Modelling gas-liquid mass transfer in wastewater treatment: when current knowledge needs to encounter engineering practice and vice-versa

Andreia Amaral, Sylvie Gillot, Manel Garrido-Baserba, Ahlem Filali, Anna Karpinska, Benedek Plosz, Chris De Groot, Giacomo Bellandi, Ingmar Nopens, Imre Takács, Izaro Lizarralde, Jose Jimenez, Justine Fiat, Leiv Rieger, Magnus Arnell, Mikkel Andersen, Ulf Jeppsson, Usman Rehman, Yannick Fayolle, Youri Amerlinck and Diego Rosso

ABSTRACT

Gas-liquid mass transfer in wastewater treatment processes has received considerable attention over the last decades both from academia and industry. Indeed, improvements in modelling gas-liquid-mass transfer can bring huge benefits in terms of reaction rates, plant energy expenditure, acid-base equilibria and greenhouse gas emissions. Despite these efforts, there is still no universally valid correlation between the design and operating parameters of a wastewater treatment plant and the gas-liquid mass transfer coefficients. That is why the current practice for oxygen mass transfer modelling is to apply overly simplified models, which come with multiple assumptions that are not valid for most applications. To deal with these complexities, correction factors were introduced over time. The most uncertain of them is the α-factor. To build fundamental gas-liquid mass transfer knowledge more advanced modelling paradigms have been applied more recently. Yet, these come with a high level of complexity making them impractical for rapid process design and optimisation in an industrial setting. However, the knowledge gained from these more advanced models can help in improving the way the α-factor and thus gas-liquid mass transfer coefficient should be applied. That is why the presented work aims at clarifying the current state-of-the-art in gas-liquid mass transfer modelling of oxygen and other gases, but also to direct academic research efforts towards the needs of the industrial practitioners.

Key words | aeration, alpha-factor, computational fluid dynamics, greenhouse gas, mass transfer coefficient

Andreia Amaral (corresponding author)
Giacomo Bellandi
Ingmar Nopens
Usman Rehman
Youri Amerlinck
BIOMATH, Department of Data Analysis and Mathematical Modelling,
Ghent University,
Coupure Links 653, 9000 Ghent,
Belgium
E-mail: *andreia.amaral@ugent.be*; *andreia.amaral@tecnico.ulisboa.pt*

Andreia Amaral
MARETEC, Instituto Superior Técnico,
Universidade de Lisboa,
Av. Rovisco Pais, 1, 1049-001 Lisbon,
Portugal

Sylvie Gillot
Irstea, UR REVERSAAL, centre de Lyon-Villeurbanne,
5 rue de la Doua, Villeurbanne cedex F-69926,
France

Manel Garrido-Baserba
Diego Rosso
Department of Civil and Environmental Engineering,
University of California,
Irvine, CA 92697-2175,
USA
and
Water-Energy Nexus Center,
University of California,
Irvine, CA 92697-2175,
USA

Ahlem Filali
Justine Fiat
Yannick Fayolle
Irstea, UR HBAN,
1 Rue Pierre-Gilles de Gennes – CS 10030, F-92761 Antony Cedex,
France

Anna Karpinska
Southern Water, Department of Operations-Optimization,
Southern House,
Lewes Road, Falmer, Brighton BN1 9PY,
United Kingdom

doi: 10.2166/wst.2019.253

Benedek Plosz
Department of Chemical Engineering,
University of Bath,
Claverton Down, Bath BA2 7AY,
United Kingdom

Chris De Groot
Department of Mechanical and Materials Engineering,
Western University,
1151 Richmond St. N., London,
Canada,
N6A 5B9

Giacomo Bellandi
Department of Civil and Environmental Engineering,
University of Florence,
via di S. Marta, 3, Florence 50139,
Italy

Imre Takács
Dynamita,
7 Lieu-dit Eoupe, La Redoute,
France

Izaro Lizarralde
Ceit-Ik4,
Manuel de Lardizábal 15, 20018 San Sebastián,
Spain

Jose Jimenez
Brown and Caldwell,
2301 Lucien Way, Suite 250, Maitland, Florida 32751,
USA

Leiv Rieger
inCTRL Solutions Inc.,
7 Innovation Drive Suite 107, Dundas, ON L9H 7H9,
Canada

Magnus Arnell
Ulf Jeppsson
Department of Biomedical Engineering (BME),
Division of Industrial Electrical Engineering and Automation (IEA),
Lund University,
P.O. Box 118, SE-221 00 Lund,
Sweden

Magnus Arnell
RISE Research Institutes of Sweden,
Gjuterigatan 1D, SE-582 73 Linköping,
Sweden

Mikkel Andersen
DHI,
Aarhus DK-8200,
Denmark

Usman Rehman
AM-TEAM, Advanced modelling for process optimization,
Okrooiplein 1 - box 601, 9000 Ghent,
Belgium

INTRODUCTION

Gas-liquid mass transfer governs dissolution and stripping phenomena of the species consumed or formed during biological and/or chemical reactions within wastewater treatment processes. Accurate gas-liquid mass transfer models are key to correctly represent reaction rates, energy expenditure, acid-base equilibria and greenhouse gas (GHG) emissions, among others. In case of biological wastewater treatment plants (WWTPs), oxygen transfer from the

gas phase to the liquid bulk is critical to provide the necessary oxidising equivalents for the aerobic microorganisms. At the same time, aeration is one of the most energy-intensive processes. Therefore, a major part of the scientific research is devoted to increase the knowledge of oxygen transfer. However, with the transition towards water resource recovery facilities (WRRFs), the transfer of other gases such as nitrous oxide, hydrogen or methane is coming on the radar as well.

The objectives of this article are: (i) to report and investigate the current models used to represent gas-liquid mass transfer in practice and to point out limitations regarding their use; (ii) to discuss the on-going developments of more advanced modelling approaches and how these can be introduced in practice. Note that the main focus of this work is on the modelling of oxygen mass transfer in aeration tanks. Nevertheless, the authors are aware of the importance of gas-liquid mass transfer for other gases and in other reactors. Hence, a dedicated section for other gases is included at the end of this article.

CURRENT PRACTICE AND LIMITATIONS

Gas-liquid mass transfer models

Several theories exist to describe the interphase gas-liquid mass transfer mechanism, e.g. the film theory (Nernst 1904), the two-film theory (Lewis & Whitman 1924), the penetration theory (Higbie 1935) and the surface-renewal theory (Dankwerts 1951). All of them assume that the flux of mass transfer is determined by a mass transfer coefficient and a driving force as a result of a concentration or pressure gradient. The two-film theory proposed by Lewis and Whitman is probably the most used among practitioners because of its straightforward interpretation. For an absorption of a gas into a liquid, the two-film theory governing equation is provided below:

$$\frac{dC(t)}{dt} = K_L a(C^* - C(t)) = K_G a(P(t) - P^*) \quad (1)$$

- $a = A/V$, with A the total gas-liquid interfacial area [m^2] and V the total liquid volume [m^3].
- According to Henry's law, equilibrium concentrations are related as follows:
  $P^* = H\ C$ and $P = H\ C^*$ with H the Henry's law constant [(m^3.Pa)/g].
- The mass transfer coefficient together with the interfacial area can be referred to as a single parameter known as $K_L a$ or the overall volumetric mass transfer coefficient [1/d].
- Multiple assumptions about the system are made to obtain Equation (1). (i) Mass transfer is controlled by two thin stagnant films at the gas-liquid interface, (ii) the mass transfer across the films is driven by molecular diffusion, and (iii) the bulks of gas and liquid phases are homogeneous with respect to the solute.
- From the underlying assumptions of the two-film theory, it follows that the inverse of the overall mass transfer coefficient $1/K_L$, also referred to as the overall resistance to mass transfer based on the liquid phase concentration, can be defined as the sum of the liquid film resistance $1/k_L$ and the gas film resistance $1/(Hk_G)$. The same is valid for $1/K_G$, the overall resistance to mass transfer based on the gas phase concentration:

$$\frac{1}{K_L} = \frac{1}{k_L} + \frac{1}{Hk_G} \quad ; \quad \frac{1}{K_G} = \frac{1}{k_G} + \frac{H}{k_L} \quad (2)$$

