Position paper – progress towards standards in integrated (aerobic) MBR modelling

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Abstract: Membrane bioreactor models are useful tools for both design and management. The system complexity is high due to the involved number of processes which can be clustered in biological and physical ones. Literature studies are present and need to be harmonized in order to gain insights from the different studies and allow a system optimization by applying a control. This position paper aims at defining the current state of the art of the main integrated MBR models reported in the literature. On the basis of a modelling review, a standardized terminology is proposed to facilitate the further development and comparison of integrated membrane fouling models for aerobic MBRs.

Keywords: MBR modelling, integrated model, terminology

Introduction

Worldwide membrane bioreactors (MBR) are employed for aerobic wastewater treatment in a strongly increasing number of installations and larger plant capacities (Brepols et al., 2017; Xiao et al., 2019). The performance of MBR processes is driven by complex interactions between biological processes, fluid (rheological) properties and membrane filtration. The nature of the membrane feed (wastewater-biomass-matrix), membrane and module characteristics and the hydrodynamic environment influence fouling behaviour by reactor set-up and load as well as numerous operating modes (Zhang et al., 2006). Various computational models have thus been used to describe and master unit processes of MBR operations under dynamic conditions (Fenu et al., 2010; Naessens et al., 2012a, 2012b).

Despite the efforts performed in MBR-based technology modelling, this topic has not yet fully matured and needs further work. Specifically, the research community has not yet reached a general consensus about some critical issues related to the biological and physico-chemical processes and their kinetics (e.g. kinetics of soluble microbial products (SMP) formation and degradation process, precipitation processes, biodegradability in terms of high sludge retention time or aerobic/anaerobic conditions), fouling propensities of components and, consequently, to translate them into mathematical expressions (e.g. SMP modelling, influent fractionation, etc.). Furthermore, up to now, a complete, clear and generally accepted nomenclature/terminology surrounding the MBR modelling field is still lacking. This complicates comparisons among different models and impedes insights from previous applications.

With this position paper, the IWA Task Group (TG) on Membrane Bioreactor Modelling and Control aims at establishing a next step towards standardised MBR modelling. This paper will mainly focus on so-called integrated MBR models which jointly take into account biological and physical (membrane filtration) processes. Modelling of the latter is often accomplished by resistance-in-series (RIS) models for membrane fouling.

Building upon previous and recent literature reviews (Chang et al., 2009; Di Bella and Di Trapani, 2019; Hamedi et al., 2019; Naessens et al., 2012a, 2012b) a brief summary and update is given to identify current trends in MBR modelling with special regard to integrated MBR models and the temporal and spatial scale of modelling applications in research and engineering.

In modelling of biological wastewater treatment processes issues with ambiguous terminologies and nomenclature have been addressed previously (Corominas et al., 2010; Rieger et al., 2013). It is examined which of these issues persist in the used MBR models. Based upon the approach of Rieger et al. (2013) a way to provide a common and unambiguous terminology for variables, parameters and processes is proposed.

Updated Literature Review

Physico-chemical or mechanical unit operations. Various computational models have been used to describe and master (physico-chemical or mechanical) unit processes of MBR operations under dynamic conditions. Simple mechanistic approaches have been used to model energy consumption of MBRs based on heuristic rules and models on pumping and aeration energy (Verrecht et al., 2008). Although they can provide information on various design options, these models generally do not predict filtration performance based on membrane fouling.

Biodegradation. Activated sludge models (ASM) are well established and widely used (Langergraber et al., 2004; Rieger et al., 2013) and have been applied to simulate biomass kinetics in MBR systems (Fenu et al., 2010). Additional sub-processes or complementary models on different or additional biological pathways can be implemented to describe e.g. greenhouse-gas (GHG) emissions (Mannina et al., 2018; Massara et al., 2018; Wisniewski et al., 2018) and energy consumption (Grau et al., 2007). ASMs have also been modified to include the presence and fate of Soluble Microbial Products (SMPs) which allegedly play an important role in membrane fouling, in so-called hybrid ASM models (Zuthi et al., 2012). Hybrid ASM models could also be used to model the fate of extracellular polymeric substances (EPS) or diluted organic matter.

