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

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ABSTRACT

Gas–liquid mass transfer in wastewater treatment processes has received considerable attention over the last decades from both 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

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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 the 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 increasing 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 two-film theory (Lewis & Whitman 1924), the penetration theory (Higbie 1935) and the surface-renewal theory (Danckwerts 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 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:

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

- C^*, the concentration in equilibrium with the bulk gas pressure as given by Henry's law; C, the concentration of the solute in the bulk of the liquid phase; P, the partial pressure of the solute being transferred; P^*, the pressure in equilibrium with the bulk liquid concentration as given by Henry's law.
- $a = A/V$, 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:

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

with k_L the liquid-phase mass transfer coefficient [m/d], H Henry's 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. In contrast, in the case where the gas is very soluble in the liquid, H is very low and consequently the main resistance for gas–liquid mass transfer is found on the gas side, i.e. $1/K_G \approx 1/k_G$.
- For the two-film theory, the liquid- and gas-phase mass transfer coefficients can be expressed as a function of the respective molecular diffusion coefficients (D) and film thickness (δ):

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

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 understanding the mechanisms of oxygen mass transfer applicable in wastewater treatment. Moreover, standardised methods exist to determine the $K_L a$ and the oxygen transfer rate (OTR).

The ASCE standard procedure (ASCE 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 OTR in clean water at standard conditions. The SOTR is expressed as:

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

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} the oxygen saturation concentration at 20 °C and 1 atm [g/m³] and V 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 influence not only the driving force in oxygen mass transfer, but also the resistance against oxygen mass transfer and the interfacial area available for exchange.

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

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 & Bridgeman 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) and 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). Although 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, 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 such as the air-flow rate, mixed liquor suspended solids concentration (MLSS), the mean cell residence time 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 analysis 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 important to accurately predict not only 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

Table 1 | Phenomena influencing the α-factor

Phenomena influencing the α-factor	References
Surfactant concentrations	Stenstrom & Gilbert (1981), Wagner & Pöpel (1998), Gillot & Héduit (2000), Loubière & Hébrard (2004), Rosso & Stenstrom (2006b), Sardeing *et al.* (2006), Gillot & Héduit (2008) and Jimenez *et al.* (2014a)
Mixed liquor suspended solids 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) and Gillot *et al.* (2005)
Daily/seasonal dynamics	Libra *et al.* (2005), Leu *et al.* (2009) and Jiang *et al.* (2017)
Mean cell residence time	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 & Stenstrom (2005), Rosso & Shaw (2015) and Garrido-Baserba *et al.* (2018)
Microbial activity	Steinmetz (1996) and Henkel *et al.* (2009)
Organic load (chemical oxygen demand)	Eckenfelder *et al.* (1956), Zlokarnik (1980), Steinmetz (1996), Leu *et al.* (2009), Jiang *et al.* (2017) and Garrido-Baserba *et al.* (2018)

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, shortcut biological nitrogen removal, ammonia-based aeration control and others, DO concentration near or below the half-saturation index K_{DO} is 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 air-flow 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).

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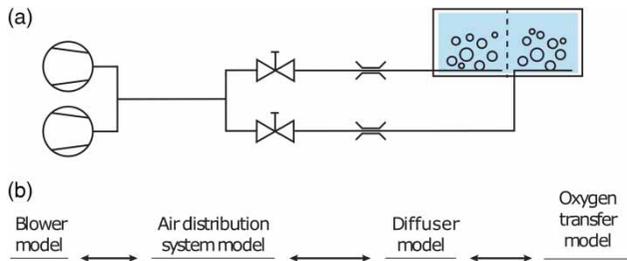
Figure 1 | (a) Schematic figure over an aeration system from blower to tank including blower, air distribution system, valves, flow meters and diffusers. (b) Principal model components and the entities required in each part. Figure adapted from Arnell (2016).