  With k_L the liquid-phase mass transfer coefficient [m/d], H the Henry constant [(m^3.Pa)/g], and k_G the gas-phase mass transfer coefficient [g/(m^2.Pa.d)].
- When the solubility of the gas in the liquid is low, H is very high and therefore the main resistance for gas-liquid mass transfer is found on the liquid side, i.e. $1/K_L \approx 1/k_L$. This is, for example, a valid assumption in the case of oxygen mass transfer. Contrarily, in case the gas is very soluble in the liquid, H is very low the main resistance for gas-liquid mass transfer is found on the gas side, i.e. $1/K_G \approx 1/k_G$.
- The liquid- and gas-phase mass transfer coefficients can be expressed in function of the respective molecular diffusion coefficients (D) and film thickness (δ). For the two-film theory that is:

$$k_L = \frac{D_L}{\delta_L}; \quad k_G = \frac{D_G}{\delta_G}; \quad (3)$$

Oxygen mass transfer

Considering that aeration is a key process from both an operational and an economic point of view, considerable attention has been paid to understand the mechanisms of oxygen mass transfer applicable in wastewater treatment. Moreover, standardized methods exist to determine the $K_L a$ and the OTR.

The ASCE Standard Procedure (2007) and its European counterpart NFEN12255-15 (2004) are well accepted for the measurement of oxygen transfer in clean water. The main objective of these procedures is to determine, in a repeatable way, the aeration performance values, e.g. the Standard

Oxygen Transfer Rate (SOTR), which is the oxygen transfer rate (OTR) in clean water at standard conditions. The SOTR is expressed as:

$$SOTR = K_L a_{CW,20} C^*_{20} V \quad (4)$$

With SOTR the standard oxygen transfer at 20 °C and 1 atm with a dissolved oxygen (DO) concentration of 0 g/L [g/d], $K_L a_{CW,20}$ the $K_L a$ in clean water at 20 °C and 1 atm [1/d], C^*_{20} is the oxygen saturation concentration at 20 °C and 1 atm [g/m³] and V is the total gas-liquid volume [m³].

To determine the actual oxygen transfer rate (AOTR) in aeration tanks, the SOTR must be corrected to account for the influence of wastewater characteristics, operational conditions, temperature and pressure (Equation (5)). These factors do not only influence the driving force in oxygen mass transfer, but also the resistance against oxygen mass transfer and the interfacial area available for exchange.

$$AOTR = \alpha F K_L a_{CW,20} (\beta \tau \Omega C^*_{20} - C(t)) \theta^{T-20} V \quad (5)$$

Here, AOTR is the AOTR [g/d], $K_L a_{CW,20}$ is the $K_L a$ in clean water at 20 °C and 1 atm, α is the ratio of the $K_L a$ for process conditions to the $K_L a$ in clean water [–], F is a fouling factor which is defined as the ratio of the aeration system performance after use to the performance of a new aeration system [–], β is the ratio of the process water oxygen saturation concentration to the clean water oxygen saturation concentration [–], τ is the ratio of the oxygen saturation concentration at the actual operating temperature to the oxygen saturation concentration at 20 °C [–], Ω is the oxygen saturation concentration pressure correction factor [–], C^*_{20} is the oxygen saturation concentration at 20 °C and 1 atm [g/m³], C(t) is the concentration of oxygen in the mixed liquor [g/m³], θ is the temperature correction factor [–], T is the mixed liquor temperature [°C], and V is the total liquid volume [m³].

α-factor: what is it? what are the advantages and disadvantages?

From all the correction factors used to calculate the AOTR, the α-factor is reported as the most uncertain oxygen mass transfer parameter which is moreover dynamic in nature (Leu *et al.* 2009; Karpinska *et al.* 2016; Jiang *et al.* 2017). Due to its high variability, it is difficult to predict the AOTR with high certainty under different process conditions, both in a single treatment facility (Amerlinck *et al.* 2016) or across different facilities (Gillot & Héduit 2008).

It is generally assumed that the most significant contributor to the decrease of the α-factor is the presence of organic surfactants (Rosso & Stenstrom 2006a; Sardeing *et al.* 2006; Gillot & Héduit 2008). Though, note that inorganic salts and alcohols can cause a gas-liquid mass transfer enhancement, as in Zlokarnik 1980. Yet, the α-factor is a composite parameter that encompasses a wide range of effects related to components and conditions, all of them affecting in different ways and magnitudes (Table 1). From chemical compounds (i.e., surfactants,

Table 1 | Phenomena influencing the α-factor

Phenomena influencing the α-factor	References
Surfactant concentrations	Stenstrom & Gilbert (1981), Wagner & Pöpel (1998), Gillot & Heduit (2000), Loubière & Hébrard (2004), Rosso & Stenstrom (2006b), Sardeing *et al.* (2006). Gillot & Héduit (2008), Tomczak-Wandzel *et al.* (2009) and Jimenez *et al.* (2014a)
MLSS concentration	Muller *et al.* (1995), Krampe & Krauth (2003), Cornel *et al.* (2003), Germain *et al.* (2007), Racault *et al.* (2010), Henkel *et al.* (2011), Durán *et al.* (2016), and Baquero-Rodríguez *et al.* (2018).
Rheological properties	Krampe & Krauth (2003), Vandu & Krishna (2004), Nittami *et al.* (2013), Durán *et al.* (2016) and Amaral *et al.* (2017).
Tank geometry	Groves *et al.* (1992), Fisher & Boyle 1999, Capela *et al.* (2002) amd Gillot *et al.* (2005).
Daily/seasonal dynamics	Libra *et al.* (2005), Leu *et al.* (2009) and Jiang *et al.* (2017).
MCRT	EPA (1989), Rosso & Stenstrom (2005), Gillot & Héduit (2008), Jiang *et al.* (2017), and Stenström & la Cour Jansen (2017)
Aeration system (types)	Kessener & Ribbius (1934), Rosso *et al.* (2005), Rosso & Shaw (2015), and Garrido-Baserba *et al.* (2018).
Microbial activity	Steinmetz (1996) and Henkel *et al.* (2009)
Organic load (COD)	Eckenfelder *et al.* (1956), Zlokarnik (1980), Steinmetz (1996), Leu *et al.* (2009), Jiang *et al.* (2017) and Garrido-Baserba *et al.* (2018).

salts, organic substrates, etc.) to physical constraints (i.e., bubble coalescence, hydrodynamic effects, etc.), but also the influence of the microbial activity (Henkel *et al.*. 2009) can potentially reduce the AOTR in wastewater treatment.

From a practitioner point of view, a straightforward expression to predict this correction factor is highly desired. This explains why it is very tempting for academic research to find empirical correlations between the measured variables and the α-factor. However, most studies relating the α-factor to process variables as the air flow rate, mixed liquor suspended solids concentration (MLSS), the mean cell residence time (MCRT) or the soluble chemical oxygen demand fall short of the mark, mainly because too many co-correlated environmental and operational conditions are lumped into a single factor.

