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Review

CFD-aided modelling of activated sludge systems – A critical review

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A R T I C L E I N F O

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A B S T R A C T

Nowadays, one of the major challenges in the wastewater sector is the successful design and reliable operation of treatment processes, which guarantee high treatment efficiencies to comply with effluent quality criteria, while keeping the investment and operating cost as low as possible. Although conceptual design and process control of activated sludge plants are key to ensuring these goals, they are still based on general empirical guidelines and operators' experience, dominated often by rule of thumb. This review paper discusses the rationale behind the use of Computational Fluid Dynamics (CFD) to model aeration, facilitating enhancement of treatment efficiency and reduction of energy input. Several single- and multiphase approaches commonly used in CFD studies of aeration tank operation, are comprehensively described, whilst the shortcomings of the modelling assumptions imposed to evaluate mixing and mass transfer in AS tanks are identified and discussed. Examples and methods of coupling of CFD data with biokinetics, accounting for the actual flow field and its impact on the oxygen mass transfer and yield of the biological processes occurring in the aeration tanks, are also critically discussed. Finally, modelling issues, which remain unaddressed, (e.g. coupling of the AS tank with secondary clarifier and the use of population balance models to simulate bubbly flow or flocculation of the activated sludge), are also identified and discussed.

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Nomenclature

c_q	mass fraction of phase q [−]
F	sum of interfacial forces shared by the phases [N]
F_q	sum of interfacial forces between the continuous and dispersed phases [N]
$J_{i'}$	diffusion flux of i' species [kg m^{-2} s^{-1}]
k	turbulent kinetic energy, [m^2 s^{-2}]
$K_L a$	volumetric mass transfer coefficient [h^{-1}]
$\dot{m}_{pq}$	mass transfer from phase p to q [kg s^{-1}]
$\dot{m}_{qp}$	mass transfer from phase q to p [kg s^{-1}]
p	pressure [Pa]
$\overline{p}$	averaged pressure field [Pa]
$R_{i'}$	net rate of production of i' species due to chemical reaction [kg m^{-3} s^{-1}]
Re	Reynolds number [−]
$S_{i'}$	source term representing rate of creation of i' species from dispersed phase and any user-defined sources [kg m^{-3} s^{-1}]
t	time [s]
t_r	particle relaxation time [s]
v	velocity [m s^{-1}]
$v_{dr,q}$	drift velocity for phase q [m s^{-1}]
v_i, v_j, v_l	velocity components [m s^{-1}]
$\overline{v}_i$	averaged velocity term [m s^{-1}]
v_i'	fluctuating velocity term [m s^{-1}]
v_m	velocity of mixture [m s^{-1}]
v_P	velocity of the particle [m s^{-1}]
v_p	velocity of phase p [m s^{-1}]
v_{pq}	velocity of phase p relative to velocity of phase q [m s^{-1}]
v_q	velocity of phase q [m s^{-1}]
x	distance [m]
x_i, x_j, x_l	spatial coordinates (displacement in the streamwise direction) [m]
$Y_{i'}$	mass fraction of the i'-th species [−]

Greek letters

α_q	phasic volume fraction [−]
α^*	damping function coefficient [−]
ε	turbulent kinetic energy dissipation rate [m^2 s^{-3}]
μ	dynamic viscosity of the fluid [Pa s]
μ_m	dynamic viscosity of the mixture [Pa s]
μ_q	dynamic viscosity of the phase q [Pa s]
μ_t	turbulent viscosity [Pa s]
ρ	fluid density [kg m^{-3}]
ρ_m	density of the mixture [kg m^{-3}]
ρ_P	density of the particle [kg m^{-3}]
ρ_p	density of the phase p [kg m^{-3}]
ρ_q	density of the phase q [kg m^{-3}]
ω	specific turbulence dissipation (frequency) [s^{-1}]

Indices

dr	refers to drift velocity
i	index or counter
i'	species index
j	index or counter
k	refers to turbulence kinetic energy
l	index or counter
m	refers to mixture
P	refers to particle
p	refers to phase p
q	refers to phase q
t	refers to turbulence

Abbreviations

ADV	Acoustic Doppler Anemomentry
AS	Activated Sludge
ASM	Activated Sludge Model
ASM1	Activated Sludge Model No. 1
ASP	Activated Sludge Plant
BOD	Biochemical Oxygen Demand
CFD	Computational Fluid Dynamics
COD	Chemical Oxygen Demand
CPU	Central Processing Unit
CSTR	Continuous Stirred Tank Reactor
DO	Dissolved Oxygen
LDV	Laser Doppler Velocimetry
LES	Large Eddy Simulation
MDV	Mono-directional Velocimetry
MLSS	Mixed Liquor Suspended Solids
MRF	Multiple Reference Frames
PBM	Particle Balance Model
PDA	Particle Dynamic Analysis
PFR	Plug Flow Reactor
PID	Proportional-Integral-Derivative
QMOM	Quadrature Method of Moments
RAM	Random Access Memory
RANS	Reynolds Averaged Navier–Stokes Simulation
RSM	Reynolds Stress Model
RTD	Residence Time Distribution
SCADA	Supervisory Control and Data Acquisition
SGS	Sub-grid Scale
SMM	Standard Method of Moments
SRT	Solids Retention Time
TSS	Total Suspended Solids
URANS	Unsteady Reynolds Averaged Navier–Stokes Simulation
WWTP	Wastewater Treatment Plant

1. Introduction

To comply with global water policy focussed on responsible management of water resources and protection of public health, wastewater collected from municipalities and communities must be treated to achieve levels imposed by discharge permits and maximum daily loads, allowing its subsequent return to receiving water bodies, or to the land or even to be reused. In the last century, the application of scientific knowledge and engineering practice led to significant developments in the wastewater sector, particularly in biological secondary treatment based on aerobic biological methods, specifically the activated sludge (AS) process (Ardern and Lockett, 1914), which is now a well-documented standard for many wastewater treatment utilities. The objectives of secondary biological wastewater treatment in the AS process have also expanded from an early emphasis on high levels of Biological Oxygen Demand (BOD) and Total Suspended Solids (TSS) removal to cover enhanced nutrients (N and P) removal, as the process itself has flexibility and numerous modifications can be tailored to meet specific requirements.

Undoubtedly, one of the foremost challenges in the wastewater sector is the successful design and reliable operation of treatment plant, which guarantee high treatment efficiencies in order to meet the effluent quality standards defined by regulators, while keeping the investment and operating cost as low as possible (Brouckaert and Buckley, 1999; Do-Quang et al., 1999). One of the characteristic features of ASP is continuous operation of the aeration process and sludge and nitrates recycling, and thus the process performance relies on a steady energy supply for operation of air blowers and sludge and mixed liquor recirculation pumps. Aeration accounts for the largest fraction of a total wastewater treatment plant's (WWTP) energy bill, ranging from 45 to 75% (Reardon, 1995; Rieger et al., 2006) and in extreme cases of stringent effluent nitrogen criterion requiring enhanced nitrification, even up to 85%. Thus, aeration has a significant effect on the operation and maintenance budget of water utilities (WEF, 2009). As a consequence of the global emphasis on the water-energy-food-climate change nexus there is an urgent need to reduce energy usage at WWTPs by imposing cost-effective energy conservation measures, engineering practices and management programs. According to guidelines (EPA, 2013; WEF, 2009) opportunities for improving energy efficiency in wastewater treatment utilities can be obtained by optimizing aeration processes or equipment upgrades, which focus on replacing items such as blowers with more efficient models; replacing the whole aeration system with less energy intensive systems (e.g. replacement of the surface aeration system by porous diffusers in full floor coverage configuration); and operational modifications, involving reduction of the energy requirements to perform specific functions by modification of the aeration control systems, e.g. on-off operation allowing formation of the anoxic conditions for denitrification. The last option facilitates greater savings than equipment upgrades, and may not require capital investment. Nevertheless, current best available aeration technology (i.e. membrane diffusers supplied by atmospheric air) are characterized by relatively low Standard Oxygen Transfer Efficiencies of around 40 up to 60% (EPA, 1989; Mueller et al., 2002; Taricska et al., 2009), which reduce with time as a result of fouling and scaling. Consequently, a wide range of multidisciplinary approaches contribute to current research aiming to improve the development, troubleshooting and management of aeration systems.

2. Current trends in engineering practice

2.1. Aeration control and design assumptions

When investigating performance and energy expenditure of AS plants it is clear that dissolved oxygen (DO) concentration is a key process variable, which controls both, nutrient removal (in the case of biological nutrient removal plants) and thus effluent quality, and the operating cost of the utility. While operating DO profiles and nitrogen patterns in the AS system are usually obtained from biokinetics modelling with Activated Sludge Model No. 1- ASM1 (Henze et al., 2000) employed by supervisory control and data acquisition (SCADA) systems, the robust modelling of the optimization strategies requires implementation of complex computational algorithms and off-line optimization techniques, which allow for coupling of the biological process with pre-defined control variables such as minimal DO concentration in the aeration tank or effluent nitrogen criterion (Åmand and Carlsson, 2012; Chachuat et al., 2005; Cristea et al., 2011; De Araújo et al., 2011; Fernández et al., 2011; Fikar et al., 2005; Holenda et al., 2007, 2008).

Although hydraulic design of wastewater treatment systems is a crucial step to assure reliable and energy-optimised operation of the process, it is usually labelled as a “low-tech” task, which is based on empirical guidelines without sound theoretical basis (Bosma and Reitsma, 2007; Pereira et al., 2012; Stamou, 2008). Thus, in the majority of designs, flow behaviour in the unit process tanks is predicted via the ideal reactor model while the actual reactor hydrodynamics are not taken into account (Stamou, 2008). The classic example for Activated Sludge Plants (ASPs) is the assumption of a completely mixed flow regime in aerobic, anoxic and anaerobic tanks. Other commonly practised rules of thumb are (Samstag and Wicklein, 2012; Tchobanoglous et al., 2003) the assumption that in AS basins equipped with diffused aeration systems, the air requirement to ensure good mixing will vary from 1.2 to 1.8 $m^3\ h^{-1}/m^3$ of tank volume; and typical power requirements for maintaining a completely mixed flow regime with mechanical aerators varies from 13 to 26 W per m^3 of tank volume. None of these assumptions consider the impact of tank hydraulics (cross-section, depth or presence of baffles), energy input, or any variable affecting mixing, such as local density gradients due to solids transport. Furthermore, none of these guidelines defines clearly hydraulic features and performance of “completely mixed” wastewater treatment systems. The one commonly used criterion for “good mixing” in AS process control is that variations of solids concentration across the complete mixed tank profile should be less than 10% (Samstag and Wicklein, 2014). However, the proper design of such “well mixed” AS systems requires a sophisticated analysis of flow behaviour accounting for mixing patterns in the tank, distribution of the oxygen, solids and determination of local densities.

