids and the impact of density gradients on fluid flow patterns have not been explored. This is critical to enhanced use of CFD in digester simulations, and may enable exploration of mechanisms such as foaming (Dalmau *et al.* 2010), which is a critical operability issue. In addition, foaming can even lead to digester-wide issues such as fluid inversion. Incorporation of biokinetic models into density coupled 3D CFD models will become increasingly important for modelling of digesters to properly consider these effects, as well as the impact of incomplete mixing on the biology, which may include formation of zones with specific activity. There is also a strong need to consider emerging processes such as plug-flow, and leach bed systems (Batstone *et al.* 2015), and the impact on ancillary processes such as heat exchangers.

Disinfection

Ultraviolet

CFD modelling of UV reactors is fast becoming a standard approach for characterizing, designing, and troubleshooting the UV disinfection performance. Moreover, growing confidence in numerical models that have been validated with extensive biodosimetry data have lead UV manufacturers to use the tool as part of an on-line algorithm for dose monitoring. Numerical UV disinfection models are complex and require the proper execution of several components so that the numerical results can be used for analysis of a UV process. UV disinfection models can be divided into three major components. These major components include: (a) fluid flow/turbulence model, (b) fluence rate distribution model, and (c) microbial transport model. As the name implies, the fluid flow/turbulence model involves characterizing the spatial variations in fluid flow and turbulent mixing that occurs in the UV reactor. The fluence rate model involves characterizing the spatial variations in the UV light intensity in the UV reactor. Finally, the microbial transport model involves characterizing the movement of the microorganisms through the UV reactor.

A number of research studies have been performed to assess CFD UV process performance as a function of the fluence rate model selection (Liu *et al.* 2004; Ducoste *et al.* 2005a, 2005b; Wols 2010), turbulence model selection (Liu *et al.* 2007; Wols 2010) and the approach used to simulate the transport of microorganisms (i.e., Eulerian or Lagrangian approaches) (Ducoste *et al.* 2005a, 2005b; Sozzi & Taghipour 2006). In drinking water treatment applications, a significant effort was made to demonstrate the accuracy of these models for several reactor designs and different microbial disinfection kinetics (Ducoste *et al.* 2005a, 2005b; Wols *et al.* 2010). In addition, the UV dose distribution, which was exclusively an output from the CFD model by simulating the transport of particles (i.e., Lagrangian approach) within the reactor and monitoring their exposure to local UV light intensity along the particle path, was only validated indirectly through the model's ability to predict the experimental effluent log inactivation. Researchers were able to develop an experimental Lagrangian approach that involved tracking fluorescent polystyrene microspheres through a UV reactor and monitor the change in fluorescence due to its cumulative exposure to UV light (Bohrerova *et al.* 2005; Blatchley *et al.* 2006; Zhao *et al.* 2009). While this approach has its limitation, it has provided additional information about the accuracy of CFD UV disinfection models and in combination with experimental log inactivation, improves the validation process of UV reactors.

A particular concern in WWT is the disinfection of water containing particle aggregates. Researchers have shown that bioflocs that shield or harbour microorganisms can reduce the UV disinfection performance (Mamane &

Linden 2006; Caron *et al.* 2007; Kollu & Ormeci 2012). Experimental results suggest that floc size, number of microbes incorporated into the floc, and the spatial location of these organisms within the floc can influence the UV dose to achieve a high log inactivation (Mamane & Linden 2006). Mamane *et al.* (2006) explored the effect of light scattering on measurement of UV absorbance and penetration of germicidal UVC irradiance in a UV reactor. As part of that study, CFD was used to evaluate the radiative transfer equation in predicting the UV fluence rate within a reactor. Mamane *et al.* (2006) results showed that the model over-predicted the fluence rate in wastewater effluent augmented with particles. The researchers hypothesized the higher model results was due to the type and size of particles in the augmented wastewater solution, which was augmented with irregular, 2–5 micron particles that scattered light anisotropically. The anisotropic nature of the scattered light was not modelled in their study.