As reported by Belia *et al.* (2009), assessing the uncertainties present in the optimisation and design of WRRFs is mandatory for good practice. Therefore, understanding the impact brought by the use of the α-factor is fundamental to achieve accurate process models. Depending on the requirements of the project at hand, the uncertainty analyse might vary from qualitatively describing the sources of uncertainty to a more in-depth sensitivity analysis all the way up to a detailed quantitative study with a stochastic dynamic model (Cierkens *et al.* 2012).

Oxygen supply, distribution and delivery

In order to have an effective aeration strategy, it is not only important to accurately predict the AOTR but also its supply, distribution and delivery, i.e. the right amount of air needs to be delivered at the right moment in time and at the right location within the aeration tank. Spatial modelling of the air delivery is thus a prerequisite to properly understand the kinetic conversion processes as well as for the prediction of energy consumption (Amaral *et al.* 2017). A main driver for the development of more detailed, as well as dynamic, air distribution models is the current trend towards low DO processes which aim at reducing the high operational costs of aeration. When the first activated sludge (AS) models were developed, DO concentrations of more than 2 mg/L were targeted, which left little room for control and resulted in major energy waste. With the rise of low DO technologies such as partial nitritation/anaerobic ammonium oxidation (ANAMMOX), simultaneous nitrification-denitrification (SND), shortcut biological nitrogen removal, ammonia-based aeration control and others, DO concentrations near or below the half-saturation index K_{DO} are often selected. Consequently, small deviations in the simulated DO concentration already have a significant impact on the biological conversion processes. To properly simulate this, simplified models are not adequate due to the lack of simulating spatial heterogeneity in air delivery. Therefore, together with the oxygen mass transfer in the bulk liquid, three other parts of the aeration system are modelled in practice: (i) air supply provided by the blowers; (ii) air distribution in the piping network; (iii) air delivery by submerged diffusers. This provides means to balance the oxygen delivery with the oxygen demand (Schraa *et al.* 2017).

Air delivery in the aeration tank depends on the pressure provided by the blowers and the pressure drop experienced due to the piping, fittings, couplings, valves, flow meters and diffusers. Ideally, the largest pressure drop is caused by valves used to redirect the airflow and the diffuser. However, pipes, fittings and others also contribute to the overall pressure profile. Hence, these can lead to uneven air distribution and therefore to higher oxygen demand than necessary, which is translated to higher energy consumption. Simplified air distribution models currently only use the diffuser distribution to estimate air splits. While these models can be sufficient for the design of conventional AS (with high DO concentration) or biofilm systems (with typically higher DO concentrations), they cannot accurately predict the actual blower capacity or constraints related to the piping network. Additional elements that need to be modelled are blowers, pipes, fittings, valves and diffusers (Figure 1; Alex *et al.* 2002; Amerlinck *et al.* 2016; Arnell 2016; Amaral *et al.* 2017; Schraa *et al.* 2017). Ideally, this is done as a dynamic network model where pressure drops are back-propagated and the pressure at every point in the system is predicted (Arnell 2016).

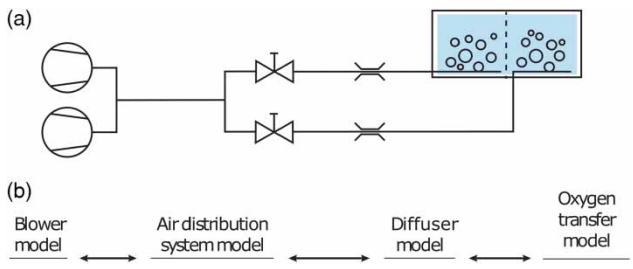

Figure 1 | (a) Schematic figure over an aeration system from blower to tank including blower, air distribution system, valves, flow meters and diffusers. (b) Principal model components and the entities required in each part. Figure adapted from Arnell (2016).

TOWARDS A NEW MODELLING FRAMEWORK

The need for new and more advanced approaches

As mentioned before, the current practice for oxygen mass transfer modelling is based on multiple assumptions, which are largely driven by the need for consistent standard tests for equipment specifications. Beside the issues related to the driving phenomena of the α-factor, current modelling practices such as the two-film theory assume that the aeration tanks encountered in WRRFs are completely mixed, i.e. no spatial variations of the DO concentration. Moreover, the effect of varying bubble sizes impacting K_L and interfacial area is not taken into account. Indeed, such assumptions result in over-simplifications which neglect the complexity of the mechanisms involved in oxygen mass transfer (Karpinska & Bridgeman 2016; Amaral *et al.* 2017). As a result of these assumptions, poor accuracy and reliability of the gas-liquid transfer models is compensated for by over-calibration of the kinetic parameters (Amerlinck *et al.* 2015).

Computational fluid dynamics

Computational Fluid Dynamics (CFD) is a powerful numerical modelling tool, which allows for flow visualisation with detailed characterisation of spatial phenomena under varying process conditions. For example, a CFD analysis can show the impact of local multiphase hydrodynamics on the gas holdup, K_L, interfacial area, K_La, AOTR, and consequently, on the local DO (Figure 2). A summary of the published work concerning CFD in wastewater aeration systems is reported in Table 2.

Gaps of CFD

Early works in the field of CFD, limited by computing power, considered the application of a neutral-density approach based on unrealistic fixed bubble sizes, to evaluate oxygen mass transfer and mixing performance in aeration tanks (Do-Quang *et al.* 1998). Consecutive studies focused on the development of an improved model applicable for different aeration tank configurations and based on the use of calibrated bubble sizes (Fayolle *et al.* 2007). Although this approach improved the prediction accuracy of the local K_La, the authors emphasised the necessity of either in-situ bubble size measurements or the application of an additional model, which estimates the bubble size at the diffuser level. A more recent CFD work performed on sequencing batch reactor (SBR) tanks equipped with jet aerators (Samstag *et al.* 2012) showed that use of clean water and air may lead to an over-prediction of the mixing, hence also the turbulence intensity and predicted K_La. This shows that density-coupling, which incorporates solids settling and transport, as well as calibration to field data, should be included in the CFD study for correct assessment of the hydrodynamic parameters affecting oxygen mass transfer.

Solids are known to affect the viscosity of the medium, the hydrodynamics along with oxygen mass transfer (Rosenberger *et al.* 2002). For tests performed in AS at different solids concentration, the solids content of the mixed liquor negatively affected the gas holdup and the K_La (Jin *et al.* 2006; Duran *et al.* 2016). Sludge is a shear-thinning fluid which is non-Newtonian pseudoplastic fluid by nature. When fine-bubbles are rising in sludge, the sludge thickness increases their coalescence. By coalescing, the bubbles rise faster, being associated with higher interfacial shear, and experience lower hydrodynamic resistance. The net result

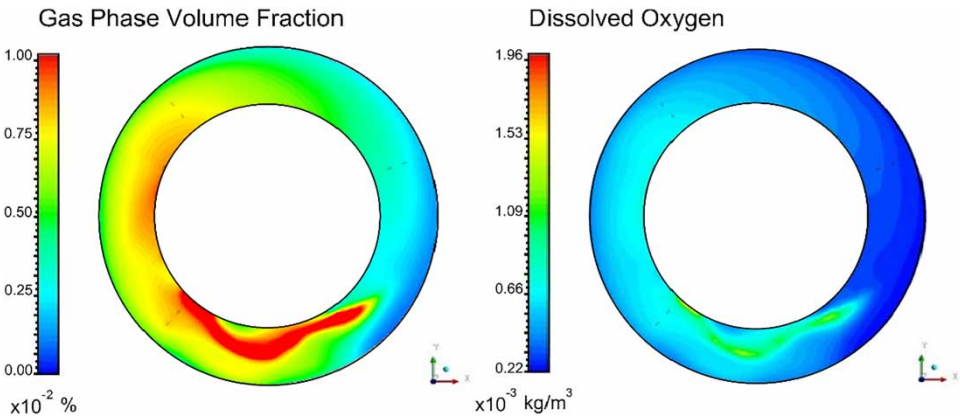

Figure 2 | CFD results for gas holdup and DO concentration at middle depth in the aeration tank of Eindhoven WRRF, The Netherlands. Figure adapted from Rehman *et al.* (2017).