Filtration. Different MBR models have been focusing on the physical aspects of the fouling process by various methods with the aim of describing several processes involved in membrane fouling. Among them, mathematical models are the most widely developed which include empirical hydrodynamic models, conventional mass transfer and tangential filtration models; fractal permeation models, sectional resistance models and RIS Models (Chang et al., 2009; Naessens et al., 2012a; Ng and Kim, 2007).

Regarding the number of publications, RIS models seem to be highly popular. Based on an application of Darcy's law non-stationary mathematical equations are used to describe the total hydraulic resistance. The filtering system (physical membrane plus internal and external fouling) is characterized by different resistance contributions which can be correlated to local parameters (cross flow velocity, MLSS concentration, etc.), the resistances to filtration and the viscosity of a Newtonian fluid. Usually, fouling analysis is based on a quantification of the total resistance as sum of different resistances-in-series, each related to a specific fouling mechanism: the so-called resistance decomposition (Di Bella and Di Trapani, 2019).

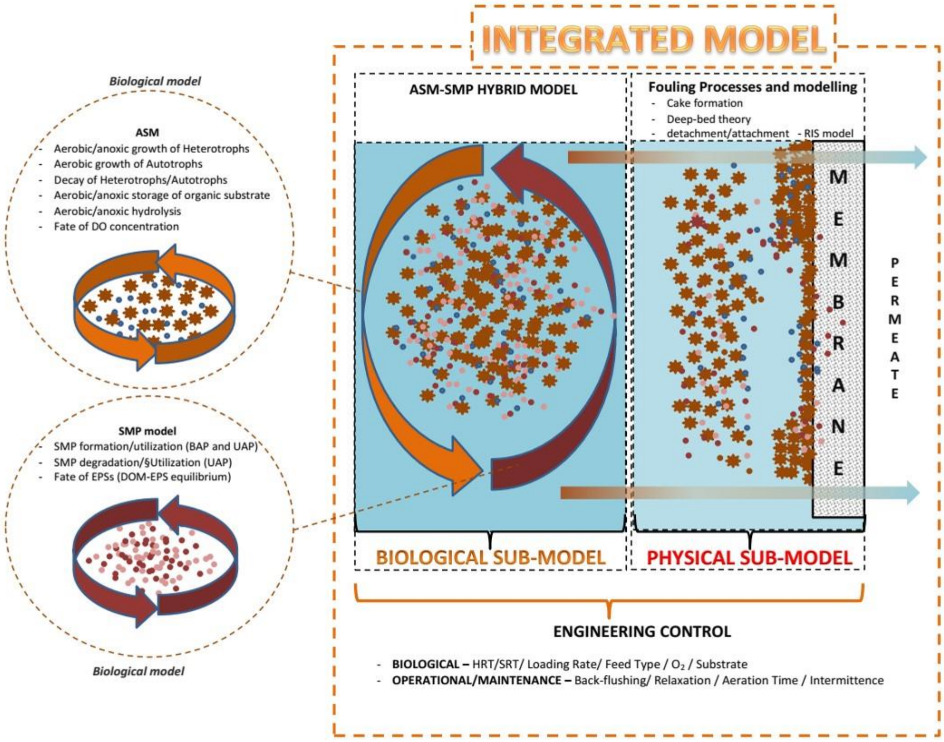

Figure 1 Integrated approach for MBR modelling (RIS: Resistance in Series, HRT: hydraulic retention time, SRT: sludge retention time.

When applied to MBR with activated sludge, the RIS concept should be used with caution (Chang et al., 2009), because the complex living suspension is not easily represented by simple addition of resistances and the additivity of components often cannot be found. Furthermore, various complementing or competing concepts on fouling phenomena in MBR have to be acknowledged (e.g.: superficial cake deposition, deep-bed fouling, complete or partial pores clogging). The analytical detection and identification of foulants is challenging. Fouling classifications and fouling mechanisms reported in literature highlight the diverse nature of membrane fouling: reversible, irreversible, irremovable fouling and cake layer deposition, intermediate blocking, concentration polarization, pore blocking, pore narrowing etc. Predicting the long-term filtration performance is further complicated by the applied membrane cleaning strategies, and by the wide range of physical scales of the examined MBR systems (Di Bella et al., 2018; Drews, 2010; Wang et al., 2014).

