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Part 2: hydrodynamic and integrated Models

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Critical review of Membrane Bioreactor models - Part 2: hydrodynamic & integrated models

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Abstract

Membrane bioreactor technology exists for a couple of decades, but has not yet overwhelmed the market due to some serious drawbacks of which operational cost due to fouling is the major contributor. Knowledge buildup and optimisation for such complex systems can heavily benefit from mathematical modelling. In this paper, the vast literature on hydrodynamic and integrated modelling in MBR is critically reviewed. Hydrodynamic models are used at different scales and focus mainly on fouling and only little on system design/optimisation. Integrated models also focus on fouling although the ones including costs are leaning towards optimisation. Trends are discussed, knowledge gaps identified and interesting routes for further research suggested.

Keywords: modelling, membrane bioreactors, hydrodynamics, CFD, integrated model, costs

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1. Introduction

Part 1 of this sequence of review papers on modelling of MBRs introduced the complexity and interactions between different processes occurring. For the readers convenience, the related figure (Fig.1) is reproduced here for clarity. Furthermore, a detailed description of sound model development and the different tools available for performing model-based analysis are provided. For the detailed description, the reader is referred to part 1 of this review. Whereas part 1 focused on biokinetic and filtration models, this paper deals with hydrodynamic models as well as integrated models. It shows where different studies have added value to process knowledge, how they can be useful for application (e.g. optimisation for design or operation, control) and what their flaws and pitfalls are. By doing this, gaps in model development and application will be pointed out and direction for future research and application with respect to modelling for MBRs will be given. Each section consists of (1) a general introduction on the type of model, (2) a review of the different literature models to date and (3) discussion and perspectives.

2. Modelling hydrodynamic processes

2.1. Introduction on CFD modelling for MBR

Monitoring and modelling of hydrodynamics in MBR is generally complex due to: (i) highly transient multi-phase flows, (ii) complex module configurations interacting with the flow, (iii) the non-transparency of the activated sludge and (iv) complex rheology of the activated sludge. Computational Fluid Dynamics (CFD) modelling is a widely used tool to investigate flow conditions in membrane processes (Ghidossi et al., 2006a,b), inspired by modelling of other reactors with somewhat comparable flow patterns such as bubble column reactors (Joshi, 2001). Extensive research has occurred in the field of CFD over the last two decades in various applications, presenting

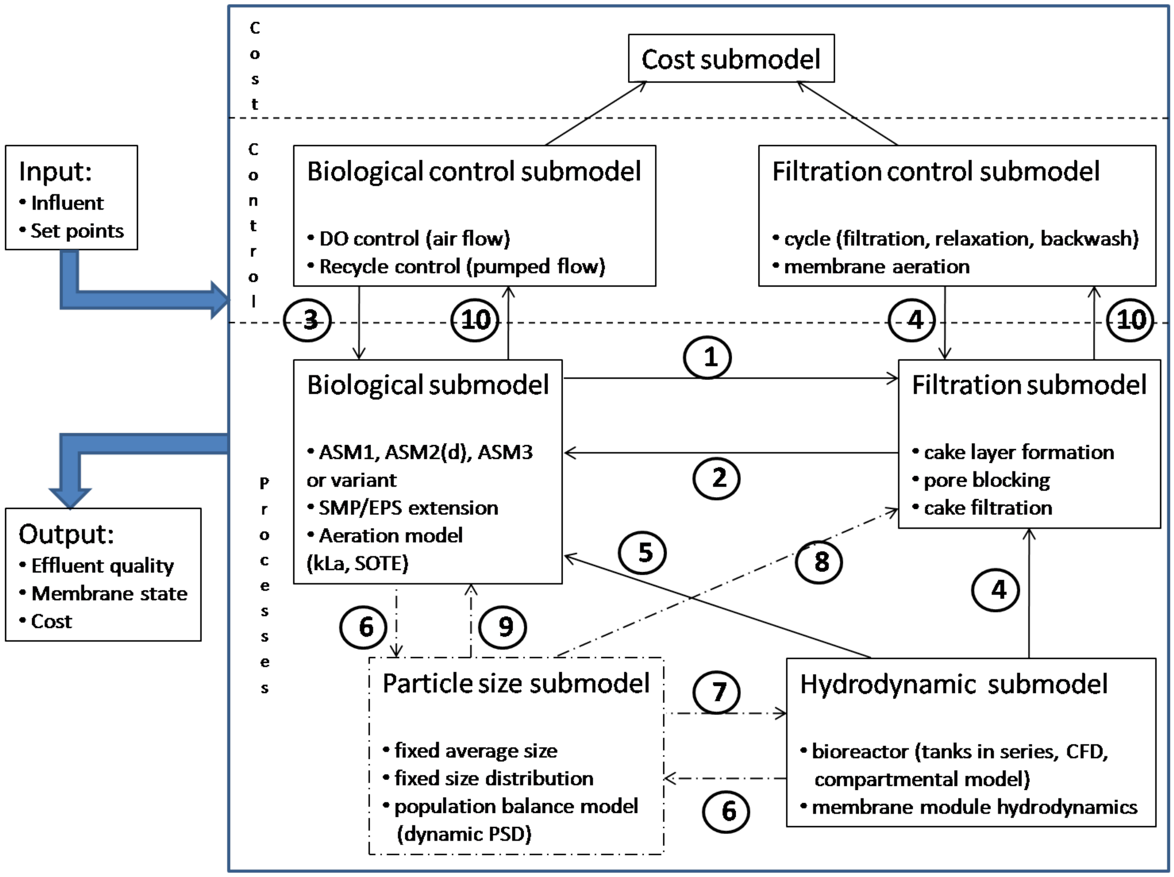

Figure 1: Illustration of the complex interactions between different processes in an MBR as well as the interaction with the control layer and costs

new approaches closer to depicting the actual physics. Basic CFD models typically comprise the overall hydrodynamics including continuity and momentum balances, possibly extended with a turbulence model. With respect to MBRs, different submodels can be linked, such as sludge transport, flocculation (population balance model), species transport (e.g. inert tracer; compounds involved in biokinetic processes) and filtration aspects, depending on the goal of the model (Fig.2), the requirement at each scale of design and the computational expense. Obviously, the degree of complexity increases

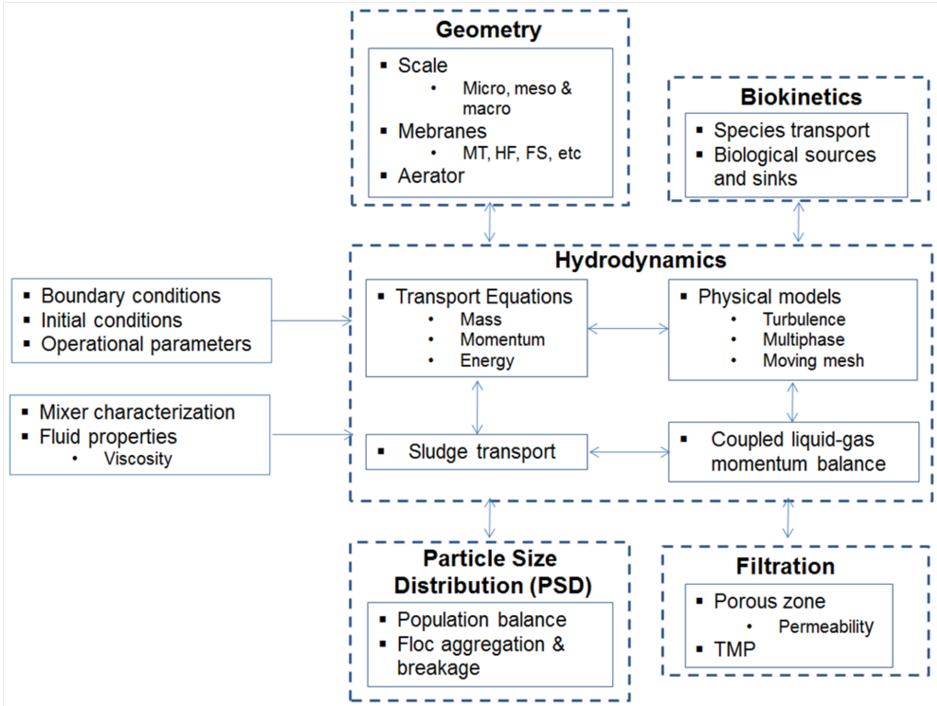

Figure 2: Schematic representation of different tiers of CFD modelling: hydrodynamic modelling as a basis extended with several submodels based on the modelling goal, scale and computational burden

gradually when including more submodels. In the remainder of this introduction, more background on the basic concepts of hydrodynamic CFD models is briefly provided.