Table 2 | Summary of CFD work on aeration tanks

Reference	CFD Platform	Multiphase Model	Turbulence Model	Bubble Size & Shape	Drag Model	Validation Study
Sanchez *et al.* (2018)	OpenFOAM	Eulerian	k-ε	Constant (sphere)	Schiller-Naumann	No
Rehman *et al.* (2017)	ANSYS Fluent	Mixture	Realizable k-ε	Constant (sphere)	Shiller-Nauman	Yes
Karpinska & Bridgeman (2017)	ANSYS Fluent	Eulerian	k-ω	Variable (ellipse, sphere)	Clift *et al.*	Yes
Rehman *et al.* (2014)	ANSYS Fluent	Mixture	Realizable k-ε	Constant (sphere)	Shiller-Nauman	Yes
Samstag *et al.* (2012)	ANSYS Fluent	Mixture	Standard k-ε	Constant (sphere)	Shiller-Nauman	Yes
Gresch *et al.* (2011)	ANSYS CFX	Eulerian	k-ω	Constant (sphere)	Ishii- Zuber	Yes
Le Moullec *et al.* (2010)	ANSYS Fluent	Eulerian	Standard k-ε	Constant (sphere)	User defined function (UDF)	Yes
Talvy *et al.* (2007)	ANSYS Fluent	Eulerian	Standard k-ε	Variable (ellipse, sphere)	Karamanev-Nikolov	Yes
Fayolle *et al.* (2007)	ANSYS Fluent	Eulerian	Sstandard k-ε	Constant (sphere)	Clift *et al.*	Yes
Do-Quang *et al.* (1998)	ASTRID	Eulerian	Standard k-ε	Constant (sphere)	UDF	No

of this coalescence is low α-factors, e.g. for MBRs and aerobic digesters (Henkel *et al.* 2009; Baquero *et al.* 2017).

Bubble size distribution (BSD) has been investigated as key factor to estimate the oxygen mass transfer since it affects both K_L and the interfacial area (McGinnis & Little 2002; Terashima *et al.* 2016; Azizi *et al.*, 2017); Sommer *et al.* 2017. Therefore, future scientific investigations must transcend the limitations of the over-simplified modelling approach with a fixed bubble size. Instead, new studies should acknowledge the nature of bubbles as an independent and separate phase with its own velocity field which is distinct from that of the liquid phase. Moreover, the BSD is dynamic in nature since it depends on variables such as the liquid viscosity, air flow rate and hydrostatic pressure. Yet, most CFD models do not consider the effect of BSD dynamics. Consequently, Karpinska & Bridgeman (2017) worked on the development of a modelling framework for aeration systems through rigorous analysis of different turbulence models and bubble flow generation models. This should account for interactions between the gas and liquid phases in a dynamic way, hence inducing bubble breakup and/or coalescence, and as a consequence, formation of bubbles with different sizes and shapes. Related to this are experimental studies that use different xanthan gum solutions to study the effect of air flow rate and viscosity on the BSD dynamics and K_La (Ciancia 2014; Amaral *et al.* 2018). Although the scale of these experiments is limited, valuable information regarding the BSD dynamics is acquired. Future studies should however attempt at investigating rheological properties at full depth. In addition, determining the BSD on-site is another challenge that needs to be tackled. To date, the only attempt to quantify BSD *in situ* was published by Fayolle *et al.* (2010). Clearly, this would represent a considerable step towards more accurate oxygen mass transfer predictions.

Population balance modelling (PBM) represents another powerful numerical modelling framework that can be used to describe the dynamics of distributed properties (Nopens *et al.* 2015). As such, the local BSD can be predicted with the help of a PBM. Such models can account for growth, coalescence and breakage of bubbles. Coupling CFD and PBM could result in improved the understanding of oxygen mass transfer and better predictions of the local AOTR. Indeed, different synergies exist between the CFD and PBM frameworks. On the one hand, the local BSD predicted by a PBM can help in determining the correct local OTR predicted by a CFD model. On the other hand, shear rate predictions provided by the CFD model help in determining the local viscosity, which in turn influences the BSD dynamics predicted by the PBM. In this respect, attempts have been made to assess the local shear rate in order to estimate the apparent viscosity and subsequently link it to the value of the K_La (Duran *et al.* 2017).

Whilst incorrect input assumptions, poor model choice, or excessive simplifications have been recognized as potential sources of CFD modelling errors, there still remains a necessity in academia to identify the appropriate modelling strategies to simulate oxygen mass transfer correctly.

Limitations of CFD

Even if academia and industry would agree on the benefits of using CFD, its current usage in the day-to-day operations

of an industrial plant are limited. There are several reasons for this. First of all, applying the mathematical concepts involved in a CFD analysis requires advanced knowledge and skills. Moreover, these studies come with a very high computational cost and thus long calculation times (with present hardware, hours to days). While these are all valid arguments, one should take into account that CFD modelling for WWTPs was never intended to be used in everyday operations. Instead, CFD should be used as a means to gather more insight into unit process performance and improve conceptualisation, calibration and validation of simpler models (Laurent *et al.* 2014).

Calibration and validation of a CFD model is an often-cited critical point, as it is expensive and labour intensive, especially for full-scale studies. Historical field samples and telemetry data are required for the accurate set up of flows and loadings. For a complete AS tank model, source data will need to account for the influent specification, feed-, return-, recycle- and air flow rates. Further model refinement and validation require dedicated sampling campaign, which enables both, telemetry data (DO, MLSS and ammonia concentration in controller location) and field data (flow-, DO- and MLSS- profiles in pre-defined control sections through the tank) obtained using portable measurement equipment, e.g. Acoustic Doppler Current Profiler, Acoustic Doppler Velocimeter, series of DO and MLSS probes. If required, effluent quality should be determined (grab sample analysis and historical sample point data). Note that in the case of CFD coupled with dynamic PBMs, validation at full-scale might not even be possible considering that BSD measurements in opaque solutions presents a challenge. However, in parallel to the kinetic parameters of lumped AS models, validation of CFD models may not be needed to guarantee CFD acceptance. Once proven valid for a number of well-studied cases, the trust of practitioners in CFD models should soon follow. Moreover, the analytical technology that can be used for such validation studies is rapidly evolving due to the needs in different industrial branches. On the other hand, use of over-simplified modelling approaches, e.g. based on standard $k-\varepsilon$ turbulence model and fixed-size spherical bubbles, yielding substantial errors in model outputs, require more rigorous calibration input. The impact of the different CFD modelling scenarios on the hydrodynamics and mass transfer prediction accuracy has been widely discussed in Karpinska & Bridgeman (2016, 2017). Consecutively, as discussed examples related to oxygen mass transfer are the recent reports on bubble size measurements in opaque solutions using acoustic bubble spectrometry (Wu *et al.* 2014).