Computational fluid dynamics (CFD) modelling in the wastewater treatment (WWT) field is continuing to grow and is used to solve increasingly complex problems. CFD models have been used to describe various aspects of the MBR filtration process (Naessens et al., 2012b) at different scales, from entire WWTPs (Brannock et al., 2009) to microscopic levels (Lohaus et al., 2018), such as the importance of fluid dynamics for MBR fouling mitigation (Böhm et al., 2012; Liu et al., 2019) or optimization of MBR design and operation (Liu et al., 2018). A proposal towards good modelling practice has been described by (Wicklein et al., 2016).

Integrated models. Combinations of hybrid models with physical filtration models (mostly RIS models) have been denoted as integrated models (Mannina et al., 2011; Zuthi et al., 2013). These models allow combined simulations of several of the above mentioned crucial aspects that are important in MBR operations (Table 1). Currently these models seem to represent the most complete and complex level for the modelling of MBR systems, considering interactions among the different parts of the system (see Figure 1), despite their limitations.

Table1 Feature comparison of selected MBR modelling studies using an integrated RIS model approach

Reference / Model features	(Lee et al., 2002)	(Wintgens et al., 2003)	(Di Bella et al., 2008)	(Zarragoitia-González et al., 2008)	(Zarragoitia et al., 2009)	(Mannina et al., 2011)	(Sarioglu et al., 2012)	(Zuthi et al., 2012)	(Janus and Ulanicki, 2016)	Mannina et al. 2018a-b
Biological sub-model										
Biomass growth (e.g. X_{TSS})				x	x		x	x		x
ASM (SMP hybrid)	x	x	x			x			x	x
SMP	x		x	x		x		x		x
EPS									x	x
Process sub-models										
Process control				x	x				x	
Energy		x							x	x
Experimental set-up										
Lab-scale					x	x		x		
Pilot-scale			x		x		x			x
Full-scale		x								
Short time series (< 1 week)		x					x			
Long time series (> 1 week)		x	x			x	x	x		x
Calibration method										
heuristic		x					x	x		
stochastic (e.g. sensitivity analysis)						x		x		x

Alternative models are based on particle size distribution (PSD). Given that the cake layer on the membrane consists of deposited particles of which the submicron sized particles have a negative effect on the structure and porosity of the layer, models are proposed that take into account the particle size distribution and its impact on cake layer build up and the resulting membrane fouling (Broeckmann et al., 2006; Cao et al., 2015; Lu and Hwang, 1993; Park et al., 2006; Picioreanu et al., 2004; Shin et al., 2013; Yoon et al., 1999). Due to the complex and somehow still unknown mechanisms for fouling development, there have been also approaches for data-driven modelling of fouling in MBRs (Ahmad Yasmin et al., 2017; Araujo Pimentel et al., 2016; Dalmau et al., 2015; Schmitt and Do, 2017).

Model based control. Several other authors have theoretically analysed and experimentally validated energy savings of different types of advanced control in aerobic MBR technology based on models or knowledge based approaches (Drews et al., 2007; Ferrero et al., 2011; González et al., 2018; Huyskens et al., 2011; Monclús et al., 2012; Villarroel et al., 2013). Process improvements and optimized MBR control strategies (improvement of effluent quality, reduction of fouling and energy costs) can be achieved through model-based methodologies (Kalboussi et al., 2018; Odriozola et al., 2017; Yusuf et al., 2016). Different open-loop and closed-loop control systems have thus been developed and validated for MBRs, even at full-scale (Smith et al., 2006; Vargas et al., 2008; Vera et al., 2014). Model-based approaches are a cost-efficient means to explore operational strategies for both control of biological processes (e.g. nitrification/denitrification) and membrane filtration (Perera et al., 2017; Robles et al., 2014; Sun et al., 2016). Additionally, model-based optimizations are tools in sensitivity and uncertainty analysis of the MBR process operation.

Depending on their experimental set-up, the spatial and temporal scale and the intention of their work authors promote various concepts for fouling modelling or RIS aggregation (see Table 1). The abovementioned papers reveal difficulties in identifying filtration resistances, their combinations and dynamics. Model calibration methods are not likely to be documented or are carried out on constrained data-sets. Models are seldom validated on alternative set-ups or time-lines. Uncertainties in experimental set-ups, analytical methods and model assumptions are generally not evaluated or discussed (Mannina and Di Bella, 2012; Mannina et al., 2017).