3. Dynamic behaviour of AS tanks

Dynamic modelling of wastewater treatment plants has been shown to be a powerful tool providing detailed insight into the unit process and system behaviour, useful for optimization studies (e.g. conceptual process design, performance evaluation, operational optimization, or controller design) and model-based process control (Langergraber et al., 2004). Nonetheless, the majority of the ASP design procedures are still limited to the empirical principles and static models, such as the ‘classic’ ATV-A-131 guideline (ATV-DVWK, 2000), while control strategies are based on a simple or cascade proportional-integral-derivative (PID) controllers for DO and ammonia. While not often used for design and control of ASP due to its complexity, the systemic approach based on well-established ASM models focuses mainly on the reactions of biochemical conversion within the ideal reactors: usually one or a cascade of Continuous Stirred Tank Reactors (CSTRs) or Plug Flow Reactor (PFR) (Abusam and Keesman, 1999; Le Moullec et al., 2011; Makinia and Wells, 2000; Pereira et al., 2009). Such approaches enable only quantitative prediction of the oxygen consumption and nutrients removal and qualitative assessment of biomass growth and decay. Nevertheless, as the overall biochemical conversion reactions occurring in AS are of orders greater than zero, the wastewater treatment efficiency in such non-ideal systems will depend on the bioreactor's hydrodynamics (Le Moullec et al., 2008), spatial distribution of oxygen, and temperature. Therefore, a more accurate forecast of the actual local scale phenomena occurring within the tank, (such as DO patterns and solids profiles) is of crucial importance to enhance system design, process efficiency and energy requirements, to predict failures of existing aeration systems and finally, to design upgrades and enhance control strategy, such as fine-tuning blower operation.

The physics of typical AS systems is complex, not only due to presence of the multiphase (gas-liquid-solid) flow, comprising mixed liquor and air/oxygen, but also due to the different length scales between the sludge flocs, bubbles and tank geometry; and furthermore, different velocities of the phases imparted by mixers and aerators yielding turbulent Reynolds numbers (Karpinska Portela, 2013; Pereira et al., 2012). The fluid flow in such bioreactors is governed by the vessel geometry, physical properties of its contents (phase, density, viscosity) and operating condition variables (flow rates and concentrations). At the same time, fluid flow governs the local concentration of components, interphase contact and mass transfer, reaction conversions and performance (Nopens and Wicks, 2012).

In engineering practice, whilst assessment of the flow regime, and thus overall mixing phenomena in AS bioreactors, can be achieved via experimental assessment of local flow velocities through a tracer technique, the dimensions of full scale units generally render this unfeasible (Pereira et al., 2012; Stamou, 2008), making simulation an attractive alternative. Several factors contribute to the increasing popularity of modelling in engineering practice, as it is a cost and time efficient solution, which allows evaluation of process performance (whether a new unit or modification will operate properly); prediction of consequences before implementation; isolation and quantification of bottlenecks in liquid or solid handling lines in the AS system. Thus, prediction of Residence Time Distributions (RTDs) of settled sewage is a fundamental tool to help understand and analyse a flow system providing realistic information on tank hydrodynamics (Danckwerts, 1953; Levenspiel, 1999; Nauman, 2007). Furthermore, the RTD yields information about the macromixing within the reactor, allowing recognition of mixing behaviours that are not plug flow or complete mixing regimes, and that are usually described by tank-in-series models or even more complex arrangements of the unit reactors (Pereira et al., 2012). Consequently, successful biological wastewater treatment modelling combining hydrodynamics, mass transfer and biochemical reactions kinetics remains one of the major goals in wastewater engineering (Le Moullec et al., 2010a, b; Morchain et al., 2014; Pereira et al., 2012).

4. Computational Fluid Dynamics

Since the 1970s, increasing computational power has been accompanied by a rapid development in the software intended for solution of fluid flow problems. Nowadays, a wide range of software suites intended for the solution of complex fluid flow problems is commercially available. Initially, CFD was almost exclusively associated with aerospace and mechanical industries allowing simulation of the processes occurring in combustion chambers of rocket engines; physico-chemical processes in the flow around rocket airframe and supersonic aircrafts. Subsequently CFD found applications with chemical engineers, mainly for design of reaction vessels, and in the last two decades, application of CFD has been extended to the civil and environmental engineering sectors (Kochevsky, 2004). Recent developments in multiphase flow research have seen a steady growth in the application of CFD modelling in wastewater treatment, with a focus on the design of pumping stations, headworks, screens, grit chambers, flow splitters, AS tanks, clarifiers and digesters. Undoubtedly, one of the great opportunities of CFD modelling of ASPs is the analysis of the multiphase flow behaviour and prediction of the impact of a wide range of operating parameters on the local scale phenomena, such as flow field coupled with interfacial mass transfer and chemical reaction. In addition to that, CFD has gained popularity over traditional wastewater treatment modelling approaches, as it is a high-precision technique allowing evaluation of the engineering systems, which are expensive, difficult or even dangerous to reproduce in laboratory-scale, pilot-scale or field conditions. Therefore, CFD-aided modelling can be used as a robust tool for the design of a new facility or the optimization or retrofitting of existing ASPs, leading to enhanced performance and energy-optimised operation of the utility, facilitating time, economic cost and manpower savings (De Gussem et al., 2014; Do-Quang et al., 1999; Essemiani et al., 2004; Guimet et al., 2004; Laurent et al., 2014).

4.1. Hydrodynamics – RANS and URANS

Various options exist for the numerical simulation of the turbulent flow with CFD codes.

In most engineering practice, time-averaged properties of the flow are able to provide the required information. Steady Reynolds Averaged Navier–Stokes (RANS) simulations and unsteady RANS (URANS) focus on the representation of the effects of turbulence on the mean flow properties by solving transport equations for the averaged flow quantities with whole range of the turbulent scales being modelled. Thus this modelling approach greatly reduces required computational effort and resources, and is widely adopted for practical engineering applications, including the wastewater sector (Karpinska Portela, 2013).

In RANS and URANS the flow patterns within the AS tank are obtained from the solution of nonlinear partial differential equations, expressing balances of mass and momentum. Therefore, the flow is governed by the following mass conservation equation:

$$\frac{\partial \rho \overline{v}_i}{\partial x_i} = 0 \tag{1}$$

and momentum conservation equation, which for RANS is:

$$\frac{\partial}{\partial x_j}\left(\rho \overline{v_i v_j}\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{v}_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{v_i' v_j'}\right) \tag{2}$$

and for time dependent, transient flow (URANS) is:

$$\frac{\partial \overline{v}_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho \overline{v_i v_j}\right) = -\frac{\partial \overline{p}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \overline{v}_l}{\partial x_l}\right)\right] + \frac{\partial}{\partial x_j}\left(-\rho\overline{v_i' v_j'}\right) \tag{3}$$

where $\overline{p}$ is the averaged pressure field, ρ and μ are the fluid density and viscosity, respectively, t is the time, x_i, x_j and x_l are the spatial coordinates, v_i, v_j and v_l are the velocity components and δ_{ij} is the Kronecker delta.

Here, the turbulent mean velocity field is described by Reynolds decomposition of the velocity using time averaged term $\overline{v}_i$, and a fluctuating term, v_i':

$$v_i = \overline{v}_i + v_i' \tag{4}$$

RANS and URANS equations are linearized and solved. The flow structures originating from the momentum transfer by the fluctuating velocity field, which are smaller than the numerical grid discretization and represented by the term $-\rho\overline{v_i' v_j'}$, namely Reynolds stresses, are unclosed, and thus they must be modelled.

4.1.1. Turbulence models

The principal turbulence models included in popular commercial CFD software suites, which are used for Reynolds stresses closure are: standard, renormalized group (RNG) and realizable $k-\varepsilon$ models; standard and shear stress transport (SST) $k-\omega$ models; and Reynolds stress model (RSM) (Bridgeman et al., 2009).

The two-equation models (i.e. $k-\varepsilon$ and $k-\omega$), solve additional transport equations for two turbulence quantities: velocity scale-turbulent kinetic energy, k, and turbulence length scale-either its dissipation rate, ε, or the specific frequency, ω (Pope, 2000). From among the two-equation models, the standard $k-\varepsilon$ ($sk-\varepsilon$) has found the broadest range of applicability in both, academia and industrial sectors, due to its robustness, relatively low computational requirements and satisfactory accuracy. The characteristic feature of all two-equation models is that modelling of the Reynolds stresses employs the Boussinesq hypothesis relating these stresses to the mean deformation rates and thus mean velocity gradients, and assuming locally isotropic turbulence (Rodi, 1993):

$$-\rho\overline{v_i' v_j'} = \mu_t\left(\frac{\partial \overline{v}_i}{\partial x_j} + \frac{\partial \overline{v}_j}{\partial x_i}\right) - \frac{2}{3}\left(\rho k + \mu_t \frac{\partial v_l}{\partial x_l}\right)\delta_{ij} \tag{5}$$

where μ_t is the turbulent viscosity computed as a function of k and ε:

$$\mu_t = \rho C_\mu \frac{k^2}{\varepsilon} \tag{6}$$

where C_μ is a model constant (variable function in a different turbulence model).

A comprehensive description of the $sk-\varepsilon$ and the relatively recently developed improved models, namely Renormalized Group (RNG) $k-\varepsilon$ and realizable $k-\varepsilon$, can be found in the literature (Launder and Spalding, 1974; Orszag et al., 1996; Shih et al., 1995).

The second widely used two-equation model, introduced by Wilcox, is the $k-\omega$ model, also based on the isotropic eddy viscosity hypothesis described by Equation (5), but where the turbulent viscosity is computed as a function of k and ω.

Knowing, that $\omega = \varepsilon/k$, Equation (6) takes the following form:

$$\mu_t = \rho\alpha^* \frac{k}{\omega} \tag{7}$$

where α^* is a coefficient related to the use of functions damping the turbulent viscosity causing a low-Reynolds-number correction.

Contrary to the $k-\varepsilon$ model, the standard $k-\omega$ model uses enhanced wall treatment to solve low-Re-number flows in the viscous layer in near-wall region. Its improved variant, SST $k-\omega$ model, considered to be the most accurate from two-equation eddy viscosity models, provides modified turbulent viscosity formulation which account for the transport of the principal turbulent shear stress. A wider discussion on the standard and SST $k-\omega$ models can be found in Wilcox (Wilcox, 1998; Wilcox and Traci, 1976) and Menter (Menter, 1993, 1994).

The Reynolds Stress Model (RSM) (Launder et al., 1975; Versteeg and Malalasekera, 1995) is the most elaborate and complex turbulence model, referred as the Second Order Closure. In RSM the isotropic eddy viscosity hypothesis is discarded and the RANS equations are closed by solving transport equations for the Reynolds stresses, together with an equation for the dissipation rate, yielding seven additional transport equations to be solved in a 3D scheme. A detailed description of the RSM turbulent closure development can be found in the literature (Launder et al., 1975), whilst a summarised description of the turbulence models commonly used for RANS closure has been summarized in Table 1 (Bridgeman et al., 2009).

4.1.2. Alternative approaches — LES and DNS

Large Eddy Simulation (LES) is an alternative approach in hydrodynamic modelling where large, three-dimensional unsteady scale motions affected by the flow geometry, i.e. large eddies, are directly and explicitly solved in time-dependent simulation using space-filtered Navier—Stokes equations. LES is one of the most expensive simulation options and requires a refined grid to accurately resolve eddies in the boundary layer. A filtering operation, analogous to the Reynolds decomposition in RANS, is based on the decomposition of the velocity into the resolved (filtered) component $\overline{v}(x,t)$ and the residual, so called subgrid-scale (SGS) component $v'(x,t)$ (Pope, 2000). The accuracy of the LES model is the result of modelling only the SGS motions-the smallest eddies, which tend to have more universal properties (Karpinska Portela, 2013). The model commonly used to model small eddies is the Smagorinsky SGS model (Smagorinsky, 1963).