Compartmental modelling

Compartmental models (CMs) can be introduced as means to improve the accuracy and reliability of current simplistic models, which assume ideal mixing, while at the same time avoiding the complexity of more advanced modelling paradigms resulting in a fit-for-purpose model. For example, upgrading the canonical 1D tanks-in-series model using a 2D scheme developed from an a priori CFD study. Indeed, this could offer solutions to choosing the number of tanks, which is still relying on rules of thumb or experimental fitting. For example, Rehman (2016) developed a CM of an aeration tank, using the CFD-ASM1 coupled model, which predicted spatial variations in the DO concentration. Regions with a homogeneous DO concentration were taken as single compartments, and subsequently modelled as continuous stirred-tank reactors (CSTRs). As such, this CM is able to provide insight in the spatial distribution of oxygen mass transfer within the aeration tank. Experimental comparison is however based on the averaged oxygen mass transfer obtained for instance with an off-gas test in each compartment. Despite the benefits, the spatial complexity reduction in CM is still a point of debate because it ignores local details. At the same time industrial practitioners might think that CMs are still overly complex as compared to the current spatially-averaged approach. A reason for the latter is the fact that the CM requires knowledge of spatial variations, which can only be answered using CFD studies. This proves that there is indeed a need to invest in more research effort into the balance between model complexity and accuracy to include the effects of spatial heterogeneity on oxygen mass transfer. There is a need to move to a fairly simple protocol to make this type of modelling accessible, also for less advanced modellers.

WHAT ABOUT THE OTHER GASES?

Gases such as NO, N_2O, H_2S, CH_4, H_2, and N_2 have received little attention with respect to gas-liquid mass transfer. This is because there are few incentives for the detailed modelling of such gases. An exception is CO_2, which is mainly studied because of its direct relation with the acid-base equilibria, which is especially important in anoxic tanks and in pH controlled biological processes (Lizarralde *et al.* 2015). Though, in the transition from WWTP to WRRFs, it is expected that not only gas-liquid mass transfer of O_2 and CO_2 can be accurately modelled, but also several other gases which relate to GHG emissions, resource

recovery, etc. A list of the gases of interest is provided in Table 3, ranked by their order of importance. Note that the solubility in water of most of these gases is low, and thus comparable to the solubility of oxygen in water.

One way of determining the gas-liquid mass transfer coefficients of these other gases is by directly relating them to the K_La, α-factor or other rate determining coefficients of oxygen gas. As an example, for gases with low solubility in water, the k_L can be calculated using the k_L of oxygen and a proportionality factor that depends on the diffusivity of oxygen and the diffusivity of the gas under study.

$$\frac{k_{L,i}}{k_{L,O_2}} = \left(\frac{D_{L,i}}{D_{L,O_2}}\right)^n \quad (6)$$

where n is an empirical coefficient that ranges from 0.1 to 1. Just like the α-factor, it lumps all the unknown phenomena of the system. Such modelling approaches typically result in over and under estimates of the transfer and emission of other gases. They should thus be taken with caution.

CFD modelling is also proposed as an approach to estimate the values of the k_L for different gases. The reason being that gas-liquid mass transfer theories such as the penetration theory (Higbie 1935), Equation (7), take into account the slip velocity of the liquid and gas phase (through the contact time), the average BSD as well as temperature effects to calculate the k_L. Hence inferring that the effect would be the same for all gases and equally bidirectional (i.e., absorption and stripping) adds to the model uncertainty. Future research should address this issue with experiments. An example for H_2S is provided by Carrera *et al.* (2017), who experimentally determined the ratio between the mass transfer coefficient of H_2S and O_2. This is subsequently used in a CFD exercise to establish a correlation between the K_La and the fluid velocity in an open channel flow.

$$k_L = 2\sqrt{\frac{D_L}{\pi . t_C}} \quad (7)$$

Recently, efforts were dedicated to develop more generic gas-liquid mass transfer models (Lizarralde *et al.* 2018; Vaneeckhaute *et al.* 2018). Experimental evaluation of some of these model parameters and hypotheses is needed, such as the value of the bubble diameter and its evolution over the reactor height; the symmetry between absorption and stripping; or the value of the empirical coefficient n used in Equation (6) and its potential variation depending on the liquid phase composition. However, the use of n is similar to the use of the α-factor in that it is essentially an artifice to lump our lack of knowledge.

In contrast, for highly soluble gases such as NH_3, oxygen gas cannot be used as a reference. Experimental estimations are thus required. Concerning the $k_{G,i}$, Sharma & Mashelkar (1968) proposed to derive its value from the diffusivity of the gas.

$$Sh_G = \frac{k_{G,i} d_b}{D_{G,i}} = 6.58 \quad (8)$$

Table 3 | Classification of gases based on their order of importance

Gas	Henry's law constant [mol/(m³ Pa)]	Solubility in water*	Importance
O_2	1.2E-5	Low	Process performance and energy i.e. effluent quality and costs
CO_2	3.3E-4	Low	pH calculations; GHG emissions
NO	1.9E-5	Low	GHG emissions
N_2O	2.4E-4	Low	
H_2S	1.0E-3	Intermediate	Corrosion, odour nuisance and inhibition effect on the anaerobic digestion
NH_3	5.9E-1	High	Odour nuisance and inhibition effect on the anaerobic digestion, resource recovery
CH_4	1.4E-5	Low	GHG emissions
H_2	2.6E-6	Low	Inhibition effect on the anaerobic digestion
Volatile organic compounds (VOC)	–	–	Health effect and odour nuisance
N_2	6.4E-6	Low	Present in air, makes up bubble volume in anoxic zones, mitigation of GHG emissions

*Sander (2015).

With Sh_G the dimensionless Sherwood number for the gas [–], $k_{G,i}$ the gas-side mass transfer coefficient [m/s], d_b the average diameter of the bubbles [m], and $D_{G,i}$ is the diffusivity of the gas in the liquid [m^2/d].

Note that the gas solubility, linking concentration and pressure, plays a key role in controlling the driving force of gas-liquid mass transfer. While the partial pressure of oxygen in the gas phase is known to be stable for moderate reactor depths, it can change substantially for gases that are much more soluble than oxygen. In these cases, it is also important to consider the gradual increase or decrease of the partial pressure in the gas bubble from the bottom to the surface of the reactor. Especially when the objective is to predict the off-gas composition. Likewise, it was found that neglecting the enrichment of N_2O in the gas phase leads to severe overestimations in stripping (Fiat *et al.* 2019).

Moreover, attention should be paid to correctly describe passive gas-liquid mass transfer in unaerated reactors with shallow dimensions. For example, N_2O might accumulate in the liquid during anoxic process conditions and can be emitted from the surface by diffusion (Marques *et al.* 2016; Bellandi *et al.* 2018).

OUTLOOK

This article looked to illustrate the current practice in gas-liquid mass transfer modelling as well as the potential of more advanced approaches. Ultimately, this should help in directing academic efforts and funds to the most rewarding research topics from a practitioner's point of view.

Most of the uncertainty associated with the design and modelling of systems involving gas-liquid mass transfer can be associated to a single parameter, i.e. the K_La. Indeed, there is no known universal correlation between the K_La and the relevant operating parameters of WRRFs. One way handling this uncertainty is by introducing correction factors to an ideal base scenario, one of them being the α-factor. This parameter is in fact an artifice, which lumps all lacks of knowledge on the system. Hence, it does not provide fundamental knowledge. Moreover, it is recognised that the α-factor is not a constant (Leu *et al.* 2009; Jiang *et al.* 2017). Therefore, a priori selection of the α-factor can only result in a good design or model if luck is involved. A good design should however rely on site-specific or site-adaptable measurements, and preferably not on literature values. In fact, one of the most common causes of error in design or process modelling of systems with gas-liquid mass transfer is the reliance on literature values and extrapolations.