Given the importance of aeration in MBRs, multiphase CFD models (modelling gas and liquid phases) are typically used. These allow calculation of different phenomena (e.g. mass, momentum and energy transport) by a set of coupled partial differential equations (PDEs) that describe the multiphase flow. These are approximated by algebraic equations and solved numerically. For this purpose, a computational grid is created, which serves as a spatial discretisation of the computational domain. A time discretisation is defined by the definition of an appropriate time step for the unsteady simulation. The current methodology of multiphase flow modelling falls into two categories: empirical correlations and numerical models. Empirical models, based on direct observation, measurements and extensive data collection, develop simplified relations between important parameters which must be evaluated by experimental data. The empirical correlations do not address any physical phenomena and behave like a black box. They can yield excellent results but their application is limited to the conditions of the experiments used to derive them.

Numerical models are based on a deeper understanding of the process behaviour. They approximate the physical phenomenon by taking into consideration the most important processes and neglecting less important effects complicating the mathematical problem without adding accuracy. Numerical models introduce multi-dimensional Navier-Stokes (NS) equations for multiphase flow. More detailed information can be obtained from numerical models such as distribution of phases, dynamic flow regime transition and turbulent effects. However, these models also have to utilize some inputs based on correlations due to the limitations of the current knowledge. There are two major approaches to model multiphase flows in CFD:

- Euler-Lagrange approach: it treats the fluid phase as a continuum while tracking every single particle, drop or bubble. It has the advantage of simple implementation for forces acting on the bubbles and the result gives a more realistic representation of the dispersed phase. However, Euler-Lagrange simulations suffer from the drawback that by tracking each particle, drop or bubble individually, high performance computers with large amounts of memory are required, resulting in long and heavy simulations. Therefore, this approach is limited to low fractions of the dispersed phase. Since in most applications of bubble columns, the gas volume fraction is generally not small, the use of Euler-Euler approach in this situation is much more suitable and practical.

- Euler-Euler approach: it treats all phases as interpenetrating continua, with volume fractions which sum to 1 in each cell. This approach solves the NS equations for each phase and coupling terms are associated to take the interaction between the phases into account. This approach is more suitable to describe any poly-phase system with dispersed phase volume fractions less than 15% and can be further subdivided in (Table 1):

- Eulerian model. This model solves a set of momentum and continuity equations for each phase, whereas all phases share one common pressure field. Significant limitations of this approach are constraints in computer capacity and lack of convergence for highly complex flow patterns. Nevertheless, the Eulerian model is known as a powerful tool for tracking the dispersed phase (Kang et al., 2008). The model is applicable to dispersed particles smaller than the grid size by predefining a uniform particle size (Ndinisa et al., 2005, 2006);
- Mixture model (or Algebraic Slip Mixture): This model is based on the solution of a single mixture momentum equation for all phases, which significantly reduces computational efforts compared to the Eulerian model. This approach takes into account slip velocities of the dispersed and the continuous phase relative to the mixture;
- Volume of fluid (VOF) model: This model is a surface tracking technique applied to immiscible fluids with particles larger than the grid size (Ndinisa et al., 2005). A single set of momentum equations is solved for the continuous phase of a two-phase flow. The corresponding solution for the dispersed phase follows directly from the closure condition of volume fraction for incompressible flows. All variables and properties of the fluid are calculated as cell-averages weighted by the corresponding volume fractions. The interpen-

etration of phases is restricted to the boundary surface, which are typically 1 or 2 grid elements thick. Slip velocities are not taken into account in the VOF model.

The choice between these three models for modelling of MBRs usually depends on the MBR configuration:

- Immersed MBR: In this type of system, a bubbly flow typically occurs in which the phases (gas and liquid) are dispersed and the volume fractions exceed 10%, and the mixture and the Eulerian multiphase models are recommended;
- Side-stream MBR: In this type of system, a slug flow pattern typically occurs and the recommended multiphase model is the VOF.

A vast amount of literature on CFD modelling of MBRs exists. A concise overview is given in Table 2. The remainder of this section aims at providing a structured overview of this literature. The following subsections are organized based on the application (part of the MBR plant or full scale). A first section (2.2) deals with CFD models related to membrane scouring at different scales, whereas a second section (2.3) treats CFD modelling at full scale. A final section (2.4) discusses knowledge gaps and perspectives. It should be noted that CFD models extended with submodels (as indicated in Fig.2) will be discussed in this section and not in the integrated model section 3, which discusses models with a lower level of complexity (i.e. not based on CFD).

2.2. Modelling hydrodynamics for membrane scouring

Membrane scouring is the process in which air bubbles are introduced underneath the membrane module in order to mitigate fouling. Table 2 illustrates that this phenomenon has been studied at different scales: large-scale flow patterns for full-scale plants; micro- and meso-scale including phenomena such as cake formation and surface

Table 1: General CFD modelling approaches for a two-phase flow system that were used in literature to study MBRs

Modelling approach	**Principle**	**Appliciation**
Eulerian model	Dispersed phase = fluid phase Continuity equation solved for each phase Coupling between the phases to consider their interaction Several model associated to the turbulence modelling	Mostly used for the description of poly-phase system for gas hold up $< 15\%$
Mixture	Close to the Eulerian-Eulerian approach Solving equations for the mixture + equation for the volume fraction of the dispersed phase	Two phase non miscible flows Dispersed phase holdup $>$ 10-15%
Volume of Fluid (VOF)	Dispersed phase = deformable Solving the Navier-Stokes equation for each phase Includes gas-liquid interface reconstruction	Interface tracking Number of inclusions < 10

Table 2: Breakdown of previous studies on CFD modelling of MBRs (*NM: Not Mentioned)

Scale	Module configuration	Multiphase model	Turbulence model	Study	References
Micro	FS	Euler	Standard $k-\epsilon$	Shear stress distribution on membrane surface	Ndinisa et al. (2006)
		VOF	NM	Bubble rise, liquid flow and wall shear and stress	Drews et al. (2010)
	HF	Single phase	Standard $k-\epsilon$ & SST $k-\omega$	Impact of fiber arrangement	Dasilva et al. (2004)
			Laminar	Pressure loss prediction for water flow through inside-out HF units	Ghidossi et al. (2006a)
		Euler-Euler & VOF	Standard $k-\epsilon$	Fine bubble & spherical-cap bubble flow	Martinelli et al. (2010)
	MT	VOF	RNG $k-\epsilon$	2D simulation of a single Taylor bubble flow (slug flow) 2D simulation of a train of Taylor bubbles (slug flow) of variable size	Taha and Cui (2002, 2006); Taha et al. (2006); Ratkovich et al. (2009a)
		Euler & VOF	Laminar	Impact of permeate extraction on the 2D bulk phase flow field	Ndinisa et al. (2005)
	RCF	Single phase	$k-\omega$	Shear stress over the membrane surface	Torras et al. (2006, 2009)
			Laminar & SST $k-\omega$	Shear stress over the membrane surface and velocity profiles	Bentzen et al. (2011b)
		NM*	NM*	TMP and velocity profiles	Li et al. (2011)
Meso	FS	Single phase	LES	Water flow in downcomer of airlift membrane contactor	Jajuee et al. (2006)
		Euler	SST $k-\omega$	Prediction of circulation velocity	Prieske et al. (2008)
		Mixture	Standard $k-\epsilon$	Shear stress distribution over the membrane wall	Khalili et al. (2009, 2011)
	HF	Euler	Standard $k-\epsilon$	Void fraction and bubble rising velocity within the reactor and air distribution within the air pipe	(Nguyen et al. 2008)
		Mixture		Bubble size impact on air distribution with the module	Liu et al. (2009, 2010)
			RNG $k-\epsilon$	Shear stress distribution over the membrane surface	Ratkovich et al. (2010, 2011)
		Single phase & VOF		Turbulent viscosity, gas fraction and mixture velocity on the tank	Buetehorn et al. (2011)
	HS	Mixture	Realizable $k-\epsilon$	Shear stress distribution over the membrane surface	Bentzen et al. (2011a)
	MT	Single phase & Mixture	RNG $k-\epsilon$	Air distribution within an airlift skid	Ratkovich et al. (2009b)
Macro	MBR	Eulerian	Realizable $k-\epsilon$	Pilot- and full-scale comparison. Mixing behaviour between phases, flow resistances (porous zones), TSS concentration effect on viscosity	Kang et al. (2008)
	MBR (FS/HF)	Mixture	RNG $k-\epsilon$	Optimization of MBR tank design and operation. Flow resistances (porous zones).	Saalbach and Hunze (2008)
			Standard $k-\epsilon$	FS vs. HF MBR units. Tracer test (RTD), Viscosity, ASM1.	Wang et al. (2009); Brannock et al. (2010b,a,c)
	MBR (MT)			Inside vs. outside submerged MT systems	Brannock et al. (2009); Wang et al. (2009)

shear. All scales can be further subdivided based on the type of membrane into multi tubular (MT), flat sheet (FS), hollow sheet (HS), hollow fiber (HF) and rotational cross-flow (RCF) configurations. Furthermore, numerous CFD approaches focussing on cake layer formation (Carroll, 2001) and the application of feed spacers were previously presented (Fimbres-Weihs and Wiley, 2007, 2008, 2010). The major findings are summarised here.