LES has been most successful for high-end applications where the RANS models fail to meet the required goals, e.g. modelling of combustion and mixing. Although it provides improved accuracy, wide application of LES approach to solve flow related issues is still limited due to the large mesh requirements and high computational costs.

Direct Numerical Simulation (DNS) is a high-fidelity tool offering the explicit solution of the whole range of turbulent time and length scales, from the Kolmogorov scales to large motion scales transporting most of the kinetic energy within the domain (Orszag, 1970). As a result, the computational cost of DNS is extremely high even at low Reynolds numbers, preventing this approach from being used as a general-purpose design tool, and making it impractical for most industrial flow conditions, especially large multiphase AS systems. Hence the CFD modelling of the AS tanks requires more computationally efficient and thus simplified methods.

4.2. Multiphase modelling

A robust understanding of the physics and biochemical processes in the gas-liquid-solid environment of the AS tank relies on accurate assessment of the transport phenomena and character of interactions between the phases. Numerical simulation of the multiphase flow in AS system is usually enabled by Euler—Euler or Euler-Lagrange approaches. Table 2 outlines the relevant characteristics of the multiphase models used in modelling of the AS systems.

In Eulerian (Eulerian—Eulerian or two-fluid) model, the phases are treated mathematically as separate and interpenetrating continua, hence the introduction of the phasic volume fractions — α_q. The sum of volume fractions is equal to unity

$$\sum_{q=1}^{n} \alpha_q = 1 \tag{8}$$

Each phase is governed by a set of continuity and momentum conservation equation, which have similar structure for all phases. Thus, considering n-phase system, the mass conservation equation for phase q is (Joshi, 2001; Ratkovich, 2010):

$$\frac{\partial}{\partial t}(\alpha_q \rho_q) + \nabla(\alpha_q \rho_q \overrightarrow{v}_q) - \sum_{p=1}^{n}(\dot{m}_{pq} - \dot{m}_{qp}) = 0 \tag{9}$$

where ρ_q is density and the term $\alpha_q\rho_q$ is the effective density of the

Table 1
Comparison of turbulence models used in ASP modelling. Adapted from Bridgeman et al. (2009) with permission from Taylor & Francis Ltd (www.tandfonline.com/).

Model	Comments	Advantages	Disadvantages
Standard $k-\varepsilon$ ($sk-\varepsilon$)	• Semi-empirical modelling of k and ε. • Valid only for fully developed turbulent flow cores (molecular diffusion ignored).	• Simplest and complete turbulence model. • Excellent performance for many flows. • Well established in academia and industry. • Robust, economic in terms of computational effort and satisfactory accuracy in diverse turbulent flow issues.	• Poor performance in some scenarios (strong streamline curvature, vortices, rotating flows, flow separation, adverse pressure gradients). • Assumes locally isotropic turbulence. • Poor prediction of the lateral expansion in 3D wall jets.
Renormalized Group (RNG) $k-\varepsilon$	• Based on the statistical methods, not observed fluid behaviour. • Mathematics is highly abstruse. Texts only quote model equations which result from it. • Effects of small-scale turbulence represented by means of random forcing function in Navier–Stokes equations. • Procedure systematically removes small scales of motion by expressing their effects in terms of larger scale motions and a modified viscosity. • Similar in form to $sk-\varepsilon$, but modified ε equation to describe high-strain flows better. • Differential equation solved for μ_t (changes C_μ from 0.09 to 0.0845 at high Re).	• Improved performance for swirling and high-strained flows compared to $sk-\varepsilon$.	• Less stable than $sk-\varepsilon$.
Realizable $k-\varepsilon$	• Recent development. In highly strained flows, the normal Reynolds stresses become negative (unrealizable condition), so μ_t uses variable C_μ. • C_μ is function of local strain rate and fluid rotation. • Different source and sink terms in transport equations for eddy dissipation. • Good for spreading rate of round jets.	• Suited for planar and rounded jets, swirling and separating flows and wall-bounded flows with strong adverse pressure gradients.	• Not recommended to use with multiple reference frames.
Standard $k-\omega$	• Specific dissipation rate is $\omega=\varepsilon/k$. • $sk-\varepsilon$ solves for dissipation of turbulent kinetic energy, $k-\omega$ solves for rate at which dissipation occurs. • Resolves near wall region without wall functions so can be applied through boundary layer.	• Valid throughout to boundary layer, subject to fine grid resolution. • Accounts for the stream-wise pressure gradients. • Applicable for detached, separated flows and fully turbulent flows.	• Pressure induced separation is typically predicted to be excessive and early.
Shear Stress Transport (SST) $k-\omega$	• As $k-\omega$ except from gradual change from $k-\omega$ to inner region of boundary layer to high Re version of $sk-\varepsilon$ in outer part. • Modified μ_t formulation to account for transport effects of principal turbulent shear stresses.	• The most accurate from two-equation eddy viscosity models. • Suitable for adverse pressure gradients and pressure-induced flow separation. • Accounts for the transport of the principal shear stresses.	• Less suitable for free shear flows.
Reynolds Stress Model (RSM)	• The most general and complex of all models solving transport of the Reynolds stresses- so called seven-equation model • Isotropic eddy viscosity hypothesis is discarded.	• Accurate calculation of the mean flow properties and all Reynolds stresses. • Accounts for the streamline curvature, rotation and rapid changes in strain rate yielding superior results to two-equation models for complex flows, e.g. with stagnation points.	• Computationally expensive. • Not always more accurate than two-equation models. • Harder to obtain converged result. • Reliability of RSM predictions are still limited by the closure assumptions employed to model pressure-strain and dissipation-rate terms.

phase q, $\vec{v}_q$ denotes its velocity, $\dot{m}_{pq}$ and $\dot{m}_{qp}$ are mass transfer mechanisms from phase p to q and from q to p, respectively.

The generalized momentum conservation equation for phase q can be written in the simplified form as (Azzopardi et al., 2011; Ratkovich, 2010):

$$\frac{\partial}{\partial t}\left(\alpha_q \rho_q \vec{v}_q\right) + \nabla\left(\alpha_q \rho_q \vec{v}_q \vec{v}_q\right) = -\alpha_q \Delta p + \nabla \mu_q \left(\nabla \alpha_q \vec{v}_q + \nabla \alpha_q \vec{v}_q^{\,T}\right) + \rho_q \vec{g} + \vec{F}_q \quad (10)$$

Table 2
Summary of approaches to multiphase modelling.

Model	Concept	Modelling	Applicability	Issues
Eulerian	Each phase modelled as a separate fluid.	A set of averaged, volume fraction-weighted Navier–Stokes (NS) equations per phase. Momentum transfer terms and constitutive equations to be modelled.	Theoretically, every type of flow; depending on the additional terms' modelization.	Additional terms' modelization is determinant, but their modelling is difficult.
VOF	Each phase modelled as a separate fluid. The interface between the phases is tracked.	Interface tracked via a continuity equation and the domains of the single phases are defined. A set of phase-specific NS equations with momentum exchange terms is solved for each domain.	Flows where the interphase surface is clearly defined (e.g. a single, large bubble inside a liquid).	Inapplicable if the interphase surface is too complex (e.g. bubbly flow where bubble dimensions are smaller than single cell size).
Mixture	Both phases treated as a whole.	Single set of NS equations. Effective mixture density and viscosity to be modelled.	Homogeneous fluids or non-homogeneous fluids that are treated as homogeneous.	Inapplicable in every case in which there is clear distinction between the phases.
Eulerian-Lagrangian	Liquid phase treated with Eulerian approach. Every particle (bubble) tracked along trajectory.	A set of averaged NS equations for the liquid phase. A set of Newton's 2nd Law (N2L) equations applied to all particles. Momentum transfer terms in both NS and N2L to be modelled.	Flows where at least one phase is clearly dispersed into a principal phase. Particles smaller than mesh cell size.	Computational expense not a priori computable, and proportional to the particles number. May be prohibitive for high particle numbers.

where p is pressure shared by all phases, μ_q denotes shear viscosity of phase q, $\vec{F}_q$ represents the sum of interfacial forces between the continuous and dispersed phases.

Considering gas–liquid system, the fluid flow around the bubbles is characterized by the occurrence of relative motion between the phases yielding local pressure and shear stress gradients. As a result, relative motion of the bubbles will be affected by a drag force which is predominant in conditions of the uniform flow. In case of non-uniform bubble motion, the concept of interfacial forces $\vec{F}_q$ needs to account for drag and various non-drag forces, such as virtual mass force, lateral lift force, wall lubrication force, turbulent dispersion force, Basset force and momentum transfer associated with mass transfer. Accordingly, the closure of Equation (11) requires correct assessment of the interfacial forces, typically using analytical models, empirical correlations and coefficients (e.g. drag coefficient), described comprehensively in Clift et al. (1978), Joshi (2001), Azzopardi et al. (2011) and Yang and Mao (2014). Many of these relations are case-specific and based on limited data what yields difficulties in exploring complex multiphase systems (Azzopardi et al., 2011; Manninen et al., 1996) and influencing the outcomes of the CFD simulations.

The Eulerian model is commonly used in multiphase systems, where momentum exchange between the phases is significant, e.g. gas–liquid flow in aeration tanks or solid–liquid flow in AS systems, especially in the case of zones with high solids concentrations, where solid–solid interactions are relevant; transitional zones with steep solids concentrations gradients (from high to low concentration), where momentum of the solid phase is relevant to model its dissipation (Samstag et al., 2015).

The Volume of Fluid (VOF) model is a single-fluid approach based on a surface tracking technique that solves the momentum equations for the continuous phase while the dispersed phase follows the closure conditions of the volume fraction for the incompressible flow (Wang et al., 2013). While the phases are immiscible, the fields for all variables and properties are shared and represented by volume-average values. Therefore, the continuity equation has the following form (Ratkovich, 2010; Vedantam et al., 2006):

$$\frac{\partial \alpha_q}{\partial t} + \nabla(\alpha_q \vec{v}_q) = 0 \tag{11}$$

where the computation of the primary-phase volume fraction is based on the constraint defined by Equation (9).

The single momentum equation, which is solved throughout the domain yielding velocity field shared by the phases, is expressed as:

$$\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla(\rho \vec{v} \vec{v}) = -\Delta p + \nabla\left[\mu\left(\nabla \vec{v} + \nabla \vec{v}^T\right)\right] + \rho \vec{g} + \vec{F} \tag{12}$$

The properties ρ and μ appearing in the transport equations are determined by the presence of the component phases in each control volume. Considering two-phase (q and p) system if the volume fraction of phase q is being tracked, the density in each cell is given by (Ratkovich, 2010; Vedantam et al., 2006):

$$\rho = \alpha_q \rho_q + (1 - \alpha_q)\rho_p \tag{13}$$

The relationship described by Equation (13) is based on the fact, that for an n-phase system, the volume-fraction-averaged density is

$$\rho = \sum \alpha_q \rho_q \tag{14}$$

All other properties (e.g. volume-fraction-averaged viscosity, μ) are computed in the same manner.

VOF is designed for modelling multiphase systems where the position of the interface between the immiscible fluids is of interest. This approach has found application in modelling of stratified and free-surface flows, filling, sloshing, and motion of large bubbles (slug flow). Examples of VOF application to model Membrane Bioreactors (MBRs) can be found in the literature (Andersson et al., 2011; Ratkovich et al., 2009; Wang et al., 2013).