Terminology and Notation

Terminologies and notations of model parameters are a source of difficulties in comparing concepts and results across reported models. RIS models show overlaps and inconsistencies in their model nomenclature (Di Bella and Di Trapani, 2019), terminology among these models can be ambiguous. These findings resemble the conclusions from an earlier examination of activated sludge models (Corominas et al., 2010; Rieger et al., 2013). It is thus attempted to draw outlines of a notational framework within this paper, while a full and unabridged framework description would exceed the limits of this publication. Still this draft is meant to be undemanding, distinctive, complete and flexible towards future requirements.

One group of state variables is used to describe bulk components which are relevant in the model and which are used in the mass balances of the model. When variables are derived from the biological (ASM) model it is recommended that their notational framework follows existing guidelines (Rieger et al., 2013). In integrated MBR models these are usually linking elements between the biological and filtration model. They can be discriminated by their nature and particle size as well as their degradability, their organic or inorganic origin, the name of the compound and other specifications. Components, which are responsible for membrane fouling can be distinguished by their actual size and nature, between particulate, colloidal and soluble compounds whose definition may depend on the actual pore-size, permeation and separation characteristics of the membrane filters in use. It is thus important that particle sizes which are relevant for the underlying theories on fouling and the model are clearly specified in the model documentation. Lumped state variables which can be obtained by grouping several variables as e.g. the total suspended solids concentration X_{TSS}, eventually need to be discriminated from composite variables which are used to compare model data with experimental data. Table 2 exemplifies the framework. Variables can be named by their main symbol and a lineage of comma-separated subscripts.

Table 2: Notation of state variables describing bulk components

Main symbol Size	**Subscript** correction factor	Nature	Name of compound	Specifications
X - particulate; C - colloidal; S - soluble	U – undegradable B – biodegradable A – abiotically convertible	Org -organic, Ig - inorganic	e.g. TSS EPS SMP	e.g. Origin, size-compartment, Sub-compound, valence

Notation of Filtration Resistances

RIS models generally employ more or less large numbers of additive resistances which are distinguished according to the applied theories on membrane fouling. Di Bella and Di Trapani (2019) provided a list of some of the most abundant resistances presented in the technical literature and come to the conclusion that despite many of the reported resistances have the same definition, they are identified with a different nomenclature due to the specific approach used. Furthermore, in some cases, the same nomenclature has been adopted to describe different fouling mechanisms. As a consequence, a more explicit notation is proposed to define the filtration resistance components of the model (Table 3). As examples intrinsic membrane resistance would be denoted $R_{It,M}$ and reversible cake layer resistance depending on TSS concentration could be denoted as $R_{Rv,CL,TSS}$. Other model parameters describe physical and chemical bulk properties, like viscosity or pH-value while other state variables describe filtration properties like flux, TMP, permeability. The main symbol can be used to specify the parameter or correction factors, while a lineage of subscripts can be used to specify, compound or reaction products and other specifications. Model parameters like hydrodynamic variables, rate coefficients and reduction factors require a notational frame of their own.

Table 3: Proposed notation of subscripts for filtration resistance R in RIS models

Classification	**Mechanism**	**Element, compound, state variable**	**Further specification**
Intrinsic - It Irreversible - Iv Irremovable - Im Reversible - Rv	Membrane - M Cake layer formation - CL Intermediate blocking - IB Concentration polarisation - CP Pore blocking - PB Pore narrowing- PN	TSS EPS SMP	Origin Compartment Sub-compound

Conclusions and future perspectives

A common RIS model framework does not exist so far. The development of a mutually accepted notation framework is thus a step towards improved exchange between researchers, modellers and practitioners longing to apply MBR models. However, the outline of a notational framework as proposed here for the biodegradation related state variables and the different resistances in the RIS based filtration model, is still a work in progress.

In accordance with previous conclusions (Naessens et al., 2012b) it can be stated that also RIS simulation studies show weaknesses regarding a good modelling practice and uncertainties in MBR modelling have not been addressed systematically. Uncertainties in wastewater treatment modelling occur during all stages of model development beginning from the scope and definition of a project through data collection and reconciliation, plant model set-up, calibration and validation to simulation and interpretation of results (Belia et al., 2009). A structured discussion on the validity of MBR models and an evaluation of possible sources, locations and levels of uncertainties seems to be inevitable. The assessment of uncertainty for MBR models needs further application to better balance model complexity between biological and physical processes.

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