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 the K_L and the 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 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 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 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 and 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; Durán *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
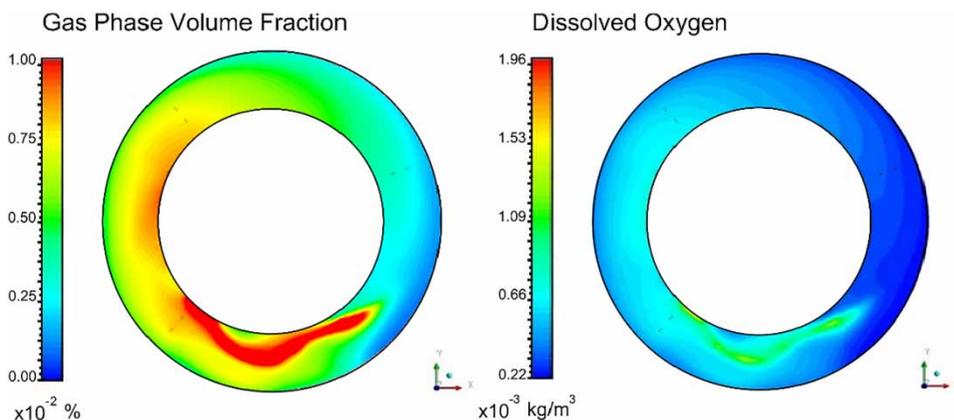

Figure 2 | CFD results for gas holdup and local DO concentration at middle depth in the aeration tank of Eindhoven WRRF, The Netherlands. Figure adapted from Rehman *et al.* (2017).

Table 2 | Summary of CFD work on aeration tanks

Reference	CFD platform	Multiphase model	Turbulence model	Bubble size & shape	Drag model	Validation study
Sánchez *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	Standard k-ε	Constant (sphere)	Clift *et al.*	Yes
Do-Quang *et al.* (1998)	ASTRID	Eulerian	Standard k-ε	Constant (sphere)	UDF	No

thickness increases their coalescence. By coalescing, the bubbles rise faster, being associated with higher interfacial shear, and experience lower hydrodynamic resistance. The net result of this coalescence is low α-factors, e.g. for membrane bioreactors and aerobic digesters (Henkel *et al.* 2009; Baquero-Rodríguez *et al.* 2018).

Bubble size distribution (BSD) has been investigated as a key factor to estimate the oxygen mass transfer since it affects both the 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 to investigate 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 improving 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 (Durán *et al.* 2016).

While incorrect input assumptions, poor model choice, or excessive simplifications have been recognised 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 a 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 present 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-ε turbulence model and fixed-size spherical bubbles, yielding substantial errors in model outputs, requires 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 one-dimensional tanks-in-series model using a two-dimensional 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. As such, this CM is able to provide insight into 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, NH_3, 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 relationship with the acid–base equilibria, which is especially important in anoxic tanks and in pH-controlled biological processes (Lizarralde *et al.* 2015). Although, in the transition from WWTPs to WRRFs, it is expected that gas–liquid mass transfer of not only 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.

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

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) and 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.

$$k_L = 2\sqrt{\frac{D_L}{\pi.t_C}} \tag{7}$$

where t_C is the contact time [s].

Recently, efforts were dedicated to developing 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

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	1.2×10^{-5}	Low	Process performance and energy, i.e. effluent quality and costs
CO_2	3.3×10^{-4}	Low	pH calculations; GHG emissions
NO	1.9×10^{-5}	Low	GHG emissions
N_2O	2.4×10^{-4}	Low	
H_2S	1.0×10^{-3}	Intermediate	Corrosion, odour nuisance and inhibition effect on the anaerobic digestion
NH_3	5.9×10^{-1}	High	Odour nuisance and inhibition effect on the anaerobic digestion, resource recovery
CH_4	1.4×10^{-5}	Low	GHG emissions
H_2	2.6×10^{-6}	Low	Inhibition effect on the anaerobic digestion
Volatile organic compounds	–	–	Health effect and odour nuisance
N_2	6.4×10^{-6}	Low	Present in air, makes up bubble volume in anoxic zones, mitigation of GHG emissions

*Sander (2015).

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 together the 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.

$$Sh_G = \frac{k_{G,i}d_b}{D_{G,i}} = 6.58 \tag{8}$$

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 $D_{G,i}$ 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 over-estimations 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 with 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 of 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. 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 perform 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 spatial models; and (v) perform rigorous regression analysis, sensitivity, and uncertainty analysis.

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