2.2.1. Multi-Tube membranes (MT)

Tubular membrane modules are usually operated in inside-out mode combined with a lumen-side slug flow (provided by introduction of air) to promote cake layer removal. This system has been modelled on different scales (both micro and meso). At the micro-scale, a detailed modelling of the slug flow is performed. A vertical Taylor bubble flow in cylindrical tubes is characterised by axi-symmetric bubbles with a round nose and a flat tail (Taha and Cui, 2002). Significantly different flow patterns were observed for horizontal or inclined tubular membranes (Taha et al., 2006). Cui et al. (2003) introduced a model to estimate mass transfer coefficients based on a computational grid with a reference frame attached to the rising bubble. A first simulation step allows a proper development of the two-phase flow and provides an estimation of wall shear stress. This outcome was linked to the filtration performance by applying polarisation and osmotic pressure models in a second simulation stage. The authors showed that the liquid is pushed sideways by the rising bubble and forms a liquid film, which accelerated along the bubble length until a terminal liquid velocity is reached. A wavy bubble tail and wall shear stress fluctuations were observed for long bubbles, leading to an increase in steady-state permeate flux. The annular film jet penetrates into the upflowing liquid slug behind the bubble and causes the formation of vortices in the wake region. It was found that the first change in flow direction close to the bubble nose is smooth, whereas the transition at the bubble tail is rather sudden. Increasing the frequency of air bubbling resulted in an increase in permeate flux. Ndinisa et al. (2005) showed that permeate extraction leads to small oscillations in wall shear stress amplitude and a slight reduction in its magnitude. The authors concluded that these alterations in wall shear stress are negligible for operating conditions typical in membrane filtration processes. Furthermore, they found good agreement with experimental data for bubble shape and terminal bubble velocity. Although the velocity profile in the wake region (behind the bubble) could not be obtained with the laminar VOF model, it produced good results in all other regions around the bubble. In addition, they pointed out the need for an extremely fine grid in this type of flow to account for larger velocity gradients. Gas slugs of variable size were studied by Ratkovich et al. (2009a). They found that the shape of the bubble fluctuates and the overall bubble shape is affected by variations in liquid viscosity and surface tension. The CFD model overestimated experimental results of shear stress measurements for high gas flow rates, which was attributed to an insufficient turbulence modelling. Ratkovich et al. (2009b) developed a CFD model of an airlift MBR system in which the membrane module was defined as a porous zone. The model was calibrated in single phase to determine resistance values of the porous zone. A disk diffuser was found to provide a better dispersion of air in the membrane module compared to a ring diffuser, providing further insight of the air dispersion within the membrane airlift module, which is one tier higher compared to the study of slug flow in a single tubular membrane.

2.2.2. Flat Sheet membrane (FS)

Ndinisa et al. (2006) investigated the impact of baffles mounted in-between flat sheet membranes on the distribution of air and wall shear stress in the system. Using baffles results in a higher degree of confinement of the flow channel, which promotes slug flow conditions. A predefined fixed bubble size was set in the simulation but varied in a series of numerical simulations. Bubbles tended to migrate from the centre of the column towards the edges, where a meandering bubble plume was formed on each side. This meandering character was presumably due to vortices in the liquid stream (Delnoij et al., 1997). The intensity of meandering was found to increase as the aeration rate or the bubble size increased. The presence of bubbles further enhanced the shear induced by a single-phase flow of water up to a critical aeration rate. Moreover, an increase in aeration rate, bubble size or number of baffles led to an increase in average shear stress. Jajuee et al. (2006) investigated the gas holdup and liquid velocity in airlift membrane contactors. In this configuration, horizontal flat sheet membranes separated aerated and unaerated compartments of the reactor. Permeation of the liquid was driven by the density difference between the unaerated (downcomer) and the aerated zone (riser). CFD simulations showed that the liquid flow enters the downcomer as a horizontal surface jet, inducing a downward liquid jet along the wall and a horizontal flow reflected from the wall towards the membrane. An increase in inter-membrane distance led to a reduction in intensity of the surface jet. An increase in bubble size was followed by a higher rise velocity and shorter residence time of the bubbles in the riser and caused a decrease in horizontal velocity in the downcomer. The circulation velocity in a FS MBR was predicted as a function of aeration rate and geometry parameters by Prieske et al. (2008) and Drews et al. (2010). Their investigations were based on a similar approach suggested by Chisti and Moo-Young (1989) for airlift loop reactors without internals. Increasing the distance between the membrane plates impeded a higher superficial liquid velocity in the riser (Prieske et al., 2008; Tacke et al., 2008). The pressure loss between down- and upflow region significantly affected the circulation velocity (Drews et al., 2010). Complementary CFD studies conducted by the same group focused on a single bubble rising in-between two membrane plates. Smaller bubbles were found to rise with the same velocity compared to unconfined conditions. An increase in bubble diameter enhanced the effect of the presence of walls on the bubble shape, which led to a smaller projected area and higher rise velocities. For a bubble rising in a stagnant liquid, the shear stress maximum was located at the largest circular circumference of the bubble. An increase in superposed circulation velocity in the riser was followed by a higher shear stress maximum and its location progressed towards the bubble wake. The predicted two-phase shear stress was much higher than that observed for a single-phase flow of the same liquid velocity, consistent with previous findings (Ducom et al., 2002, 2003). Drews et al. (2010) found that the wall shear stress either decreases or increases with increasing bubble size depending on the distance between the membrane sheets. Furthermore, it was experimentally observed that an increase in cross-flow velocity leads to a decrease in critical flux. This unexpected observation was attributed to a decrease in critical cut diameter as the tangential liquid velocity increased. Therefore, a selective particle deposition took place, leading to a reduced average particle size and a higher specific filtration resistance of the cake layer. Finally, Khalili et al. (2009) and Khalili et al. (2011) found a relationship between the permeate flux and shear stress near the membrane surface. They suggested that imposing a proper shear stress on the surface of the membrane would result in fouling control. Values of resistances were determined experimentally and revealed that the resistance was due to cake formation on the surface of the membrane and was linked with the predicted shear stress.