The Eulerian-algebraic (slip mixture or algebraic slip) model is a simplified multiphase model used for two or more phases, treated as interpenetrating continua. This single-fluid approach can be used to model phases moving at different velocities-by using concept of slip (or drift) velocities.

Here, the continuity and momentum equations are solved for the mixture and algebraic equations are used to solve relative velocities to describe the dispersed phases. Thus, the continuity equation for the mixture is (Manninen et al., 1996):

$$\frac{\partial \rho_m}{\partial t} + \nabla(\rho_m \vec{v}_m) = 0 \tag{15}$$

where the mixture density, ρ_m is defined as:

$$\rho_m = \sum_{q=1}^{n} \alpha_q \rho_q \tag{16}$$

and the mass-averaged mixture velocity $\vec{v}_m$ is:

$$\vec{v}_m = \frac{1}{\rho_m} \sum_{q=1}^{n} \alpha_q \rho_q \vec{v}_q \tag{17}$$

The mass fraction of phase q is defined as:

$$c_q = \frac{\alpha_q \rho_q}{\rho_m} \tag{18}$$

The momentum equation for the mixture is obtained from the following formula (Ratkovich, 2010):

$$\frac{\partial}{\partial t}(\rho_m \vec{v}_m) + \nabla(\rho_m \vec{v}_m \vec{v}_m) = -\Delta p + \nabla\left[\mu_m\left(\nabla \vec{v}_m + \nabla \vec{v}_m^T\right)\right] + \rho_m \vec{g} + \vec{F} + \nabla\left(\sum_{q=1}^{n} \alpha_q \rho_m \vec{v}_{dr,q} \vec{v}_{dr,q}\right) \tag{19}$$

where μ_m is mixture viscosity equal to:

$$\mu_m = \sum_{q=1}^{n} \alpha_q \mu_q \tag{20}$$

and $\vec{v}_{dr,q}$ is drift velocity for the secondary phase q expressed as follows:

$$\vec{v}_{dr,q} = \vec{v}_q - \vec{v}_m \tag{21}$$

The slip velocity of the secondary phase (p) relative to the velocity of the primary phase (q) is computed as follows:

$$\vec{v}_{pq} = \vec{v}_p - \vec{v}_q \tag{22}$$

The relation between drift and slip velocities can be written as:

$$\vec{v}_{dr,q} = \vec{v}_{pq} - \sum_{q=1}^{n} c_q \vec{v}_q \tag{23}$$

The basic assumption of the algebraic slip mixture model is that a local equilibrium between the phases should be reached over a short spatial length scale. For the phases moving with the same velocity, the mixture approach can be used to model homogeneous multiphase flow (Manninen et al., 1996; Wicklein and Samstag, 2009). However, this approach is usually not recommended in cases when the interface laws are not well known (Ratkovich, 2010). This model has been successfully used to simulate sediment-induced density currents, and thus solid–liquid mixing in AS tanks, and turbulent transport of suspended solids in secondary clarifiers (Samstag et al., 2015; Wicklein and Samstag, 2009; Yeoh and Tu, 2009), but also a gas–liquid turbulent flow in closed loop bioreactors (Xu et al., 2010; Yang et al., 2011).

Another method to deal with multiphase flow in AS systems is via the modelling of turbulent transport of the secondary phase within a continuous primary phase. The transported phase (species) is treated as an active or passive scalar (density, viscosity, temperature, dissolved oxygen or solids), hence the effects of its gradients across the domain can be either coupled to the momentum equation as an equation of state or treated as a passive property transported by the fluid flow.

Therefore prediction of local mass fraction of each species, $Y_{i'}$, is modelled by solving conservation equation describing convection and diffusion of the i'-th species (Cartland Glover et al., 2000):

$$\frac{\partial}{\partial t}(\rho Y_{i'}) + \nabla(\rho \vec{v} Y_{i'}) = -\nabla \vec{J}_{i'} + R_{i'} + S_{i'} \tag{24}$$

where $\vec{J}_{i'}$ is the i'-th diffusive mass flux of species; $R_{i'}$ is net rate of production of i'-th specie due to chemical reaction; $S_{i'}$ is the source term which injects i'-th specie into the domain by addition from the dispersed phase plus any user-defined sources.

The active/passive scalar approach is used to model solid–liquid interactions in the systems with lower solids concentrations (Combest et al., 2011; De Clercq, 2003; Samstag et al., 2015; Wicklein and Samstag, 2009) and to model oxygen mass transfer in aerated tanks (Fayolle et al., 2007).

In the Lagrangian model, the governing phase (fluid) is treated as a continuum by solving time-averaged Navier–Stokes equations (Eulerian reference frame), while the behaviour of secondary phase (e.g. solids) is predicted by tracking a large number of particles using random-walk Lagrangian trajectory calculations for dispersed phase through the flow field of the continuous phase. Here, the particles can exchange momentum, mass, and energy with the fluid phase. The particles' trajectories are predicted by integrating the force balance on the single particle and recording the particle position. This force balance, which equates the particle inertia with the forces acting on it is defined as (Bridgeman et al., 2009):

$$\frac{\partial \vec{v}_P}{\partial t} = \frac{\vec{v} - \vec{v}_P}{t_r} + \frac{\vec{g}(\rho_P - \rho)}{\rho_P} + \vec{F} \tag{25}$$

where $\vec{v}_P$ is particle velocity and $\vec{v}$ is fluid phase velocity, the term $\vec{v} - \vec{v}_P/\tau_r$ represents drag force per unit particle mass, t_r is particle relaxation time, ρ_P and ρ are particle and fluid densities, respectively; and $\vec{F}$ relates to additional forces that are relevant under special circumstances; for example virtual mass and pressure gradient forces, or forces on particles that arise due to rotation of the reference frame.

Additionally, particle–particle interactions, such as collisions and momentum exchange can be enabled through the introduction of drag coefficients (Bridgeman et al., 2009; Karpinska Portela, 2013). This approach is suitable to simulate gas–liquid flow in aeration tanks, however should not be used when the volume fraction of the secondary (particulate) phase exceeds 10–12% (Sokolichin et al., 1997), as e.g. solid–liquid flow in complete mixed AS systems.

Apart from multiphase modelling, particle tracking within the Lagrangian reference frame is a useful tool to simulate RTDs in process tanks (Danckwerts, 1953; Levenspiel, 1999), and so to assess the macromixing, established by convective flow patterns (Karpinska Portela, 2013; Le Moullec et al., 2008). However, the main limitation here is the number of particles being tracked within the simulated system, and in the case of a full-scale AS tank, tracking too many particles will result in extensive computational times. Thus, when comparing workability of different approaches in multiphase modelling, the Lagrangian approach is the most expensive, involving long computational times and requiring a large number of CPUs (Central Processing Units), so limiting its popularity in the simulation of wastewater treatment tanks.

5. Application of CFD in ASP

Biological wastewater treatment systems require enhanced transfer of oxygen into the AS tanks to maintain aerobic processes occurring in biodegrading-nitrifying biomass. Enhanced oxygen mass transfer in most common ASP configurations i.e. channel or closed-loop bubbly flow AS reactors aerated by diffusers, can be achieved by maximisation of the surface area of the interface between the dispersed phase (air/oxygen bubbles) and the continuous phase (mixed liquor). Nonetheless, in most wastewater utilities, designs of AS tank and aeration system, and furthermore process control are based on static models and simple PID controllers, and so a major concern remains the accurate determination of tank hydrodynamics and its impact on DO profiles within the basin. Therefore, improvement of biochemical conversion efficiencies, hydraulic and process design, and reliable operation of AS systems rely on an improved understanding of the bioreactors' behaviour, with emphasis on micro- and macro-scale mixing and, in particular, on the analysis of the interactions between the mixed liquor circulation imparted by mechanical agitation and the fluid and sludge flocs motions induced by the air bubbles. The key advantage of CFD as a virtual modelling technique is powerful visualization capability allowing detailed characterization of the local-scale phenomena in varying operating conditions. Hence, CFD can be used as a robust tool for the design of either new efficient and energy optimised unit processes at WWTPs or for "tune for benefit" optimization of performance and even retrofitting of existing AS systems.

The complete CFD simulation of a biologically active gas-liquid-solid AS system is challenging, due to the complex hydrodynamics and biochemical reactions of conversions involved, resulting in massive computational resources required in terms of RAM and CPU usage and with long computational times involved. Furthermore, increasing complexity of the model involved, mesh resolution and solution accuracy may lead to distinctly higher costs of the CFD analysis, yet lower than a capital investment in a new layout. To avoid overly long and complex CFD runs (Karpinska Portela, 2013; Le Moullec et al., 2010b), common engineering practice has been to model the AS processes separately (e.g. aeration system performance or flow field within the basin) and afterwards to couple the results (Pereira et al., 2012). In addition to that, depending on the purpose of the CFD analysis, data collection for model calibration and validation using advanced measurement techniques, may be absolutely required and yet time and resource consuming (Nopens et al., 2012).

It is worth mentioning, that despite the current successful spread and usage of CFD modelling, potential risk of its misuse due to poor model choice, wrong setup assumptions or interpretation of the results, has been also recognized (Nopens et al., 2012).

5.1. Development of new aeration devices

CFD simulations have been used as a high-tech design tool in the development of new aeration devices and optimisation of their spatial arrangement in wastewater treatment tanks.

A computationally inexpensive modelling procedure, based on 3D steady-state and single-phase flow simulations with the $sk{-}\varepsilon$ turbulence model was used by Morchain et al. (2000) to study the impact of the spatial distribution of the cross-flow hydro-ejectors on the recirculation and the oxygen mass transfer in a large tank for wastewater treatment. Although the cross-flow hydro-ejectors generate two-phase flow, it was shown experimentally that the momentum transfer is not significantly affected by the presence of bubbles and thus the velocity field could be obtained using a single-phase model, while the oxygen transfer in the tank was enabled by the introduction of transport species.

The same single-flow modelling scheme was applied to modify geometry and operating scenarios of a curved blade mechanical aerator intended for use in oxidation ditches (Bhuyar et al., 2009). The results, which were in good agreement with the experimental data, allowed optimization of blade design and the aerators' submergence, and reductions to rotational speed range, yielding enhanced aeration efficiencies when compared with conventional mechanical devices.

Despite higher computational costs, transient gas–liquid simulations involving URANS with the $sk{-}\varepsilon$ turbulence model and one of the Euler–Euler multiphase models have found applications in the development of new aeration techniques, as they provide direct and more accurate analysis of the multiphase reactor systems. Xu et al. (2010) simulated an oxidation ditch equipped with cylindrical airlift aerators. Here the CFD simulations of the fluid flow in an airlift oxidation ditch served to verify the feasibility of the preliminary design and to assess its applicability for municipal wastewater treatment. The results from the simulations (which were validated in a bench-scale ditch) emphasized the suitability of the proposed aeration system for deep tank ditch configurations.

Karpinska Portela (2013) used CFD to focus on overcoming oxygen transfer efficiency limitations of membrane diffusers via the introduction of an independent external aeration unit, designed as a continuous flow component included in the mixed liquor recirculation loop. Similar to the previous work, CFD simulations of aeration within several device configurations provided an excellent design tool for selection of the most efficient geometry, characterized by the highest value of SOTE. The aeration process parameters determined from pilot-scale aeration tests matched the predictions obtained from the CFD simulations.