Disinfection

Chemical oxidation

Greene (2002) researched the fate of chlorine and bacterial pollutants in chlorine contact tanks treating wastewater effluent. An Euler-Euler approach was used for simulation of microbial inactivation with the spatial distribution of microorganisms in the reactor viewed as a continuous field, similar to a dissolved species. Disinfection models were implemented in the general purpose commercial CFD software. Reactor tanks were modelled in 3D using a k-epsilon turbulence model. Buoyant forces were assumed to be negligible. Grid independence checks were undertaken with a mesh of 132,000 cells selected for the influent piping and 790,000 cells for the reactor. Santoro *et al.* (2015) used CFD as a deterministic tool to identify probabilistic curves for pathogen deactivation by peracetic acid, identifying the value of CFD for protyping of systems where there are complex mechanisms present, and enabling simple tools for end-user application.

Research needs. Application of CFD to disinfection is relatively well developed. It is normally assumed that disinfection flows are not affected by solids density or other buoyant forces. Hence neutral density simulations are typical and this has seemed to be a reasonable assumption. To date, no CFD model has been developed to explore the performance of UV disinfection in wastewater containing particle aggregates. The ability to model such a system may require the simulation of continued aggregation within UV reactor, the floc size distribution, and UV light path length, absorbance, and potential scattering due to the presence of these aggregates.

CONCLUSIONS

Analysis of the general use of CFD in WWT has identified that the sophistication of the technique is highly variable between different units. In particular, CFD simulation of secondary sedimentation is highly mature, while work in anaerobic digestion is less well developed. Nowhere (except possibly disinfection) is CFD used in a widespread or routine way as a design, risk-management, or trouble-shooting tool. This offers clear opportunities to further develop the value of CFD in wastewater process evaluation.

1. While projects which assess the general flow distribution between units are widespread in engineering practice there is a need for more peer-reviewed research specific to flow splitting and head loss determination in water and WWT processes. The potential impacts of solid and gas phases on flow distribution should be addressed in future models.
2. The common assumption that grit settlement is not affected by density gradients should be demonstrated by comparative studies.
3. There is little work on the analysis of sludge blankets for primary sedimentation. CFD models in 3D, incorporating the entire tank domain and including discrete and compressive settling and improved flocculation and rheology models, should be considered in future work.
4. Alternative models for flocculation should be compared to the dominant empirical model and these included more routinely in CFD analysis of activated sludge basins and final sedimentation.
5. CFD coupled to activated sludge biochemical models has been demonstrated to be very valuable compared with simpler mixed tank models. This should be further expanded to include models such as the ASM2d and ASM3 models incorporating phosphorus removal. Incorporation of density-coupled solids transport should be included in future suspended growth reactor CFD models since solids settling affects the solids concentration, density and velocity profiles and resulting reactant concentrations. There is also a continuing need to use CFD models for validation of biokinetic models based on simpler hydraulic assumptions.
6. More sedimentation tank modelling should be done in 3D incorporating full GSM and models for flocculation

and rheology. Alternative physically based models for compression settling should be compared to the dominant empirical models.

7. Future work in modelling of digestion should include the effects of density couple, hindered settling, compression and rheology. Incorporation of biokinetic models into anaerobic digestion study is in its infancy and could be critical to advanced issues such as foaming and inactive zones.
8. Disinfection modelling using CFD is relatively well developed but modelling of floc aggregates should be explored in future work.
9. There are potential applications for CFD outside of the areas considered here, such as final dewatering; particularly through screens, which may avoid primary unit elevation and reduce catchment pumping costs and centrifuges (enabling reduced energy and polymer consumption and unit wear); other solids handling units such as screws and conveyor belts, centrifugal and positive displacement transport of liquids and gases and behaviour of fluids and particulates during transport (mainly in pipes).
10. Whole plant hydraulic modelling is also a major opportunity for the optimisation of design and operating costs, although this is obviously a significant computational challenge.

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