2.2.3. Hollow Fiber membrane (HF)

Dasilva et al. (2004) investigated the impact of fiber arrangement on the overall flow pattern for both square and triangular fiber arrays, modelling the fibers as solid cylinders. They observed low flow areas for a relatively short inter-fiber distance in a square-type configuration, indicating that the maximum packing density for a square fiber array is lower than that for a triangular fiber arrangement. Square arrays led to symmetrical flow patterns, whereas the flow through a triangular fiber array of short fiber distance was sinusoidal. Moreover, the friction factor decreased significantly as the boundary layer separated from the fiber surface. A reduction in outer diameter of the membrane was followed by more significant back-currents and higher friction factors. Nguyen Cong Duc et al. (2008) predicted the flow distribution from a pipe sparger in a pilot HF unit. It was found that the higher the gas flow rate, the less uniform the distribution of the air occurs (same flow of air in each hole) and vice versa. Numerical results were in good agreement with experimental data. However, at elevated gas flow rates, the predicted profiles of the void fraction and bubble velocity were shifted, showing the influence of the flow distribution by the sparger. Liu et al. (2009) and Liu et al. (2010) conducted two types of measurements: i) hydrodynamics of the water flow using a particle image velocimetry (PIV) system, and ii) air bubble size distribution and movement using a high-speed camera (HSC). They found that the water flows upward in the center part of the MBR unit and goes downward along the side walls. Furthermore, fiber vibration only occurred when combining water flow and aeration. Due to the aeration induced oscillation the water velocity profile becomes more homogeneous. Air bubble sizes were in between 3 to 5mm in diameter (66% in this range) and increased in size when moving upward due to reduced water pressure leading to coalescence. They compared these results with CFD for different bubble sizes and found a good agreement for small bubbles at the lower part of the MBR tank, and for larger bubbles at the upper part of the MBR tank. It was recommended that a CFD model should be able to account for the phenomenon of variable bubble size, possibly reducing the error induced by assuming constant bubble size. Martinelli et al. (2010) applied two different CFD approaches for a detailed modelling of fine and spherical cap bubble flows. Interestingly, very low wall shear stress values were observed for all aeration conditions simulated. No significant benefit of using spherical cap instead of fine bubbles was found, which is in contrast to a number of previous studies (Cui et al., 2003). The authors attributed this finding to a horizontal flow induced by a rising bubble, which led to an enhanced particle transport to the membrane. Ghidossi et al. (2006a) derived a pressure loss correlation for a flow through inside-out HF ultrafiltration units as a function of membrane characteristics and operating conditions. It was shown that the pressure drop increased as the inlet velocity increased, while the inlet pressure increased and the internal diameter or the permeability of the membrane decreased. The pressure was found to drop linearly along the membrane length. The resulting correlation served as an adaptation of the well-known Hagen-Poiseuille equation. Ratkovich et al. (2010) and Ratkovich et al. (2011) used a CFD model to gain insight into the shear stresses induced by air sparging on HF MBR system. It was found that the shear stresses obtained by the CFD model and experimentally were similar in magnitude (0 - 0.3 Pa) but the shear distribution differed significantly especially for large shear stresses. This was attributed to the fact that the CFD model only considers the two-phase flow and not the movement and collision of fibers within the system, which is likely to impose additional shear, especially in the large shear stress range. Buetehorn et al. (2011) investigated irregular HF arrangement on submerged membrane units. This geometry model was based on CT scans to map the instantaneous displacement of HF at different heights of a membrane bundle. The HFs in the bundles were arranged irregularly, which exposed an anisotropic resistance to the flow. This resistance was implemented in a CFD model through porosity and a friction factor. CFD results showed that the distribution of cross-flow velocity and turbulent viscosity highly depended on the local fiber arrangement, the superficial inlet velocity and the total suspended solids (TSS) concentration.

2.2.4. Hollow Sheet membrane (HS)

Bentzen et al. (2011a) performed a proper validation of a CFD model in terms of velocity measurements using micro-propellers. An error less than 11% on velocity profiles was found. Wall shear stress measurements were not performed. However, based on the validation of the velocity profiles, it was inferred that the shear stress results from the CFD simulations were accurate and showed a homogeneously distributed shear over the HS membrane surface.

2.2.5. Rotation Cross-Flow membrane (RCF)

Torras et al. (2006) and Torras et al. (2009) performed CFD simulations of the flow in a membrane module equipped with a rotating disk. It was found that the velocity and shear stress profiles were dominated by centrifugal forces at angular rotating velocities greater than 2000 rpm. Furthermore, the flow distribution in the module did not contain dead zones. At lower rotation rates, membrane wall shear stress distribution was considerably affected. Angular velocities of 2000 rpm gave a good balance between energy consumption and permeate flux. Bentzen et al. (2011b) develop a CFD model of a RCF system, they performed a proper validation of the CFD model in terms of velocity measurements using laser doppler anemometry (LDA) with water. They found an error of less than 8% between experimental measurements and CFD simulations. The CFD model was used to determine shear stress values over the membrane surface. Further simulations were performed including the non-Newtonian behaviour of activated sludge, resulting in 10 times larger shear stresses. Li et al. (2011) performed CFD simulations to study how the collection-tube size, spacer thicknesses and TMP affects the fluid flow through a disk-type membrane module. 24 different combinations were modelled and a special combination (collection-tube size of 15-20 mm and a spacer thickness of 0.75-1.00 mm) was found to improve the permeate flux.

2.3. Modelling hydrodynamics of full-scale MBRs

When modelling the full-scale hydrodynamics behaviour of immersed MBRs, the membrane module cannot be ignored and needs to be modelled as such. Kang et al. (2008) investigated differences in flow behaviour between pilot- and full-scale MBR units by representing HF modules as porous zones. The study highlighted the importance of performing both simulations using the same methodology as subtle differences occurred. They observed that the mixed liquor velocity in the full-scale unit was significantly lower (50-80%) compared to that in the pilot plant. Moreover, the air velocities were found to be 15-40% lower and an increase in tank size resulted in a more pronounced internal circulation flow. Good agreement between the simulated mixed liquor velocity and air hold-up of the pilot system with experimental data was found. Saalbach and Hunze (2008) used a similar approach and provided recommendations related to the design and operation of an MBR. Modules were taken as zones of porous media with resistance values according to the type of membrane module installed. Whereas HF modules were represented by a homogeneous porous medium each, every single plate of a FS system was modelled individually. Resistance values were determined on the basis of velocity measurements. A calibration of the CFD model was achieved by defining a single set of friction factor values for all three spatial coordinates. Two full-scale MBR plants demonstrated that the modelling technique used was suitable for investigations of flow structures in MBR tanks. Furthermore, circulation flows were investigated for a HF MBR operated in air-cycling mode. Upflow regions were observed in aerated and downflow regions in unaerated modules. Interestingly, a downflow occurred in the innermost aerated module due to the proximity to the unaerated compartment of the tank.

Brannock et al. (2009) and Wang et al. (2009) found that the main mixing mechanism in MBRs was the aeration system when comparing two submerged system configurations, inside vs. outside. In the former, the membranes were immersed directly in the aerobic tank, whereas the latter configuration had the membranes immersed in a seperate tank. It was also found that certain inlet positions pushed the system towards a plug-flow system, in which short circuiting and dead zones did not occur, as there is a proper internal recirculation within the system. In addition, it was found that for the outside configuration, the recycle pumped flow, baffle and outlet positioning were crucial for proper mixing. For both configurations, having a low aeration favoured plug-flow conditions, which is advantageous for pollutant removal. However, a minimum level of aeration is required for oxygen supply and membrane scouring.

Hydrodynamics in vessel design are commonly accounted for using the residence time distribution (RTD). For given reaction rate kinetics and reactant loading rate, the RTD studies yield the actual reactor performance in a reliable manner. Wang et al. (2009); Brannock et al. (2010a); Brannock et al. (2010b) and Brannock et al. (2010c) compared RTDs of FS and HF MBR units. They performed inert tracer tests (in multitude) which provided reproducible results with high recovery of tracer to measure the RTD. Their experiments suggested that the two MBRs studied, both with respect to the bioreactor and membrane filtration vessel, had different effects on the RTD. RTD profiles indicated that both MBRs are close to complete mixing conditions. They learned that HF membranes are more energy efficient in terms of creating completely mixed conditions compared to FS membranes. This resided in the fact that HF membranes consumed 50% less aeration energy compared to the FS membranes to create the same amount of permeate. This is caused by the larger volume of filtration vessels required by the FS membrane due to the larger size of membrane modules (i.e. lower packing density) and higher sludge retention time. A CFD model was developed to optimise mixing energy and assess the effect of membrane configuration. They found that the CFD model is able to accurately predict the RTD and mixing of the two MBRs. In addition, the CFD model was extended with bioreactions using the Activated Sludge Model No. 1 (ASM1) Benchmark (Copp, 2002). This allows prediction of how full-scale reactor design features (e.g. size and position of inlets, baffles or membrane orientation) affect hydrodynamics and hence overall performance (i.e. energy) at a certain set level of pollutant removal. Brannock et al. (2010c) investigated the impact of sludge settling and found that the Froude Number ratio between sludge and gas buoyancy forces indicated that sludge settling had minimal impact on the hydrodynamics and the coupled sludge transport equations. Also, it was found that the sludge viscosity was at minimum 5 times higher than that of water. For this reason, a calibrated sludge rheological model was incorporated into the CFD model. The results showed that the sludge rheology had minimal effect on the hydrodynamics. This was attributed to the high turbulent viscosity ratio present within the system (at high turbulent viscosities the non-Newtonian behaviour tends to disappear and activated sludge behaves like a Newtonian liquid).