As such, new and more advanced modelling approaches are required to provide additional insight into the oxygen mass transfer mechanisms in order to increase model accuracy. A solution might be found in more advanced modelling paradigms being CFD, PBM, and CM. The advantage of these approaches is the fact that they account for the distributed nature of important process variables. For example with the help of CFD, it is possible to understand the actual gas distribution. Hence, the higher the detail in the temporal and spatial domains, the higher will be the modelling accuracy for gas-liquid mass transfer. Even if the use of CFD, PBM, or CM does not widely spread among industrial practitioners, it is still possible to use the knowledge derived from such models. For instance, the knowledge obtained from a CM can be used to define the location of gas measurements. Indicating that there is indeed a need to develop such more complex models.

The question remains however on how to ideally bridge the gap between practical yet accurate models for gas-liquid mass transfer. That is, link the fundamental scientific work (e.g., mapping the oxygen mass transfer phenomena in time and space within the aeration tank) with design parameters that can be measured in practical and repeatable ways such as the current practice of measuring K_La in clean water. As such, it is still too early to completely abandon correction factors such as the α-factor for industrial design and operation.

That is why a set of actions is listed to assure that practice-driven needs related to gas-liquid mass transfer are met: i) Assess reactor hydraulics and mixing; ii) Locate sensors in reactor and performing concurrent and high-frequency data collection; iii) Quantify soluble and particulate fractions, influencing mass transfer; iv) Assess bubbles in the reactor (gas holdup, bubble diameter, path length, velocity vectors, size distribution) and include them in a spatial models; v) Perform rigorous regression analysis, sensitivity, and uncertainty analysis.

ACKNOWLEDGEMENTS

This work is the product of the discussion at the Gas-Liquid Mass Transfer Modelling Workshop of the 6th IWA/WEF Water Resource Recovery Modelling Seminar, Canada, 2018.

REFERENCES

Alex, J., Binh To, T. & Hartwig, P. 2002 Improved design and optimization of aeration control for WWTPs by dynamic simulation. *Water Science and Technology* **45** (4–5), 365–372.

Alex, J., Rieger, L. & Schraa, O. 2016 Comparison of fine-bubble aeration control concepts with respect to energy efficiency and robustness. In: *89th Water Environment Federation (WEF) Technical Exhibition and Conference (WEFTEC), New Orleans, LA, USA*.

Amaral, A., Schraa, O., Rieger, L., Gillot, S., Fayolle, Y., Bellandi, G., Amerlinck, Y., Mortier, S. T. F. C., Gori, R., Neves, R. & Nopens, I. 2017 Towards advanced aeration modelling: from blower to bubbles to bulk. *Water Science and Technology.* **75** (3), 507–517.

Amaral, A., Bellandi, G., Rehman, U., Neves, R., Amerlinck, Y. & Nopens, I. 2018 Towards improved accuracy in modeling aeration efficiency through understanding bubble size distribution dynamics. *Water Research.* **131**, 346–355.

Amerlinck, Y., De Keyser, W., Urchegui, G. & Nopens, I. 2016 A realistic dynamic blower energy consumption model for wastewater applications. *Water Science and Technology.* **74** (7), 1561–1576.

Arnell, M. 2016 *Performance Assessment of Wastewater Treatment Plants – Multi-Objective Analysis Using Plant-Wide Models. Thesis PhD compilation*, Department of Biomedical Engineering, Lund University, Lund, Sweden.

Aymerich, I., Rieger, L., Sobhani, R., Rosso, D. & Corominas, L. 2015 The difference between energy consumption and energy cost: modelling energy tariff structures for water resource recovery facilities. *Water Research.* **81**, 113–123.

Baquero-Rodríguez, G. A., Lara-Borrero, J. A., Nolasco, D. & Rosso, D. 2018 A critical review of the factors affecting modeling oxygen transfer by fine-pore diffusers in activated sludge. *Water Environ. Res.* **90**, 431–441.

Belia, E., Amerlinck, Y., Benedetti, L., Johnson, B., Sin, G., Vanrolleghem, P. A., Gernaey, K. V., Gillot, S., Neumann, M. B., Rieger, L., Shaw, A. & Villez, K. 2009 Wastewater treatment modelling: dealing with uncertainties. *Water Science and Technology.* **60** (8), 1929–1941.

Bellandi, G., Amerlinck, Y., Hoey, S., Amaral, A. & Nopens, I. 2016 Image analysis procedure to derive bubble size distributions for better understanding of the oxygen transfer mechanism. In: *3rd International Water Association Conference on New Developments in it in Water; Jointly Organized with the 7th International Conference and Exhibition on Water, Wastewater and Environmental Monitoring (WWEM 2016)*. International Water Association (IWA).

Bellandi, G., Porro, J., Senesi, E., Caretti, C., Caffaz, S., Weijers, S., Nopens, I. & Gori, R. 2018 Multi-point monitoring of nitrous oxide emissions in three full-scale conventional activated sludge tanks in Europe. *Water Science and Technology.* **77** (4), 880–890.

Capela, S., Héduit, A. & Roustan, M. 2002 Influence of the water depth on fine bubble aeration efficiency in the presence of surfactants. In: *Proceedings of the International Water Association 3rd World Water Congress, Melbourne, Australia*, April.

Carrera, L., Springer, F., Lipeme-Kouyi, G. & Buffiere, P. 2017 Sulfide emissions in sewer networks: focus on liquid to gas mass transfer coefficient. *Water Science and Technology.* **75** (8), 1899–1908.

Cierkens, K., Plano, S., Benedetti, L., Weijers, S., de Jonge, J. & Nopens, I. 2012 Impact of influent data frequency and model structure on the quality of WWTP model calibration and uncertainty. *Water Science and Technology* **65** (2), 233–242.

Clift, R., Grace, J. & Weber, M. 2005 *Bubbles, Drops, and Particles. Dover Civil and Mechanical Engineering Series*. Dover Publications.

Cornel, P., Wagner, M. & Krause, S. 2003 Investigation of oxygen transfer rates in full scale membrane bioreactors. *Water Sci. Technol.* **47**.

Do-Quang, Z., Cockx, A., Liné, A. & Roustan, M. 1998 Computational fluid dynamics applied to water and wastewater treatment facility modeling. *Environmental Engineering and Policy.* **1** (3), 137–147.

Domingo-Félez, C., Mutlu, A. G., Jensen, M. M. & Smets, B. F. 2014 Aeration strategies to mitigate nitrous oxide emissions from single-stage nitritation/anammox reactors. *Environmental Sci. Technol.* **48**, 8679–8687.

Durán, C., Fayolle, Y., Pechaud, Y., Cockx, A. & Gillot, S. 2016 Impact of suspended solids on the activated sludge non-newtonian behaviour and on oxygen transfer in a bubble column. *Chem. Eng. Sci.* **141**, 154–165.

Eckenfelder Jr., W. W., Raymond, L. W. & Lauria, D. T. 1956 Effect of various organic substances on oxygen absorption efficiency. *Sewage and Industrial Wastes* 1357–1364.

EPA, U. 1989 *Design Manual: Fine Pore Aeration Systems.* US Environmental Protection Agency, Office of Research and Development, Risk Reduction Engineering Laboratory.

Fabiyi, M. E. & Novak, R. 2008 Evaluation of the factors that impact successful membrane biological reactor operations at high solids concentration. *Proc. Water Environ. Fed.* 503–512.