A more detailed description of the CFD approaches used in the development of aeration devices is shown in Table 3.

5.2. Evaluation of the performance of the existing aeration systems

Robust and energy efficient operation of complex AS reactor systems relies on an understanding of the multiphase nature of the AS tank and on the assessment of the impact of the aeration system on the mixing, biological treatment efficiency and associated energy expenditure, while taking into account the number, type and spatial distribution of the aeration and mixing devices. This section considers CFD approaches used to determine the dynamic behaviour of aeration tanks, and for which descriptions are summarized in Table 4.

5.2.1. Gas-liquid models

When considering fluid flow within an aeration tank, the use of gas–liquid CFD models enables relatively fast and straightforward

Table 3
CFD studies of new aeration devices.

Author	Code	Device	Scale	Dim.	Turbulence model	Extra model	Validation
Bhuyar et al. (2009)	Fluent	Curved blade mechanical aerator	Lab	3D	RANS + $sk{-}\varepsilon$	Transport species + chemical reaction	K_La measurements
Xu et al. (2010)	Fluent	Airlift aerator	Lab	3D	URANS + $sk{-}\varepsilon$	Mixture	Particle Dynamic Analysis (PDA)
Karpinska Portela (2013)	Fluent	Pressurized Aeration Chamber	Lab	3D	URANS + $sk{-}\varepsilon$	Mixture	K_La measurements

Table 4
CFD modelling of aeration in activated sludge tanks.

Aim	Reference	Code	Scale	Dim.	Mesh size	Model	Multiphase model	Extra model	Validation
Numerical modelling of an oxidation ditch aerated with diffusers and agitated by impellers.	Cockx et al. (2001), Do-Quang et al. (1999)	Astrid	Full	2D	n/a	RANS + $sk{-}\varepsilon$	Gas-liquid Eulerian	Transport eq. for oxygen	–
CFD studies of the oxidation ditches-coupling of hydrodynamic with biokinetics modelling.	Glover et al. (2006)	Fluent	Lab pilot, full	3D	n/a	RANS + $sk{-}\varepsilon$	Gas-liquid Eulerian	Lagrangian, transport eq. for oxygen + complete biokinetics (ASM1)	DO, COD, NH_4, NO_3 measurements
Prediction of the oxygen transfer in oxidation ditches.	Fayolle et al. (2007)	Fluent	Pilot, full	3D	29k–452k	URANS + $sk{-}\varepsilon$	Gas-liquid Eulerian	Transport eq. for oxygen (each phase)	MDV, DO measurements
RTD of an aerated channel bioreactor.	Le Moullec et al. (2008)	Fluent	Lab	3D	350k	RANS + $sk{-}\varepsilon$/RSM	Gas-liquid Eulerian	Lagrangian	LDV, tracer experiments
Simulation of the hydrodynamics and reactions in activated sludge channel reactor.	Le Moullec et al. (2010a), b), Le Moullec et al. (2011)	Fluent	Lab	3D	50k	RANS + $sk{-}\varepsilon$	Gas-liquid Eulerian	Transport eq. for	
	oxygen + biokinetics (ASM1)	LDV,	bubble size			measurements	Impact of the surface aeration on the solids distribution in the oxidation ditch.	Fan et al. (2010)	Fluent
Lab	3D	70.3k	RANS + $sk{-}\varepsilon$		Solid-liquid Eulerian	–	PDA		
Effect of aeration patterns on the flow field in the conventional AS tank.	Gresch et al. (2011)	CFX	Full	3D	400k	URANS + SST $k{-}\omega$	Gas-liquid Eulerian	Biokinetics-consumption of NH_4	ADV, reactive tracer experiments
Modification of the operation conditions in the oxidation ditch to enhance energy efficiency.	Yang et al. (2011)	Fluent	Full	3D	1.66M	RANS + $sk{-}\varepsilon$	Gas-liquid mixture	Transport eq. for oxygen + biokinetics-consumption of BOD	MDV, DO measurements
Evaluation of jet aeration and mixing in sequence batch reactors.	Samstag et al. (2012)	Fluent	Full	3D		URANS + $sk{-}\varepsilon$	Gas-liquid mixture	Density-coupled model- solids settling	MLSS measurements
RTD of an oxidation ditch aerated with hydrojets.	Karpinska Portela (2013); Karpinska et al. (2015)	Fluent	Pilot	3D	600k	RANS + $sk{-}\varepsilon$, URANS + $sk{-}\varepsilon$, LES + Smagorinsky SGS	–	Lagrangian	–
Studies on flow field and sludge settling in Carrousel oxidation ditch.	Xie et al. (2014)	Fluent	Full	3D	1.53M	URANS + $sk{-}\varepsilon$	Solid-liquid mixture	Slip velocity-sludge settling	MDV, MLSS measurements
A complete model to predict hydrodynamics, oxygen transfer and biokinetic reactions in an oxidation ditch.	Lei and Ni (2014)	Fluent	Pilot	3D	162k	RANS + $sk{-}\varepsilon$	Gas-liquid-solid mixture	Transport eq. for oxygen + biokinetics- (ASM1)	ADV, DO, COD, MLSS, NH_4, NO_3 measurements

ADV – Acoustic Doppler Velocimetry, MDV – Mono-directional Velocimetry, PDA – Particle Dynamic Analysis, LDV – Laser Doppler Velocimetry.

prediction of the multiphase velocity field induced by the aerators and mixers, bubble sizes and local gas hold-up, i.e. process parameters that have significant impact on the oxygen mass transfer in bioreactors, but either require time- and resource-expensive experimental techniques or are not taken into account in the analysis of the experimental results (Fayolle et al., 2007; Gillot et al., 2005; Gillot and Héduit, 2000; Le Moullec et al., 2008; Vermande et al., 2007).

Hence the focus of early CFD works was on a better understanding of mass transfer phenomena in full scale closed-loop aeration tanks equipped with membrane diffusers and agitated by means of horizontal slow speed impellers (Cockx et al., 2001; Do-Quang et al., 1999). 2D two-phase flow in the aeration tank was simulated using an Eulerian model for imposed, constant gas bubble size. To simplify numerical simulations, an equivalent uniform liquid velocity field was imposed in the section of the impellers. The oxygen mass transfer was obtained via introduction of the global volumetric mass transfer coefficient, K_La, determined experimentally, as a transport source term. Here, the correct estimation of the absolute values of oxygen transfer requires assessment of the most uncertain aeration process parameter, i.e. the alpha-factor, quantifying the impact of the contaminants and process conditions on the oxygen transfer rates-in this work-the impact of the imposed constant bubble diameter on the gas–liquid interface surface area (Nopens et al., 2015; Rosso et al., 2011; Rosso and Stenstrom, 2006).

The results from the simulations showed that the hydrodynamics of these tanks was controlled by mutual competition between vertical gas plume and horizontal fluid flow currents. Thus, in the absence of the horizontal flow motion, the interactions between gas plumes released by diffusers generate vertical, massive liquid loop circulations, i.e. spiral flow, yielding low gas hold-up. Contrary to that, under conditions of horizontal liquid motion imparted by e.g. rotating impellers, the increase in wastewater velocity causes neutralization of the spiral flow patterns, inclination of the vertical gas plume, and dispersion of the bubbles and, as a consequence, longer contact times between the phases yielding better gas retention in the tank. As a result, the increase of the global mass transfer coefficient in the closed-loop tanks was found to be associated exclusively with fluid circulation.

The impact of the fluid velocity on oxygen mass transfer was later confirmed in experimental studies (Abusam et al., 2002). It was reported that even small changes in the axial velocity may have a dramatic effect on the oxygen profiles, and thus on the ammonia removal in oxidation ditches. Therefore in these closed-loop AS systems, horizontal fluid velocity should be treated as an important process variable to control total nitrogen removal efficiency.

A clear shortcoming of the discussed work (Cockx et al., 2001; Do-Quang et al., 1999) is that the 2D modelling is insufficient to represent mutual interactions between the neighbouring gas plumes causing formation of the more complex, three-dimensional flow structures. Moreover, the impact of the flow circulation on the size of the bubbles released by membrane diffusers was neglected; yet this plays a key role in the oxygen mass transfer within the aeration tank. Nevertheless, despite these weaknesses and the lack of experimental validation, conclusions from this work provided valuable research background for many successive numerical and experimental studies.

Subsequent studies (Fayolle et al., 2007) addressed development of a more complete numerical tool, to predict oxygen mass transfer in a number of pilot- and full-scale oxidation ditches of various configurations and where aeration is dissociated from mixing by the introduction of membrane diffusers and slow speed mixers. The aeration was simulated using Eulerian model for water and air. Mixing was modelled using fixed value method by imposing flow characteristics induced by agitation on the grid zones corresponding to mixers location. This method gives good prediction of the average experimental axial velocity. Similar to earlier CFD works (Cockx et al., 2001; Do-Quang et al., 1999), Fayolle et al. (2007) showed that oxygen mass transfer in closed-loop AS basins aerated with diffusers is linked to the number, type, spatial distribution and performance of the agitators (Fayolle et al., 2007, 2010, 2006; Vermande et al., 2007), The impact of the ascending bubbles released by the diffusers on the velocity profile along the oxidation ditch can be seen in Fig. 1. It was also showed that implementation of more complex modelling approach accounting

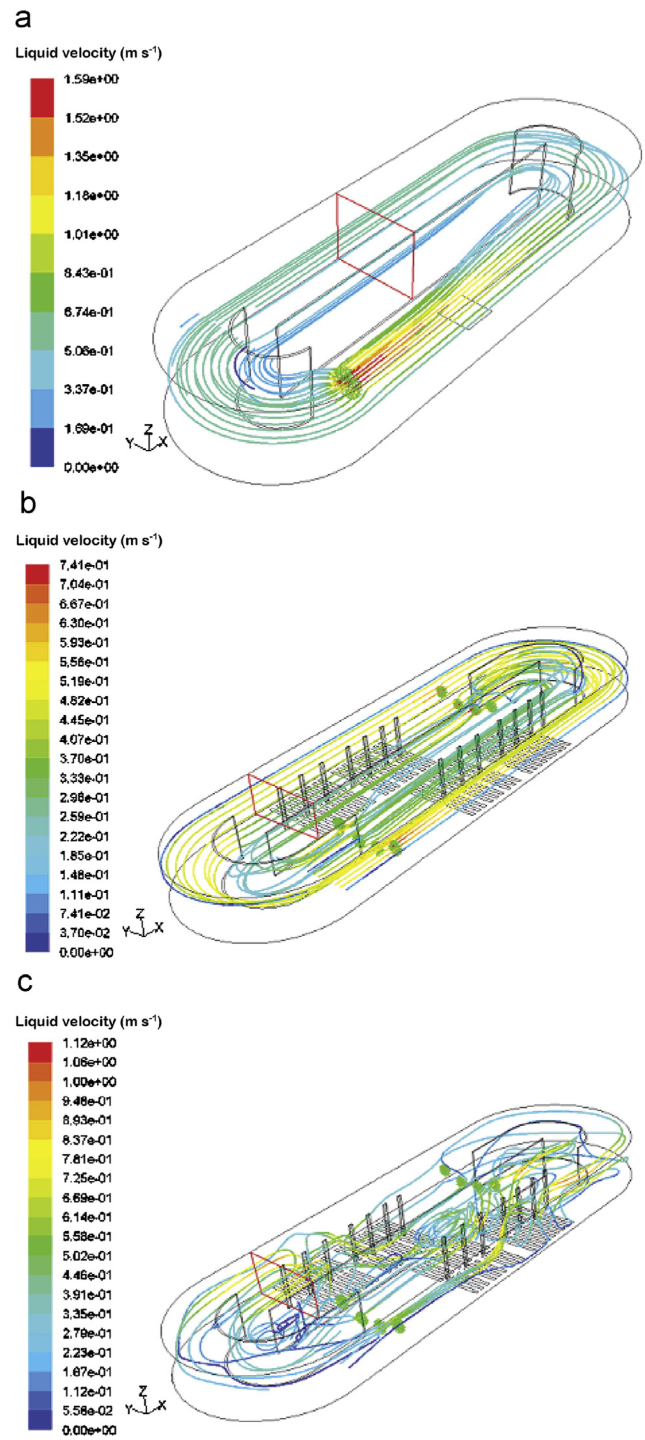

Fig. 1. Streamlines coloured by liquid velocity magnitude U_L in tank (a) without aeration ($U_L = 0.35$ ms^{-1}) (b) without aeration ($U_L = 0.27$ ms^{-1}) and (c) with aeration ($U_L = 0.23$ ms^{-1}). Reprinted from Fayolle et al. (2007). Copyright (2007) with permission from Elsevier.