2.4. Discussion and perspectives

The CFD modelling studies reported in literature had ample focus on membrane scouring, covering scales from micro over meso to macro. Despite the fact that most of these efforts aimed at knowledge buildup, the entire mechanisms are not completely understood due to the complexity of the problem and the difficulty of collecting non-invasive and representative experimental data needed for validation. This often leads to contradictory observations. However, the magnitude of shear near membrane surface is now approximately known for different types of membranes. Meso-scale observations revealed that air diffusers provide a good distribution of air over the membrane surface for different systems. However, little papers focus on this more practical aspect. Given the knowledge gathered, more focused research towards operation and optimisation of spargers would be useful (e.g. possible use of air pulses to save energy without loss of filtration efficiency). However, to accomplish this, more quantitave knowledge about the interaction between shear produced by scouring and the actual behaviour of the filtration process is required. In most studied CFD models in this review filtration is not included. This is based on the simplifying assumption that the filtration flow is rather low (<10%) compared to the cross-flow. Although this is a valid assumption for meso- and macro-scale, it could have a significant effect at the micro-scale. An additional advantage of including filtration is that the frequently measured and easily accessible TMP could be used as validation variable for these models. It should be noted that certain filtration models (as discussed in part 1 of this review) aim at introducing hydrodynamic effects and actually are pursueing the same.

Next to scouring, the remnant of the reported CFD studies focused on general mixing behaviour of bioreactors and the impact of the membrane module on this. Supporting measurements are limited to RTDs derived from inert tracer tests although in some occasions velocity measurements have been performed. This type of studies are crucial as the mixing behaviour is important with respect to bioprocess performance. In this sense, the coupling of CFD with ASM models should be further investigated, a trend that can also be observed in CAS studies. The reason behind is that simple models that model mixing with the tanks in series approach is too crude and too much of an oversimplifaction. The use of compartmental models, calibrated based on CFD models, is being explored (Le Moullec et al., 2010) but no applications to MBRs is reported to date.

Advanced experimental techniques have been used to acquire data for model validation, although it seems that the limits of what is measureable are constantly being pushed. Acceptable comparison is mostly found in terms of model validation with experimental flow data at different scales. It is noteworthy though that mostly water systems are used due to difficulties with measuring in activated sludge. Surrogates for activated sludge can be used but their representativeness can be questioned. One of the major challenges remains viscosity as no consensus has been reached with regard to measurement and model. This deserves further attention and is crucial as all current CFD models use this assumption. In highly turbulent situations this might not be a big issue as mentioned by Brannock et al. (2010c).

Most of the proposed literature models have been used for process understanding, whereas only little contributions offer suggestions towards process optimization or design at specific scales. The main objective of the CFD models to date has been to understand the hydrodynamics of the system, to determine flow patterns, dead zones and improve/optimize design. The translation of the gathered knowledge to practice needs attention. The major problems are (1) transfer over scales and the aspect of validity as well as (2) computational burden. The former would require rebuilding of the model at a larger scale and data collection at large scale which are expensive and sometimes impossible. The latter is true for a single simulation (either steady state) as well as for repeated simulations that seek optimisation. However, in order to build knowledge and methods to achieve this, this type of studies are urgently needed.

The imposed membrane shear has an (unwanted) impact on sludge particle size distribution (PSD), which in turn impacts sludge filterability, and is considered crucial in fouling control and required energy input to establishe the appropriate membrane shear. Here resides another powerful application of CFD, albeit combined with a Population Balance Equation (PBE). The latter framework allows description of PSD dynamics due to aggregation and breakage phenomena, which are typically driven by velocity (shear) gradients in the liquid computed by the CFD model. In the available literature, only few studies are reported on PSD dynamics in MBRs, and none of them combine this information with CFD, making this an open research domain for further process knowledge buildup.

In summary, further research is required in two directions: (1) more complex models to further improve our understanding of the process as a whole and (2) reduced models that include the knowledge obtained from more complex models, being more rigorous than the simple models available to date. The former should explore extensions of the plain CFD with other submodels for biokinetics (ASM) or (de)flocculation (PBE) in more detail. The latter type of models are important for conducting optimisation studies. Current models are often not well balanced (complex and simple submodels are linked) leading to significant calibration efforts in which degrees of freedom of the complex model are being used to compensate for lack of detail of simple models. However, the reduction step should be based on the knowledge obtained from more complex models. Once these reduced models are in place, a powerful optimisation tool will be available.

3. Integrated modelling

3.1. Introduction

In the previous section and part 1 of this sequence of papers, the described models were mainly dedicated to single processes (e.g. biokinetics, filtration, hydrodynamics) of the total complex MBR system. This was a valid approach as most of these models were intended to build new knowledge of the different (sub)processes. However, as shown in Fig. 1, these processes are heavily linked and, hence, impact their distinct behaviour. The danger of using these separate models for optimisation of the entire system lies in the fact that optimal conditions for one process might not at all be optimal for another process (e.g. optimising SRT for biological performance might result in increased SMP and deteriorated filtration). Therefore it is important when optimising the entire system, all separate process models should be combined to a single system model which can be used for the optimisation. The challenge lies in the computational burden of the higher complexity models that are obtained, the balancing of these models, the definition of the goal(s) and the collection of sufficient data for model calibration and validation. First steps in combining different models were reported in literature and are reviewed here. Note that integrated models combining ASM and SMP dynamics are reported in the biokinetic section of part 1 of this review sequence as these are both bioprocess models and are considered as ASM extensions instead of truly integrated models. Furthermore, integrated models with a high level of complexity (mostly CFD models and their extensions) are also not considered as being useful for system optimisation due to their computational burden. Therefore, these models have been discussed earlier in section 2 and will not be included in this section.

3.2. Combined biological and filtration models

First attempts of this type of models, as reported by Ng and Kim (2007), were proposed by Lee et al. (2002) and Wintgens et al. (2003). The former coupled an ASM1-SMP model with a RIS model using Total Suspended Solids (TSS) as the main contributor to fouling (cake resistance), whereas SMP was considered to be negligible (no pore blocking included). The latter used an ASM3 model without extension and coupled it to a resistances in series (RIS) model including both cake resistance and pore blocking. The study included a successful calibration and validation based on permeability data, apart from a period where load was considered to have risen which was not accounted for in the model. Saroj et al. (2008) also acknowledged the usefulness of integrated models with regard to MBR system optimisation for both biological and filtration performance. They presented an extension of ASM3 with EPS dynamics and coupled it to the EPS based filtration model of Ognier et al. (2004). However, they only simulated the EPS dynamics and did not illustrate the link with the filtration model. Zarragoitia-González et al. (2008) described a detailed and rigorous conceptual model to simulate several biological-filtration links. A modified ASM1-SMP model (Lu et al., 2001; Cho et al., 2003) was used for the kinetics while the filtration model was based on the model of Li and Wang (2006), extended with dynamics regarding the influence of MLSS concentration, specific cake resistance and coarse bubble aeration. However, the integrated model was only confronted with a limited (though informative) set of biological and filtration data from a small lab-scale MBR. The biokinetic model was not calibrated nor validated, except for the oxygen transfer ($k_L a$) which was measured, though, did not include the adverse effects of elevated sludge concentrations on aeration efficiency. Hence, conclusions should be handled with care. Di Bella et al. (2008) also presented a rigorous integrated model in which, similar to Zarragoitia-González et al. (2008), ASM1 extended with the SMP model of Lu et al. (2001) was combined with a filtration model inspired by Li and Wang (2006), including a force balance for attachment and detachment and, for the first time in an integrated model, COD removal by the cake layer based on deep-bed filtration theory. On the other hand, some processes described in Zarragoitia-González et al. (2008) were not included nor did the model predict membrane resistances. The calibration was performed step-wise by using reactor MLSS and COD and effluent NH_4 and NO_3 for the biological model calibration and effluent COD for the calibration of the filtration model, also keeping in mind the realism of the cake layer thickness. A Monte Carlo based automated calibration technique was adopted using the Nash-Sutcliffe criterion for parameter sets that were selected based on a sensitivity analysis. Data were obtained from a relatively small aerobic pilot-scale MBR using a buffered influent flow rate, showing little dynamics in the effluent. A good description of the data and a cake layer between 0 and 35 μm were obtained. 20 parameters were calibrated in the model which seems questionable especially since little dynamics are present in the data. Moreover, there is no clear evidence that the model structure is valid as there are no detailed measurements available about the filtering efficiency of the cake layer. Hence, the removal by this mechanism predicted by the model could compensate for the SMP production dynamics or the SMP retention differences by the membranes themselves as these processes are clearly correlated in the model. Including it in the model is not sufficient to claim the process is actually taking place. This hypothesis needs further confirmation, though intuitively the mechanism seems realistic. Some of the aforementioned issues were recognized by the authors and led to the effort of Mannina et al. (2011). The model extension for SMP was replaced by a modified version of the approach of Jiang et al. (2008) for the reasons of a COD leak and introduction of too many parameters by the model of Lu et al. (2001). The considerations of Fenu et al. (2011) regarding the model of Jiang et al. (2008) were not yet adopted. The filtration model was again based on Li and Wang (2006), but also included the sectional approach of calculating local shear values instead of a constant along the membrane. Furthermore, the model was extended to predict different resistances to flux. The calibration procedure was modified and was based on Monte Carlo simulation in conjunction with standardised regression coefficients (SRC) (Saltelli et al., 2008). The integrated model had 45 parameters and 9 output variables were used for calibration. The number of estimated parameters was reduced to 25 via the sensitivity analysis. They were grouped and separately estimated in a step-wise approach: MLSS followed by TMP and resistances, COD and TN. This specific order seems arguable since an expert knowledge based calibration likely would tackle the biology first and then the filtration behaviour. Furthermore, not all parameters that are influential according to the sensitivity analysis should necessarily or automatically be calibrated: touching stoichiometric coefficients is not regarded as good modelling practice (Rieger et al., 2012). Total resistance was well predicted, but the individual contributions showed some (serious) deviations. Predictions of resistances along the membrane were given as well showing the resistances to increase towards the top of the membrane module due to lower shear. The latter was not backed up with measurements and, hence, remains merely a hypothesis that again can impact the remainder of the modelling exercise. The conclusion by the authors that the model is now ready to be used for design and optimisation is very premature and should be illustrated first.