Fayolle, Y., Cockx, A., Gillot, S., Roustan, M. & Héduit, A. 2007 Oxygen transfer prediction in aeration tanks using CFD. *Chemical Engineering Science.* **62** (24), 7163–7171.

Fiat, J., Filali, A., Fayolle, Y., Bernier, J., Rocher, V., Spérandio, M. & Gillot, S. 2019 Considering the plug-flow behavior of the gas phase in nitrifying BAF models significantly improves the prediction of N_2O emissions. *Water Research* **156**, 337–346.

Fisher, M. J. & Boyle, W. C. 1999 Effect of anaerobic and anoxic selectors on oxygen transfer in wastewater. *Water Environ. Res.* **71**, 84–93.

Garcia-Ochoa, F. & Gomez, E. 2009 Bioreactor scale-up and oxygen transfer rate in microbial processes: an overview. *Biotechnol Adv* **27**, 153–176.

Garrido-Baserba, M., Asvapathanagul, P., McCarthy, G. W., Gocke, T. E., Olson, B. H., Park, H.-D., Al-Omari, A., Murthy, S., Bott, C. B., Wett, B. *et al.* 2016 Linking biofilm growth to fouling and aeration performance of fine-pore diffuser in activated sludge. *Water Research* **90**, 317–328.

Garrido-Baserba, M., Asvapathanagul, P., Park, H.-D., Kim, T.-S., Baquero-Rodriguez, G. A., Olson, B. H. & Rosso, D. 2018 Impact of fouling on the decline of aeration efficiency under

different operational conditions at WRRFs. *Science of the Total Environment* **639**, 248–257.

Germain, E., Nelles, F., Drews, A., Pearce, P., Kraume, M., Reid, E., Judd, S. J. & Stephenson, T. 2007 Biomass effects on oxygen transfer in membrane bioreactors. *Water Res.* **41**, 1038–1044.

Gillot, S. & Heduit, A. 2000 Effect of air flow rate on oxygen transfer in an oxidation ditch equipped with fine bubble diffusers and slow speed mixers. *Water Research* **34** (5), 1756–1762.

Gillot, S. & Héduit, A. 2008 Prediction of alpha factor values for fine pore aeration systems. *Water Sci. Technol.* **57**, 1265–1269.

Gillot, S., Capela-Marsal, S., Roustan, M. & Héduit, A. 2005 Predicting oxygen transfer of fine bubble diffused aeration systems – model issued from dimensional analysis. *Water Research* **39** (7), 1379–1387.

Gresch, M., Armbruster, M., Braun, D. & Gujer, W. 2011 Effects of aeration patterns on the flow field in wastewater aeration tanks. *Water Research.* **45** (2), 810–818.

Groves, K. P., Daigger, G. T., Simpkin, T. J., Redmon, D. T. & Ewing, L. 1992 Evaluation of oxygen transfer efficiency and alpha-factor on a variety of diffused aeration systems. *Water Environment Research* **64** (5), 691–698.

Hebrard, G., Destrac, P., Roustan, M., Huyard, A. & Audic, J. M. 2000 Determination of the water quality correction factor α using a tracer gas method. *Water Res.* **34**, 684–689.

Henkel, J., Lemac, M., Wagner, M. & Cornel, P. 2009 Oxygen transfer in membrane bioreactors treating synthetic greywater. *Water Res.* **43**, 1711–1719.

Henkel, J., Cornel, P. & Wagner, M. 2011 Oxygen transfer in activated sludge–new insights and potentials for cost saving. *Water Science and Technology* **63** (12), 3034–3038.

Higbie, R. 1935 The rate of absorption of a pure gas into a still liquid during short periods of exposure. *Trans. Am. Inst. Chem. Eng.* **31**, 365–377.

Jiang, L.-M., Garrido-Baserba, M., Nolasco, D., Al-Omari, A., DeClippeleir, H., Murthy, S. & Rosso, D. 2017 Modelling oxygen transfer using dynamic alpha factors. *Water Res.* **124**, 139–148.

Jimenez, M., Dietrich, N., Grace, J. R. & Hébrard, G. 2014a Oxygen mass transfer and hydrodynamic behaviour in wastewater: determination of local impact of surfactants by visualization techniques. *Water Research* **58**, 111–121.

Ju, L.-K. & Sundararajan, A. 1994 The effects of cells on oxygen transfer in bioreactors: physical presence of cells as solid particles. *Chem. Eng. J. Biochem. Eng. J.* **56**, B15–B21.

Karpinska, A. M. & Bridgeman, J. 2016 CFD-aided modelling of activated sludge systems e A critical review. *Water Research.* **88**, 861–879.

Karpinska, A. M. & Bridgeman, J. 2017 Towards a robust CFD model for aeration tanks for sewage treatment – a lab-scale study. *Engineering Applications of Computational Fluid Mechanics.* **11** (1), 371–395.

Kessener, H. J. N. H. & Ribbius, F. J. 1934 Comparison of aeration systems for the activated sludge process. *Sewage Works Journal* 423–443.

Krampe, J. & Krauth, K. 2003 Oxygen transfer into activated sludge with high MLSS concentrations. *Water Sci. Technol.* **47**, 297–303.

Kulkarni, A. A. & Joshi, J. B. 2005 Bubble formation and bubble rise velocity in gas – liquid systems: a review. *Industrial & Engineering Chemistry Research.* **44** (16), 5873–5931.

Laurent, J., Samstag, R. W., Ducoste, J. M., Griborio, A., Nopens, I., Batstone, D. J., Wicks, J. D., Saunders, S. & Potier, O. 2014 A protocol for the use of computational fluid dynamics as a supportive tool for wastewater treatment plant modelling. *Water Science and Technology.* **70** (10), 1575–1584.

Le Moullec, Y., Gentric, C., Potier, O. & Leclerc, J. P. 2010 CFD simulation of the hydrodynamics and reactions in an activated sludge channel reactor of wastewater treatment. *Chemical Engineering Science.* **65** (1), 492–498.

Leu, S.-Y., Rosso, D., Larson, L. E. & Stenstrom, M. K. 2009 Real-Time aeration efficiency monitoring in the activated sludge process and methods to reduce energy consumption and operating costs. *Water Environ. Res.* **81**, 2471–2481.

Lewis, W. K. & Whitman, W. G. 1924 Principles of gas absorption. *Industrial and Engineering Chemistry.* **16** (12), 1215–1220.

Libra, J. A., Sahlmann, C., Schuchardt, A., Handschag, J., Wiesmann, U. & Gnirss, R. 2005 Evaluation of ceramic and membrane diffusers under operating conditions with the dynamic off-gas method. *Water Environ. Res.* **77**, 447–454.

Lizarralde, I., Fernández-Arévalo, T., Brouckaert, C., Vanrolleghem, P., Ikumi, D. S., Ekama, G. A., Ayesa, E. & Grau, P. 2015 A new general methodology for incorporating physico-chemical transformations into multi-phase wastewater treatment process models. *Water Res.* **74**, 239–256.

Lizarralde, I., Fernández-Arévalo, T., Beltrán, S., Ayesa, E. & Grau, P. 2018 Validation of a multi-phase plant-wide model for the description of the aeration process in a WWTP. *Water Res.* **129**, 305–318.

Loubière, K. & Hébrard, G. 2004 Influence of liquid surface tension (surfactants) on bubble formation at rigid and flexible orifices. *Chemical Engineering and Processing: Process Intensification* **43** (11), 1361–1369.