for the impact of the bubble size on the axial fluid velocities and on the global gas hold-up profile within the tank, was able to reproduce precisely the values of K_La with high accuracy ($\leq$5%). Nonetheless, it was found, that the predicted accuracy depends on the assumed value of inlet bubble size, emphasizing the necessity either to measure *in situ* bubble diameter or apply an appropriate numerical model estimating bubble sizes at the diffuser level. A shortcoming of Fayolle et al. (2007) is that although the proposed CFD protocol appears to be suitable for the prediction and optimization of oxygenation capacities in a full scale AS tank, it is based on clean water–air simulations. However, for robust analysis of agitation system performance, the impact of the velocity on the local solids content and density gradients should be considered.

Yang et al. (2011) focused on predicting the flow pattern and oxygen mass transfer in a multichannel oxidation ditch aerated with horizontal rotors and agitated with submerged mixers (a Carrousel). Experimental field data showed that under existing operational conditions, DO concentration in the anoxic zone exceeded 1.0 mg/L, inhibiting the denitrification process. Thus, the aim of the CFD study was to determine an operational regime for the surface aerators, which would lead to formation of stronger DO gradients in the anoxic zone, yielding a reduction in energy expenditure for aeration while maintaining high treatment efficiencies. The modelling procedure involved a two-phase mixture approach, enhanced with additional transport equations related to the transfer of oxygen introduced by rotors and biochemical reaction of oxygen consumption for BOD removal. To reduce computational expenses related to the modelling of a number of rotating devices, the large surface aerators were simulated using moving wall model, while actuator disk (fan) approach was used to simulate submerged mixers. Although an energy efficient operating scheme for the ditches was developed, this study was based on average flow and constant influent quality parameters, thus the validity of the optimal operating conditions deduced from the steady-state is limited.

More recent CFD studies on the aeration of conventional AS tanks (Gresch et al., 2011) provided further and more detailed analysis of the flow field induced by porous diffusers. The CFD approach proposed in this work consisted of the gas–liquid Eulerian multiphase model, where the physical properties of the continuous phase were approximated to those of activated sludge.

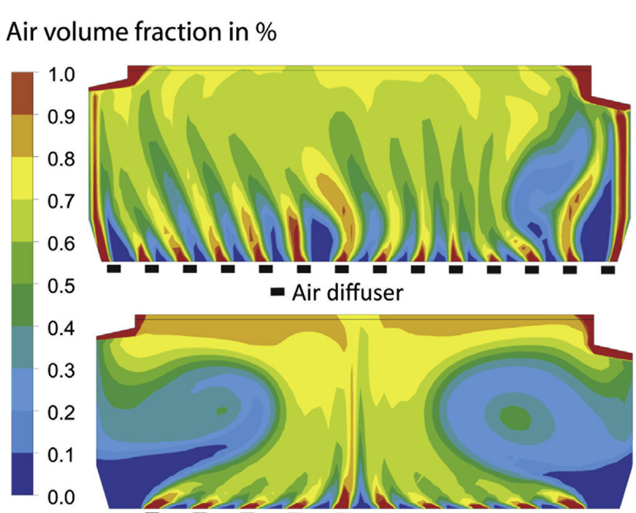

Fig. 2. Snapshot of air volume fractions at two cross sections with different diffuser patterns. Reprinted from Gresch et al. (2011). Copyright (2011) with permission from Elsevier.

Moreover, instead of solving additional transport equations for oxygen transfer, hydrodynamic simulations were enhanced with a biokinetic model for nitrification. The results from CFD studies validated experimentally in a full-scale plug flow AS tank complemented conclusions from earlier work (Cockx et al., 2001; Do-Quang et al., 1999) and provided a comprehensive description of the spiral flow generated by changing diffuser layout, its impact on the velocity field, air hold-up (Fig. 2), and ammonia degradation. It was also shown that, contrary to the closed-loop basins, in plug flow AS lanes without flow boosters, the flow field determines the aeration efficiency and the intensity of the longitudinal mixing, which are significantly reduced by either occurrence of non-aerated zones at the sidewalls or the rolling motion of the fluid generated by changes in diffusers layout.

5.2.2. Density-coupled models

In recent years, multiphase modelling of AS tanks based on gas–liquid neutral density simulations has become common practice for evaluation of both aeration and mixing, mainly because it enables faster setup of the lab-scale validation, usually involving use of tap water and air only. However, CFD studies on a sequencing batch reactor equipped with conventional jet aeration system (Samstag et al., 2012) showed that use of neutral density may lead to over-prediction of the degree of mixing. In this work, a density-coupled CFD model incorporating solids settling and transport was calibrated to field data and used to evaluate capacity of the jet aeration system in keeping the solids suspended and to determine power consumption for pumping considering two operating modes: mixing with and without air. The authors found that in order to generate complete information about activated sludge mixing, complementary CFD studies based on density-couple modelling are required to predict local density gradients due to the impact of the flow regime on solids transport. While this work underlines the importance of the analysis of the aeration systems with respect to the activation sludge mixing, the approach is rarely used by the wastewater modelling community for AS tanks, and only limited works can be found in the literature (Jensen et al., 2006; Laursen, 2007; Samstag et al., 1992, 2012, 2015; Wicklein and Samstag, 2009).

Recently Xie et al. (2014) considered prediction of the mixing and suspended solids distribution in a full-scale Carrousel ditch equipped with surface aerators and submerged impellers. The simulation procedure involved a solid–liquid mixture model, where the sludge settling was coupled through the slip velocity. Similar to the earlier work by Yang et al. (2011), surface rotors and submerged mixers were simulated using moving wall and fan models. The resulting mixing patterns and solids profiles throughout the ditch, shown in Fig. 3, facilitated identification of the stagnation regions affected by the sludge settling, and resulted in optimization of the operation scenario.

Previously, Fan et al. (2010) simulated a single-channel oxidation ditch aerated by means of inversed umbrella surface aerators using a solid–liquid two-fluid Eulerian model. The operating aerators were simulated using Multiple Reference Frames (MRF) approach. This work also focused on a detailed description of the mixing regime induced by the operating aeration system, aiming to select the optimal range of aerator speed ensuring the most uniform distribution of the solids within the ditch, and thus prevents solids settling.

Thus, the literature shows that the use of density-coupling is well founded to assess sludge mixing in agitated AS systems, however its applicability to study bubbly bioreactors is still uncertain.

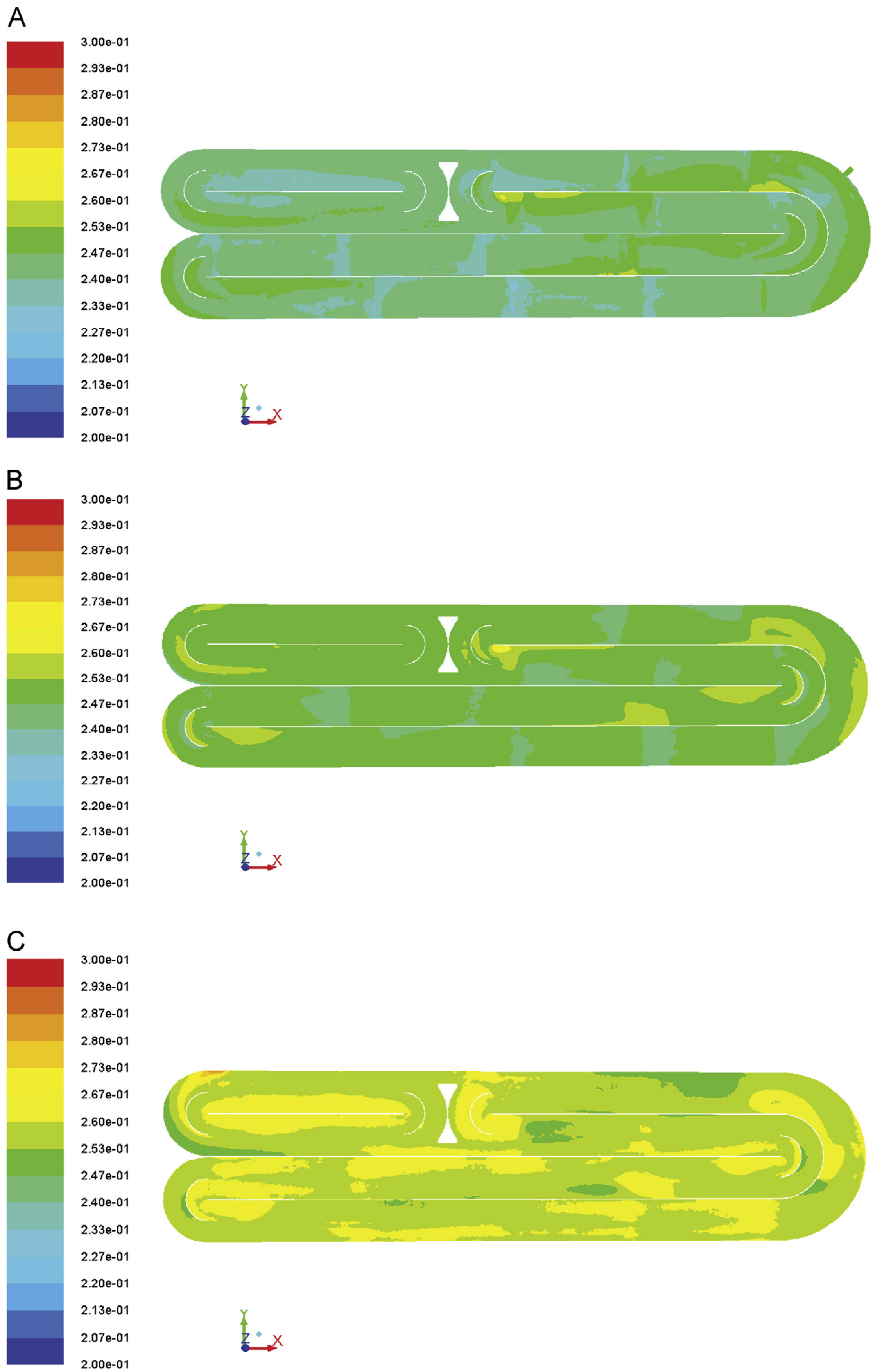

Fig. 3. Contours of volume fraction of solid phase at different height: (A) top of the tank, (B) middle of the tank, and (C) bottom of the tank. Reprinted from Xie et al. (2014). Copyright (2014) with permission from Elsevier.