Moreover, a validation of the model, preferably on a highly dynamic extensive data set, is missing. Finally, a recent study by Tian et al. (2011) integrated an ASM3 based model, extended with their own SMP model, including features similar to Jiang et al. (2008), with a filtration model based on a force balance inspired by literature models (Busch et al., 2007; Li and Wang, 2006) to predict COD removal by the cake layer and membrane. They collected experimental data on lab scale and spent additional batch experiments (e.g. respirometry, SMP) to determine as many model parameters as possible, ruling out the need for their subsequent calibration (considered as good modelling practice). They used a local sensitivity analysis to further strip down the number of parameters for calibration. The steady state calibration included MLSS, supernatant COD and SMP, NH_4 and NO_3 and yielded good results. Especially the distinction between supernatant COD and effluent COD could be captured by the model. The simulation of the cake layer yielded strange results as thicknesses up to 2 cm were predicted which seems not realistic (no data available) and might question the correctness of the remainder of the model. The authors concluded that further studies are needed to confirm the model validity and cure some limitations like (1) dynamic and local shear as function of aeration intensity and (2) inclusion of membrane pore characteristics.

3.3. Integrated biokinetic and population balance model

In the biokinetic section of part 1 of this review sequence it appeared that current biokinetic models needed significant calibration of half saturation constants, often postulated as being caused by the smaller floc size in MBRs. Kostoglou and Karabelas (2011) used the framework of population balance modelling (PBM), which is applied for modelling the dynamics of a distributed property of individuals in a population, to explicitly model floc size. In conjunction to that, they modelled the bioreaction effectiveness as function of the particle size, assuming that smaller sized particles would suffer less from diffusion limitation. They included aggregation and breakup in the PBM which govern the particle size distribution. From the latter they then derived the process efficiency, average particle size and the dispersivity of the suspended biomass and investigated the impact of several operational conditions like hydraulic residence time, energy dissipation rate and total system biomass. Although the approach is interesting, the study has several flaws due to oversimplification of the biological process kinetics (it only includes one equation and is nowhere near to the mostly used ASM models for biokinetics). Moreover, the conclusion that particle breakup is recommendable for MBR performance improvement (with regard to effluent quality) is not accounting for the impact of small particles on the filtration process which was recently found to be affected by small particles (Van den Broeck et al., 2010). Moreover, the story changes significantly for systems exploiting the benefit of SNDN, which requires larger flocs. Nevertheless, the study could be inspiring for further research in this direction.

3.4. Integration of cost models

Since operational cost is the major bottleneck for market breakthrough of MBRs, it is important to have accurate cost models to test new strategies for energy optimisation. All previously discussed models focused on understanding of processes and their interrelationship, leading to proposals for optimisation from a process point of view. It is, however, crucial to be able to calculate the implication with regard to cost. Since the major operational cost in an MBR is related to aeration, it is not surprising that models for energy reduction prioritised aeration. Verrecht et al. (2008) proposed a steady state model including a thorough energy cost computation for both membrane aeration as well as sludge aeration to sustain biological processes. They concluded that significant operational cost reductions could be achieved by lowering flux (keeping more membranes in operation when possible) and, accordingly, lowering membrane aeration. A sensitivity analysis revealed that loading, SOTE, MLSS and the air upflow velocity in the membrane tanks are the most important parameters. Operating at low MLSS concentrations was considered beneficial as it increases oxygen transfer efficiency. However, this would result in higher capital cost as more biological tank volume would be needed for maintaining treatment capacity. Not increasing the tank volumes would result in lower SRT and higher sludge production costs (Schaller et al., 2010; Yoon et al., 2004). As steady state tools are interesting to investigate this problem, a more accurate energy prediction is attainable by using a dynamic model. Verrecht et al. (2010a) illustrated this for a small-scale MBR for reuse by calibrating an ASM2d model and linking this to dynamic operational cost based on empirical energy models of the major unit processes (e.g. aeration). With a scenario analysis the impact of DO controller set point, SRT and recirculation flow on effluent quality, MLSS and aeration demand was tested and revealed, inter alia, that decreasing membrane aeration and SRT were most beneficial towards total energy consumption. A model validation was performed by implementing the optimal scenario to the plant, which lead to a 23% energy reduction without compromising effluent quality. A similar approach was adopted by Fenu et al. (2010) to investigate the energy consumption of a full-scale MBR. Maere et al. (2011) performed a more detailed simulation study using the framework of Benchmark Simulation Models (BSM) originally outlined by Copp (2002) with BSM1. This framework is comprised of (1) a virtual plant configuration, (2) a set of influent files and (3) performance criteria with regard to effluent quality and operational cost. It was developed to perform fair comparisons of control strategies, but can also be used for comparing operational scenarios. The bioprocess model behind BSM1 is ASM1 and a settler model is included as it was developed for CAS systems. Maere et al. (2011) extended the concept for MBR by introducing MBR specificities (e.g. complete solids retention, fine bubble and coarse bubble aeration) and adapting operational costs specifically for MBR systems. Steady state and dynamic simulations confirmed better effluent quality at higher energy cost compared to CAS. Results were also compared to three full-scale systems and were found to be realistic. Two simple control strategies were tested to illustrate the usefulness of the approach. These lead to significant energy savings without compromising effluent quality. However, as membrane fouling was not modelled, the impact of reducing membrane aeration on membrane filtration could not be assessed. Verrecht et al. (2010b) used features of the BSM concept to investigate the capital and operational costs of MBRs. A life-cycle cost analysis revealed the importance of buffer tanks for peak flows, membrane lifetime, SRT, etc. However, also here membrane fouling was not modelled precluding the assessment of design or operational choices on filtration performance and costs. Hence, a route that should be further explored is merging this type of models with models linking biological and filtration processes (section 3.2).

3.5. Conclusions and perspectives

When it comes to integrated modelling for MBR systems, three distinct types can be distinguished. The first one couples existing literature models on biokinetic and filtration processes. However, there is not yet consensus on which models to choose mainly caused by the fact that the exact fouling mechanism is not fully understood. However, interesting work is being performed and these efforts should be further stimulated in order to test several hypotheses. When doing so, authors should follow good modelling practice (see section 1 of part 1 of this paper sequence) and prefer either calibrated submodels or submodels that do not suffer from overparameterisation. One vital missing link is detailed experimental data about the process in order to either confirm or reject proposed hypotheses. There are many contributions that seem interesting from a conceptual point of view, but are worthless without experimental validation as the hypothesis can neither be confirmed, nor rejected. Furthermore, most studies were performed on lab or (small) pilot scale operated at pseudo steady state which are severe drawbacks (although justified as a first simplified step). The outlook in different papers suggesting that models can be used for optimisation is a step that is premature at this stage as first models need to be validated at full scale as well. The move to dynamic situations is also to be made, but will most probably further complicate the issue. A second integrated model is quite distinct from the others, but is nevertheless worthwhile mentioning. It seeks to understand required calibration of half saturation values in ASM models through the explicit modeling of particle size using a population balance framework. A first stab was made, but the model needs to be developed further as the biokinetic model was oversimplified in comparison with the rigour in the modeling of the particle size dynamics. Finally, a third type of integrated model integrates cost models with biological models both in steady state and dynamic. Simulation studies show the potential savings and this was even implemented once. However, major efforts in these papers went to the development of the cost models themselves, leaving the filtration model to be very basic. One interesting route to explore is to merge the first and third integration approaches and couple the more complex biological-filtration models with dedicated cost models. Moreover, these models should then be run under dynamic conditions. One important issue that should be regarded when integrating models is to keep a healthy balance between the complexity of all included submodels and not just link existing models with very different complexity. Especially when calibrating, a submodel with many control handles (degrees of freedom; parameters) might easily start correcting for flaws in more simplistic sub-models. Moreover, the calibration procedure should always be performed in a rigorous way using the tools at hand as demonstrated by Di Bella et al. (2008) and Mannina et al. (2011) and using rigorous experimental data as collected by Tian et al. (2011). Another recommendation is that when extending a model, one should focus on the "easy" bit to add, i.e. the process that has already received ample attention in literature instead of further increasing model complexity with adding additional processes. A hidden integrated model not discussed here is the way mixing is modelled in biokinetic models. This was briefly touched on in section 2 and deserves more attention as well. Quite some knowledge is available and should be used.