Marques, R., Rodriguez-Caballero, A., Oehmen, A. & Pijuan, M. 2016 Assessment of online monitoring strategies for measuring N_2O emissions from full-scale wastewater treatment systems. *Water Res.* **99**, 171–179.

Metcalf and Eddy 2014 *Wastewater Engineering: Treatment and Resource Recovery*, 5th edn.

McGinnis, D. F. & Little, J. C. 2002 Predicting diffused-bubble oxygen transfer rate using the discrete-bubble model. *Water Res.* **36** (18), 4627–4635.

Muller, E., Stouthamer, A., van Verseveld, H. W. & Eikelboom, D. 1995 Aerobic domestic wastewater treatment in a pilot plant with complete sludge retention by cross-flow filtration. *Water Research* **29** (4), 1179–1189.

NFEN-12255-15 2004 *European Standard: Wastewater Treatment Plants – Part 15: Measurement of the Oxygen Transfer in Clean Water in Aeration Tanks of Activated Sludge Plants*. p. 17.

Nittami, T., Katoh, T. & Matsumoto, K. 2013 Modification of oxygen transfer rates in activated sludge with its characteristic changes by the addition of organic polyelectrolyte. *Chem. Eng. J.* **225**, 673–678.

Nopens, I., Torfs, E., Ducoste, J., Vanrolleghem, P. A. & Gernaey, K. V. 2015 Population balance models: a useful

complementary modelling framework for future WWTP modelling. *Water Science and Technology.* **71** (2), 159–167.

Ozdemir, B. & Yenigun, O. 2013 A pilot scale study on high biomass systems: energy and cost analysis of sludge production. *J. Memb. Sci.* **428**, 589–597.

Plósz, B. G., Jobbágy, A. & Grady Jr., C. P. L. 2003 Factors influencing deterioration of denitrification by oxygen entering an anoxic reactor through the surface. *Water Res.* **37** (4), 853–863.

Racault, Y., Stricker, A.-E., Husson, A. & Gillot, S. 2010 Effect of mixed liquor suspended solids on the oxygen transfer rate in full scale membrane bioreactors. *Proc. Water Environ. Fed* 5853–5865.

Redmond, D., Groves, K., Daigger, G., Simpkin, T. & Ewing, L. 1992 Evaluation of oxygen transfer efficiency and alpha-factor on a variety of diffused aeration systems. *Water Environ. Res.* **64**, 691–698.

Rehman, U. 2016 *Next Generation Bioreactor Models for Wastewater Treatment Systems by Means of Detailed Combined Modelling of Mixing and Biokinetics*. Thesis PhD *compilation*, Ghent University, Belgium.

Rehman, U., Audenaert, W., Amerlinck, Y., Maere, T., Arnaldos, M. & Nopens, I. 2017 How well-mixed is well mixed? hydrodynamic – biokinetic model integration in an aerated tank of a full scale water resource recovery facility. *Water Science & Technology* **70** (10), 1575–1584 (in press).

Rosso, D. & Shaw, A. R. 2015 *Framework for Energy Neutral Treatment for the 21st Century Through Energy Efficient Aeration*. IWA Publishing.

Rosso, D. & Stenstrom, M. K. 2005 Comparative economic analysis of the impacts of mean cell retention time and denitrification on aeration systems. *Water Res.* **39**, 3773–3780.

Rosso, D. & Stenstrom, M. 2006a Economic implications of fine-pore diffuser aging. *Water Environ. Res.* **78**, 810–815.

Rosso, D. & Stenstrom, M. K. 2006b Surfactant effects on α-factors in aeration systems. *Water Research* **40** (7), 1397–1404.

Rosso, D., Lothman, S. E., Jeung, M. K., Pitt, P., Gellner, W. J., Stone, A. L. & Howard, D. 2011 Oxygen transfer and uptake, nutrient removal, and energy footprint of parallel full-scale IFAS and activated sludge processes. *Water Research* **45** (18), 5987–5996.

Samstag, R. W., Wicklein, E., Reardon, R. D., Leetch, R. J., Parks, R. M. & Groff, C. D. 2012 Field and CFD analysis of jet aeration and mixing. In: *Proceedings of WEFTEC 2012 - 85th Annual WEF Technical Exhibition and Conference*. Proc., WEFTEC 2012 4113-4139.

Sánchez, F., Rey, H., Viedma, A., Nicolás-Pérez, F., Kaiser, A. & Martínez, M. 2018 CFD simulation of fluid dynamic and biokinetic processes within activated sludge reactors under intermittent aeration regime. *Water Research* **139**, 47–57.

Sander, R. 2015 Compilation of Henry's law constants (version 4.0) for water as solvent. *Atmos. Chem. Phys.* **15** (8), 4399–4981.

Sardeing, R., Painmanakul, P. & Hébrard, G. 2006 Effect of surfactants on liquid-side mass transfer coefficients in gas–liquid systems: a first step to modeling. *Chem. Eng. Sci.* **61**, 6249–6260.

Schraa, O., Rieger, L. & Alex, J. 2015 A comprehensive aeration system model for WRRF design and control. In: *88thWater Environment Federation (WEF) Technical Exhibition and Conference (WEFTEC)*. Water Environment Federation, Chicago, IL, USA, pp. 5091–5120.

Schraa, O., Rieger, L. & Alex, J. 2017 Development of a model for activated sludge aeration systems: linking air supply, distribution, and demand. *Water Science and Technology.* **75** (3), 552–560.

Sharma, M. M. & Mashelkar, R. A. 1968 Absorption with reaction in bubble columns. *Inst. Chem. Eng. Symp. Ser.* **28**, 10–21.

Stenstrom, M. K. & Gilbert, R. G. 1981 Effects of alpha, beta and theta factor upon the design specification and operation of aeration systems. *Water Res.* **15**, 643–654.

Stenström, F. & la Cour Jansen, J. 2017 Impact on nitrifiers of full-scale bioaugmentation. *Water Science and Technology* **76** (11), 3079–3085.

Talvy, S., Cockx, A. & Line, A. 2007 Modeling of oxygen mass transfer in a gas-liquid airlift, reactor. *AIChE Journal.* **53** (2), 316–326.

US EPA 1989a *Respirometric Methods for Determination of Biodegradability*. Cincinnati, Ohio.

USEPA, U.S.E.P.A. 1989b *Fine Pore (Fine Bubble) Aeration Systems*. Cincinnati, Ohio.

Vandu, C. O. & Krishna, R. 2004 Volumetric mass transfer coefficients in slurry bubble columns operating in the churn-turbulent flow regime. *Chem. Eng. Process. Process Intensif.* **43** (8), 987–995.

Vaneeckhaute, C., Claeys, F. H. A., Tack, F. M. G., Meers, E., Belia, E. & Vanrolleghem, P. A. 2018 Development, implementation, and validation of a generic nutrient recovery model (NRM) library. *Environmental Modelling and Software.* **99**, 170–209.

Wagner, M. R. & Pöpel, H. J. 1998 Oxygen transfer and aeration efficiency – influence of diffuser submergence, diffuser density, and blower type. *Water Sci. Technol.* **38**, 1–6.

Wu, Q., Knowles, R. & Niven, D. F. 1994 O2 regulation of denitrification in Flexibacter Canadensis. *Can J Microbiol.* **40**, 916–921.

Wu, X.-J., Wendel, M., Chahine, G. L. & Riemer, B. 2014 Gas bubble size measurements in liquid mercury using an acoustic spectrometer. *Journal of Fluids Engineering.* **136** (3), 031303.

First received 27 January 2019; accepted in revised form 15 July 2019. Available online 25 July 2019