5.2.3. Residence time distribution of AS tanks

Although rarely used to simulate the aeration process itself, CFD modelling based on the Lagrangian multiphase approach with particle tracking can be used as a tool for evaluation of the aeration system performance through the assessment of the macromixing, and thus the overall transport phenomena in a bioreactor. The literature offers numerous examples of studies on aeration and/or agitation systems responsible for different flow patterns within the tank, and thus having an impact on the mixing at micro- and macro-scale in AS systems. Considering different advection paths of the fluid elements within an aerated continuous flow channel or closed-loop bioreactors for wastewater treatment, RTD data obtained from CFD simulations can be used successfully to predict such adverse phenomena as segregation of the flow resulting in short-circuiting (channelling), recycling of the flow, or formation of dead zones. RTD data can also be used to assess the mixing time, which can be of crucial importance for oxygen transfer and impact on chemical and biochemical reaction yield. Data can also be used for troubleshooting of the reactor and improved design of the future vessels (Brannock, 2003; Karpinska et al., 2015; Karpinska Portela, 2013; Kjellstrand, 2006).

Glover et al. (2006) considered oxidation ditches aerated by bottom diffusers and agitated by slow-speed rotors and determined reactor model structure by implementation of a CFD-generated RTD curve in Fluent into WEST® software environment based on the systemic approach. The fluid flow in the ditch was obtained from the Eulerian gas–liquid model, and the turbulence simulated with $sk-\varepsilon$ model. It was found that the RTDs of the ditch behaviour can be approximated by 90 CSTRs (plug flow) for non-aerated conditions and by 20 CSTRs (perfectly mixed) for aerated conditions (Glover et al., 2006). The work showed that closed-loop reactors with different internal recycling rates, such as oxidation ditches, can be modelled by one or series of CSTRs, the number of which can be determined from CFD-RTD studies. In this way, a suitable reactor model structure for ASM studies can be predicted.

Le Moullec et al. (2008) considered the assessment of RTDs in a cross-flow channel reactor aerated with porous tube, in which the hydrodynamics was modelled using a gas–liquid Eulerian model and the turbulence models used were $sk-\varepsilon$ and RSM. It was shown that in the channel-type reactors for wastewater treatment, turbulence has a dominant role in axial dispersion (90%), while dispersion due to convection is negligible. Furthermore it was shown that only the RTDs obtained from the RSM model are in good agreement with the experimental data treated by curve fitting for a plug flow with axial dispersion model, while the $sk-\varepsilon$ model underestimated the value of dispersion coefficient by around 50%, as seen in Fig. 4. This particular case is the effect of the default constants in Lagrangian stochastic particle motion model, which are determined by different closure assumptions. Thus, both models, $sk-\varepsilon$ and RSM, will use different C_μ which are directly linked to the modelling of the turbulent dispersion, what emphasizes the need for careful attribution of values to parameters, through the proper model calibration.

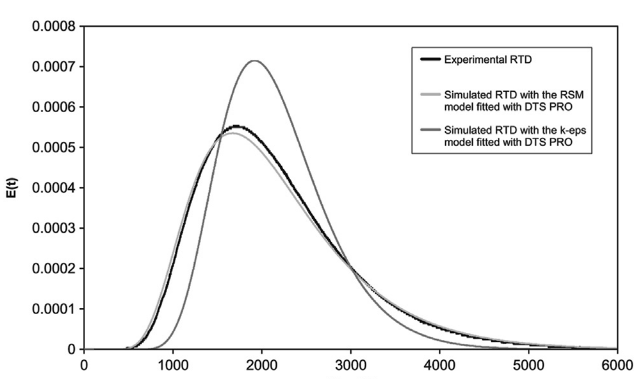

Fig. 4. Comparison between experimental and simulated RTD obtained with the RSM and the k–ε turbulence models and the particle tracking method for a liquid flowrate of 3.6 L min^{-1} and a gas flowrate of 15 L min^{-1}. Reprinted from Le Moullec et al. (2008). Copyright (2008) with permission from Elsevier.

Macromixing assessment is a useful tool to describe actual reactor performance. CFD studies assessing the impact of turbulence model selection on the RTDs of oxidation ditches aerated with slot injectors (Karpinska Portela, 2013; Pereira et al., 2012), considered the fluid flow simulated with RANS and URANS with the $sk-\varepsilon$ model and also LES with Smagorinsky's SGS model. This work shows the limitations of some approaches in computation of the RTD, as the turbulence model involved to simulate hydrodynamics has a large impact on prediction of the tracer's trajectories. The RTD simulations based on the average flow field, RANS and URANS, led to overestimation of channelling effects. The flow dynamics underlies mixing at all scales, both macro- and micro-, and thus this should always be accounted for. Furthermore, is has been shown that CFD data for AS modelling must align with all dynamic components of the flow, thus LES simulations, which demand more computational resource, should be used for some specific purposes.

5.2.4. Full model: CFD-ASM

Few workers have focused on the development of a complete three-phase CFD model to simulate actual physical-chemical-biological processes within different AS system configurations (Glover et al., 2006; Le Moullec et al., 2010a, b; Le Moullec et al., 2011; Lei and Ni, 2014). Here, the integration of hydrodynamics with biokinetics is accomplished by embedding an ASM model (e.g. ASM1) in a CFD model through introduction of the additional species of transport with source terms comprising bioreaction rates. The CFD-ASM simulations permit the quantification of interactions and transport phenomena between the water-gas, water-sludge and gas-sludge phases occurring within the AS reactor and accounting for the flow field, oxygen mass transfer, growth, decay and metabolic activity of the AS biomass, and sludge settling. Therefore it is possible to predict simultaneously the system hydrodynamics and its impact on the reactions occurring in nitrifying-denitrifying-biodegrading biomass and represented by the concentration profiles, in order to optimize aeration, mixing or system layout leading to efficient process operation with reduced exploitation costs.

The first attempt at CFD-ASM1 coupling reported in the literature (Glover et al., 2006), based on the Eulerian gas–liquid approach, facilitated prediction of poor performance of the diffused aeration system in a full scale oxidation ditch system, giving low nitrifying capacity of the sludge. These studies demonstrated the robustness of the CFD-ASM1 approach; however it was emphasized, that the validity of this modelling procedure requires further work to study different AS systems and aeration/agitation scenarios.

Le Moullec et al. (2010a) provided a robust discussion on the modelling issues concerning simulations of the hydrodynamics and biokinetics in a channel AS tank aerated by porous tube using Eulerian two-fluid model coupled to the ASM1. The authors discussed the trade-off between a model which can be implemented and run in the realistic time, and the extent of simplifications required to facilitate this. The authors assumed that the channel reactor was in a pseudo steady-state with constant biomass content; air bubbles with constant diameter; and the activated sludge flocs being perfectly soluble in the liquid phase. These simplifications gave rise to a series of errors in model output; specifically,

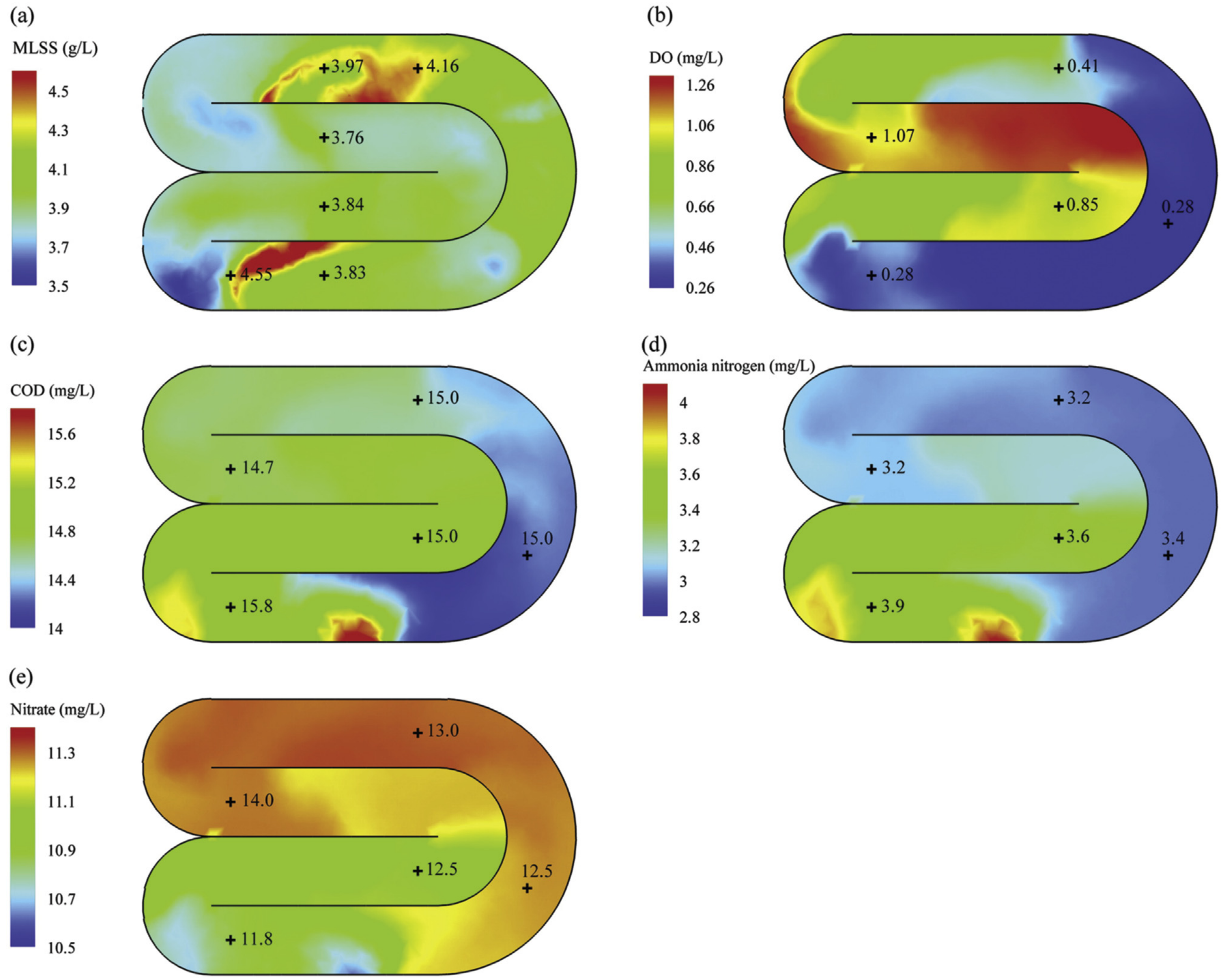

Fig. 5. The contour plots of: (a) MLSS, (b) DO, (c) COD, (d) ammonia and (e) nitrate concentration distribution, where "+" indicates measured data values at the sampling points in a Carrousel oxidation ditch. Reprinted from Lei and Ni (2014). Copyright (2014) with permission from Elsevier.

incorrect estimation of the local K_La value; underestimation of the nitrate and overestimation of the ammonia values (wrong estimation of the autotrophic fraction of biomass in the system).