4. Conclusions and perspectives

Hydrodynamic and integrated models for MBRs are critically reviewed. Hydrodynamic models span the spectrum from micro- to macro-scale, but tend to mainly focus on fouling. The interaction with biokinetics is important and models at full-scale yield interesting insights. It is recommended to start using these models in design/optimization and explore further extensions and model reduction. Integrated models with potential use for design/optimization (i.e. moderate complexity) should be based on calibrated submodels with a minimal number of parameters (apply good modeling practice). Further routes for integration of multiple submodels should be explored and research in this area is encouraged.

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References

Bentzen, T.R., Ratkovich, N., Rasmussen, M.R., Heinen, N., Hansen, F., 2011a. Energy efficient aeration in a single low pressure hollow sheet membrane filtration module. GWF - Wasser, Abwasser 152, 104–107.

Bentzen, T.R., Ratkovich, N., Rasmussen, M.R., Madsen, S., Jensen, J.C., Bak, S.N., 2011b. Numerical modelling of non-Newtonian fluid in a rotational cross-flow MBR, in: 6th IWA Specialist Conference on Membrane Technology for Water & Wastewater Treatment.

Brannock, M., De Wever, H., Wang, Y., Leslie, G., 2009. Computational fluid dynamics simulations of MBRs: Inside submerged versus outside submerged membranes. Desalination 236, 244–251.

Brannock, M., Leslie, G., Wang, Y., Buetehorn, S., 2010a. Optimising mixing and nutrient removal in membrane bioreactors: CFD modelling and experimental validation. Desalination 250, 815–818.

Brannock, M., Wang, Y., Leslie, G., 2010b. Evaluation of full-scale membrane bioreactor mixing performance and the effect of membrane configuration. Journal of Membrane Science 350, 101–108.

Brannock, M., Wang, Y., Leslie, G., 2010c. Mixing characterisation of full-scale membrane bioreactors: CFD modelling with experimental validation. Water Research 44, 3181–91.

Buetehorn, S., Volmering, D., Vossenkaul, K., Wintgens, T., Wessling, M., Melin, T., 2011. CFD simulation of single- and multi-phase flows through submerged membrane units with irregular fiber arrangement. Journal of Membrane Science 384, 184–197.

Busch, J., Cruse, A., Marquardt, W., 2007. Modeling submerged hollow-fiber membrane filtration for wastewater treatment. Journal of Membrane Science 288, 94–111.

Carroll, T., 2001. The effect of cake and fibre properties on flux declines in hollow-fibre microfiltration membranes. Journal of Membrane Science 189, 167–178.

Chisti, Y., Moo-Young, M., 1989. On the calculation of shear rate and apparent viscosity in airlift and bubble column bioreactors. Biotechnology and Bioengineering 34, 1391–92.

Cho, J., Ahn, K.H., Seo, Y., Lee, Y., 2003. Modification of ASM No.1 for a submerged membrane bioreactor system: including the effects of soluble microbial products on membrane fouling. Water Science & Technology 47, 177–81.

Copp, J., 2002. The COST simulation benchmark - Description and simulator manual. Technical Report. Office for Official Publications of the European Communities. Luxembourg.

Cui, Z., Chang, S., Fane, A., 2003. The use of gas bubbling to enhance membrane processes. Journal of Membrane Science 221, 1–35.

Dasilva, A., Sinfort, C., Heran, M., Grasmick, A., 2004. Optimization of flow shear stress through a network of capillary fibers with the use of CFD. International Journal of Chemical Reactor Engineering 2, 1–11.

Delnoij, E., Kuipers, J., van Swaaij, W., 1997. Computational fluid dynamics applied to gas-liquid contactors. Chemical Engineering Science 52, 3623–3638.

Di Bella, G., Mannina, G., Viviani, G., 2008. An integrated model for physical-biological wastewater organic removal in a submerged membrane bioreactor: Model development and parameter estimation. Journal of Membrane Science 322, 1–12.

Drews, A., Prieske, H., Meyer, E.L., Senger, G., Kraume, M., 2010. Advantageous and detrimental effects of air sparging in membrane filtration: Bubble movement, exerted shear and particle classification. Desalination 250, 1083–1086.

Ducom, G., Puech, F., Cabassud, C., 2002. Air sparging with flat sheet nanofiltration: a link between wall shear stresses and flux enhancement. Desalination 145, 97–102.

Ducom, G., Puech, F.P., Cabassud, C., 2003. Gas/liquid two-phase flow in a flat sheet filtration module: Measurement of local wall shear stresses. The Canadian Journal of Chemical Engineering 81, 771–775.

Fenu, A., Roels, J., Wambecq, T., De Gussem, K., Thoeye, C., De Gueldre, G., Van De Steene, B., 2010. Energy audit of a full scale MBR system. Desalination 262, 121–128.

Fenu, A., Wambecq, T., Thoeye, C., De Gueldre, G., Van de Steene, B., 2011. Modelling soluble microbial products (SMPs) in a dynamic environment. Desalination and water treatment 29, 211–217.

Fimbres-Weihs, G., Wiley, D., 2007. Numerical study of mass transfer in three-dimensional spacer-filled narrow channels with steady flow. Journal of Membrane Science 306, 228–243.

Fimbres-Weihs, G., Wiley, D., 2008. Numerical study of two-dimensional multi-layer spacer designs for minimum drag and maximum mass transfer. Journal of Membrane Science 325, 809–822.

Fimbres-Weihs, G., Wiley, D., 2010. Review of 3D CFD modeling of flow and mass transfer in narrow spacer-filled channels in membrane modules. Chemical Engineering and Processing: Process Intensification 49, 759–781.

Ghidossi, R., Daurelle, J., Veyret, D., Moulin, P., 2006a. Simplified CFD approach of a hollow fiber ultrafiltration system. Chemical Engineering Journal 123, 117–125.

Ghidossi, R., Veyret, D., Moulin, P., 2006b. Computational fluid dynamics applied to membranes: State of the art and opportunities. Chemical Engineering and Processing 45, 437–454.

Jajuee, B., Margaritis, A., Karamanev, D., Bergougnou, M.A., 2006. Measurements and CFD simulations of gas holdup and liquid velocity in novel airlift membrane contactor. AIChE Journal 52, 4079–4089.

Jiang, T., Myngheer, S., De Pauw, D.J.W., Spanjers, H., Nopens, I., Kennedy, M.D., Amy, G., Vanrolleghem, P.A., 2008. Modelling the production and degradation of soluble microbial products (SMP) in membrane bioreactors (MBR). Water Research 42, 4955–64.

Joshi, J., 2001. Computational flow modelling and design of bubble column reactors. Chemical Engineering Science 56, 5893–5933.

Kang, C., Hua, J., Lou, J., Liu, W., Jordan, E., 2008. Bridging the gap between membrane bio-reactor (MBR) pilot and plant studies. Journal of Membrane Science 325, 861–871.

Khalili, A., Mehrnia, M., Mostoufi, N., Sarrafzadeh, M., 2009. Flow characteristics in an airlift membrane bioreactor. Chemical Product and Process Modeling 4.

Khalili, A., Mehrnia, M.R., Mostoufi, N., Sarrafzadeh, M.H., 2011. Analyze and control fouling in an airlift membrane bioreactor: CFD simulation and experimental studies. Process Biochemistry 46, 1138–1145.

Kostoglou, M., Karabelas, A., 2011. On population balance modeling of membrane bioreactor operation with periodic back-washing. AIChE Journal 57, 2274–81.