The conclusions from this work emphasized the importance of the bubble size distribution for the oxygen mass transfer and for the molar diffusivity of oxygen in mixed liquor. Furthermore, a new concept for the approximation of AS floc properties (highly hydrated solid phase) to a liquid phase, was proposed. The authors also highlighted that, as the hydrodynamics-biokinetics coupling requires high number of CPUs and long computational times, a compromise between mesh resolution and solution accuracy has to be found.

In more recent work on three-phase CFD-ASM1 simulations of a Carrousel oxidation ditch aerated and agitated by means of mechanical aerators and mixers, Lei and Ni (2014) treated the AS flocs as a pseudo-solid phase. Here, the solid-liquid-gas flow field was obtained with a three-phase mixture model. The results from the simulations, (i.e. velocity, DO, organics and nutrients profiles) are in good agreement with the validation data. Crucially, this modelling approach allowed the prediction of physical kinematics of sludge settling. Concentration maps of the solids (near the bottom), DO, COD, ammonia and nitrates (in the mid-depth) in the horizontal cross-section through the oxidation ditch, are shown in Fig. 5.

It can be concluded, that the CFD-ASM1 simulations provide more reliable results than those obtained from oversimplified ASM models, which fail to represent the flow dynamics within a system, particularly regarding DO profiles along an AS basin, which have an impact on the biological nutrient removal (Pereira et al., 2009). Thus, the CFD-ASM data can be considered more suitable for the design and scale-up of bioreactors. However, besides high computational costs, another emerging drawback of CFD-ASM modelling approach is its limited feasibility due to stringent convergence criteria and equilibrium solution (Nopens and Wicks, 2012). As a result, the procedures of coupling hydrodynamics data obtained from CFD simulations with the ASM simulations have been also intensively studied (Glover et al., 2006; Karpinska Portela, 2013; Le Moullec et al., 2010b; Pereira et al., 2012). Here the RTD curves, actual HRT values, corrected recycle ratio, local velocities and other hydrodynamics characteristics obtained from the CFD simulations of an analysed AS system can be used to generate a suitable reactor model, i.e. in terms of number of CSTRs in series, recirculation rate and the flow pattern between each of the reactors, where the ASM can be implemented.

Nowadays, an alternative modelling approach using a compartmental model, based on the description of the AS reactor system using a network of interconnected sections, i.e. compartments, is emerging. The bi-directional flow rates between the compartments are computed from the flow field obtained in the

CFD simulations and accounting for the local values of velocities and mixing due to turbulence. When comparing with CFD models, compartmental models are inexpensive in terms of RAM and CPU usage. Nevertheless, as they are derived from steady-state CFD simulations, the results must be experimentally validated. In addition, it is still necessary to develop a more detailed biokinetic model to apply this approach in modelling of the full-scale industrial bioreactors, including ASPs (Le Moullec et al., 2010b; Le Moullec et al., 2011; Nopens and Wicks, 2012; Pereira et al., 2012).

6. Unaddressed issues in CFD modelling of AS tanks

Despite the fact that work has taken place on the CFD modelling of AS systems for over 15 years now, there are a number of issues which remain unaddressed and which, if successfully overcome, would enhance model fidelity and robustness further.

6.1. Secondary settler

In engineering practice, the behaviour of the AS tanks is inseparably linked to the performance of the secondary settler, as the efficient removal of BOD and nutrients in AS process depends on the Solid Retention Times (SRTs), concentration of Mixed Liquor Suspended Solids (MLSS), and the composition of biomass. The rationale behind the dynamic modelling of a coupled aeration tank-clarifier system is the prediction of interconnected flow and mass transport in unsteady flow loading conditions, and thus evaluation of the impact of dynamic changes in return sludge flow rates on the concentration patterns (Patziger et al., 2012).

Secondary settling is referred to in the literature as “the most sensitive and complicated process in activated sludge plants” (Ji et al., 1996). In fact, the complete CFD modelling of a clarifier is not a feasible task, since many physico-biochemical phenomena must be considered simultaneously, i.e. hydrodynamics, turbulence, flocculation, sludge rheology, settling characteristics, heat exchange and temperature, and finally, biokinetics (Plósz et al., 2012). The most critical issue in the modelling of clarifiers is the inherent unpredictability of activated sludge settleability and missing data regarding the particulate fraction. Additionally, even the most advanced models for clarifiers are still based on empirical equations describing sludge settling. The variability of settling behaviour which is not predicted by models affects the actual SRTs of AS system, yielding a potential source of error in wastewater treatment plant models (Plósz et al., 2011, 2012). Consequently, there is always a risk that the simultaneous modelling of clarifiers may affect the results obtained for the AS tank. Nonetheless, a CFD simulation of a simplified 2D AS tank-clarifier system has been reported in the literature (Patziger et al., 2012), where the focus was on the solids transport between both units in conditions of variable inflow and wet weather, but neglecting biokinetics and oxygen mass transfer. The necessity for further model enhancement and validation was also emphasized.

When considering the complexity of CFD models predicting clarifier behaviour simultaneously with a complete solid-liquid-gas model of the AS tank, computing time, availability of CPU resources and predictive capability must be recognised as confounding issues. As a result, common modelling practice is to avoid the interference between the two unit processes, and assume constant separation efficiency for the clarifier performance (Le Moullec et al., 2010a, b; Le Moullec et al., 2011) predicted in agreement with the guideline (Copp, 2001). Moreover, in engineering practice, the design of clarifiers is based on assumption of certain sludge properties, hence the CFD models of settlers only have been frequently used for optimization of design and retrofitting purposes (De Clercq, 2003; Stamou et al., 2009). However, it will be worthwhile to pursue CFD analysis of integrated aeration tank-secondary settler systems, when models capable of predicting the character of activated sludge flocculation are regularly incorporated into sludge settling models.

6.2. Population balance model

The AS system can be described as an ensemble of populations of individual entities (bubbles, flocs, biomass cells), having specific properties (size, density, viscosity, enzymatic activity). In such a system, two kinds of behaviour may be recognized: interactions of the individual entities with the environment (e.g. interfacial oxygen transfer, shear induced break-up), and mutual interactions between the individual entities (e.g. coalescence, aggregation). The character of these interactions is a function of one or more properties of the entities, which vary within the population. Thus, it is more correct to refer to this variation as “distributed properties”, as they can be represented by a distribution instead of a scalar (Nopens et al., 2015). Nevertheless, in order to reduce overall complexity of the model framework associated with aeration tanks, a common procedure is to assume non-distributed scalar properties implying that all individuals behave in exactly the same way (Nopens et al., 2015; Sobremisana et al., 2011). The classic example is the assumption of fixed bubble diameter (Fayolle et al., 2007; Glover et al., 2006; Gresch et al., 2011; Le Moullec et al., 2010a) and uniform floc size (Fan et al., 2010).

When considering an AS tank, recent experimental studies have demonstrated the influence of floc size on the flocculation behaviour and thus settleability of the activated sludge (Nopens et al., 2015), as well as on the biokinetic reaction environment within the AS floc (Sobremisana et al., 2011). Therefore estimation of floc size distribution may provide further insight into modelling of the activated sludge mixing (Samstag et al., 2012) and assessment of aeration tank settling, an important process parameter allowing the prediction of hydraulic capacity and treatment efficiency during high hydraulic loads associated with wet weather flows (Nielsen et al., 2000; Sharma et al., 2013).

Depending on the bubble flow regime in an AS tank, the intensity of collisions, agglomerations, breakups and deformation promotes a large diversity in the shapes and sizes of the bubbles (Karpinska Portela, 2013; Shaikh and Al-Dahhan, 2007; Takács, 2005). At the same time, the impact of the bubble size on K_La, superficial gas velocity, and thus gas hold-up and oxygen mass transfer in aeration tanks has been also recognized (Fayolle et al., 2006; Vermande et al., 2007). However, in some cases involving modelling of aeration in conventional AS tanks, the assumption of non-distributed scalar properties is still predominant, while in others, i.e. modelling of clarifiers or bubble columns, it may lead to predictions that diverge significantly from the real systems (Sobremisana et al., 2011). Consequently, multiphase models which incorporate bubble/particle size distributions require the use of population balance models (PBM) to describe variations in populations of entities. An assessment of several solution methods for PBM, namely the discrete class size method (Hounslow et al., 1988), the standard method of moments- SMM (Randolf and Larson, 1971) and the quadrature method of moments- QMOM (Marchisio et al., 2003), can be found in the literature (Bridgeman et al., 2009). It should be highlighted, that although development of PBMs is at advanced stage and the coupling of QMOM with hydrodynamics requires only a small number of computationally inexpensive scalar equations to be tracked, its application in modelling of aeration systems with suspended solids is still scarce and limited to very few examples (Bridgeman et al., 2009; Nopens et al., 2015; Sobremisana et al., 2011), associated almost exclusively with secondary settlers (Griborio and McCorquodale, 2006; Nopens et al., 2005). However, PBM-CFD coupling has been successfully exploited by the chemical engineering community to study bubble columns, airlift and stirred bioreactors (Dhanasekharan et al., 2005; Morchain et al., 2014; Wang, 2011).

7. Conclusions

In the last few years, as a result of increasing availability and accessibility of commercial and open-source software suites, the use of CFD has evolved into a robust and precise technique for design, optimization and control of the AS systems. The following key conclusions can be put forward from this review:

- 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/URANS closed by $sk{-}\varepsilon$ turbulence model has been adopted as the standard for the modelling of AS tanks;
- Different CFD models serve different applications. Examples from the literature have demonstrated the potential and robustness of single flow simulations in design and optimization of the AS systems equipped with mechanical and jet aeration systems;
- The Euler–Euler approach has been extensively explored for the prediction and optimization of oxygenation capacities in AS tanks equipped with diffused aeration systems;
- Lagrangian approach with particle tracking has been used to determine RTDs of the tanks-a tool for evaluation of the aeration and mixing performance and troubleshooting of the reactor design;
- The neutral density modelling of AS tanks became common practice used for design and evaluation of aeration and mixing systems, despite leading to over-prediction of the degree of mixing. Hence the necessity to include density-coupled modelling of aeration tanks to predict accurately local density gradients due to the impact of the flow regime on solids transport;
- A small number of works concerns a complete three-phase CFD model coupled with ASM1 aiming to quantify the transport and mutual interactions between water-gas-sludge phases within the AS reactor. Despite providing more reliable results than those obtained from ASM, this approach relies on the trade-off between a model which can be implemented and run in a realistic timeframe, and the extent of simplifications and the solution accuracy, which may lead to a series of output errors;
- Potential possibilities of coupling of the CFD data with ASM based codes have been explored in order to generate a suitable tank-in-series model, where the biokinetic model can be implemented;
- There are several areas in modelling practice, which remain unaddressed and require further study, e.g. modelling of coupled aeration tank-clarifier system to predict interconnected flow and mass transport in unsteady flow conditions and CFD-PBM coupling to assess the impact of the AS floc/air bubble size on mixing, settling, gas hold-up and oxygen mass transfer in the aeration tank.

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