Le Moullec, Y., Gentric, C., Potier, O., Leclerc, J., 2010. Comparison of systemic, compartmental and CFD modelling approaches: Application to the simulation of a biological reactor of wastewater treatment. Chemical Engineering Science 65, 343–350.

Lee, Y., Cho, J., Seo, Y., Lee, J.W., Ahn, K.H., 2002. Modeling of submerged membrane bioreactor process for wastewater treatment. Desalination 146, 451–457.

Li, X.y., Wang, X.m., 2006. Modelling of membrane fouling in a submerged membrane bioreactor. Journal of Membrane Science 278, 151–161.

Li, Y.L., Lin, P.J., Tung, K.L., 2011. CFD analysis of fluid flow through a spacer-filled disk-type membrane module. Desalination 283, 140–147.

Liu, N., Zhang, Q., Chin, G.L., Ong, E.H., Lou, J., Kang, C.W., Liu, W., Jordan, E., 2010. Experimental investigation of hydrodynamic behavior in a real membrane bio-reactor unit. Journal of Membrane Science 353, 122–134.

Liu, W., Jordan, E., Kippax, V., Kang, C.W., Lou, J., Zhang, Q., Liu, N., 2009. Using Computational Fluid Dynamics (CFD) and Particle Image Velocimetry (PIV) to characterize air and water two phase plug flow membrane clean system, in: WEFTEC, pp. 2798–2811.

Lu, S.G., Imai, T., Ukita, M., Sekine, M., Higuchi, T., Fukagawa, M., 2001. A model for membrane bioreactor process based on the concept of formation and degradation of soluble microbial products. Water Research 35, 2038–48.

Maere, T., Verrecht, B., Moerenhout, S., Judd, S., Nopens, I., 2011. BSM-MBR: a benchmark simulation model to compare control and operational strategies for membrane bioreactors. Water Research 45, 2181–90.

Mannina, G., Di Bella, G., Viviani, G., 2011. An integrated model for biological and physical process simulation in membrane bioreactors (MBRs). Journal of Membrane Science 376, 56–69.

Martinelli, L., Guigui, C., Line, A., 2010. Characterisation of hydrodynamics induced by air injection related to membrane fouling behaviour. Desalination 250, 587–591.

Ndinisa, N., Wiley, D., Fletcher, D., 2005. Computational Fluid Dynamics simulations of Taylor bubbles in tubular membranes - Model validation and application to laminar flow systems. Chemical Engineering Research and Design 83, 40–49.

Ndinisa, N.V., Fane, A.G., Wiley, D.E., Fletcher, D.F., 2006. Fouling control in a submerged flat sheet membrane system: part II - Two-phase flow characterization and CFD simulations. Separation Science and Technology 41, 1411–1445.

Ng, A.N.L., Kim, A.S., 2007. A mini-review of modeling studies on membrane bioreactor (MBR) treatment for municipal wastewaters. Desalination 212, 261–281.

Nguyen Cong Duc, E., Levecq, C., Fournier, L., Lesjean, B., Grelier, P., Tazi-Pain, A., 2008. Modelling the two phase flow in a pilot submerged membrane bioreactor, in: 10th World Filtration Congress, Leipzig (Germany).

Ognier, S., Wisniewski, C., Grasmick, A., 2004. Membrane bioreactor fouling in subcritical filtration conditions: a local critical flux concept. Journal of Membrane Science 229, 171–177.

Prieske, H., Drews, A., Kraume, M., 2008. Prediction of the circulation velocity in a membrane bioreactor. Desalination 231, 219–226.

Ratkovich, N., Chan, C., Berube, P., Nopens, I., 2009a. Experimental study and CFD modelling of a two-phase slug flow for an airlift tubular membrane. Chemical Engineering Science 64, 3576–3584.

Ratkovich, N., Fulton, B., Hunze, M., Berube, P., Nopens, I., 2010. Experimental validation of a hydrodynamic CFD model of a hollow fiber MBR using shear intensity measurements, in: Proceedings of the Water Environment Federation, pp. 526–538.

Ratkovich, N., Fulton, B., Hunze, M., Berube, P., Nopens, I., 2011. Detailed hydrodynamic study of a hollow fiber membrane bioreactor using CFD and shear stress measurements in the bundle .

Ratkovich, N., Hunze, M., Futselaar, H., Nopens, I., 2009b. Use of CFD to model and optimize the hydrodynamics of an airlift MBR side-stream module, in: Proceedings of the Water Environment Federation, pp. 2812–2818.

Rieger, L., Gillot, S., Langergraber, G., Ohtsuki, T., Shaw, A., Takács, I., Winkler, S., 2012. Guidelines for using Activated Sludge Models. IWA Scientific and Technical Report. Technical Report. IWA Publishing. London.

Saalbach, J., Hunze, M., 2008. Flow structures in MBR-tanks. Water Science & Technology 57, 699–705.

Saltelli, A., Ratto, M., Andres, T., Campolongo, F., Cariboni, J., Gatelli, D., Saisana, M., Tarantola, S., 2008. Global sensitivity analysis. The primer. John Wiley & Sons.

Saroj, D., Guglielmi, G., Chiarani, D., Andreottola, G., 2008. Modeling and simulation of membrane bioreactors by incorporating simultaneous storage and growth concept: an especial attention to fouling while modeling the biological process. Desalination 221, 475–482.

Schaller, J., Drews, A., Kraume, M., 2010. Development of a cost model for membrane bioreactors including sludge handling costs. Desalination and Water Treatment 18, 315–320.

Tacke, D., Pinnekamp, J., Prieske, H., Kraume, M., 2008. Membrane bioreactor aeration: investigation of the velocity flow pattern. Water Science & Technology 57, 559–65.

Taha, T., Cheong, W., Field, R., Cui, Z., 2006. Gas-sparged ultrafiltration using horizontal and inclined tubular membranes - A CFD study. Journal of Membrane Science 279, 487–494.

Taha, T., Cui, Z., 2002. CFD modelling of gas-sparged ultrafiltration in tubular membranes. Journal of Membrane Science 210, 13–27.

Taha, T., Cui, Z., 2006. CFD modelling of slug flow in vertical tubes. Chemical Engineering Science 61, 676–687.

Tian, Y., Chen, L., Jiang, T.L., 2011. Simulation of a membrane bioreactor system for wastewater organic removal: biological treatment and cake layer-membrane filtration. Industrial and Engineering Chemistry Research 50, 1127–1137.

Torras, C., Pallares, J., Garcia-Valls, R., Jaffrin, M., 2009. Numerical simulation of the flow in a rotating disk filtration module. Desalination 235, 122–138.

Torras, C., Pallarès, J., Garcia-Valls, R., Jaffrin, M.Y., 2006. CFD simulation of a rotating disk flat membrane module. Desalination 200, 453–455.

Van den Broeck, R., Van Dierdonck, J., Caerts, B., Bisson, I., Kregersman, B., Nijskens, P., Dotremont, C., Van Impe, J., Smets, I., 2010. The impact of deflocculation-reflocculation on fouling in membrane bioreactors. Separation and Purification Technology 71, 279–284.

Verrecht, B., Judd, S., Guglielmi, G., Brepols, C., Mulder, J.W., 2008. An aeration energy model for an immersed membrane bioreactor. Water Research 42, 4761–70.

Verrecht, B., Maere, T., Benedetti, L., Nopens, I., Judd, S., 2010a. Model-based energy optimisation of a small-scale decentralised membrane bioreactor for urban reuse. Water Research 44, 4047–56.

Verrecht, B., Maere, T., Nopens, I., Brepols, C., Judd, S., 2010b. The cost of a large-scale hollow fibre MBR. Water Research 44, 5274–83.

Wang, Y., Brannock, M., Leslie, G., 2009. Membrane bioreactors: overview of the effects of module geometry on mixing energy. Asia-Pacific Journal of Chemical Engineering 4, 322–333.

Wintgens, T., Rosen, J., Melin, T., Brepols, C., Drensla, K., Engelhardt, N., 2003. Modelling of a membrane bioreactor system for municipal wastewater treatment. Journal of Membrane Science 216, 55–65.

Yoon, S.H., Kim, H.S., Yeom, I.T., 2004. The optimum operational condition of membrane bioreactor (MBR): cost estimation of aeration and sludge treatment. Water research 38, 37–46.

Zarragoitia-González, A., Schetrite, S., Alliet, M., Jáuregui-Haza, U., Albasi, C., 2008. Modelling of submerged membrane bioreactor: Conceptual study about link between activated slugde biokinetics, aeration and fouling process. Journal of Membrane Science 325, 612–624.