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Modeling MBR fouling: A critical review analysis towards establishing a framework for good modeling practices

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ABSTRACT

This study critically analyses filtration process modeling in membrane bioreactor (MBR) technology. More specifically, the variety of approaches and assumptions considered within a curated selection of resistance-inseries (RIS) filtration models found in the literature is critically assessed. Aimed to move towards good filtration process modeling practices, the basis for establishing a unified framework rooted in the fundamentals of membrane fouling is defined in this work, considering fouling classifications, process dynamics, and underlying processes used by different authors for elucidating membrane fouling phenomena. Systematically analyzing these factors should be considered as a basic step for efficiently comparing the performance of different models. This involves a detailed examination of the processes applied within each model and their interplay with the involved resistances and fouling types. A lack of homogeneity in RIS-based filtration modeling has been observed. To address this, basic guidelines towards good modeling practices are proposed aimed at balancing model accuracy and complexity. Specifically, seven model processes, six resistances, and three subgroups for types of fouling, further divided into four or five categories are proposed to guide the selection of processes and state variables in the model structure. Hence, this study facilitates the understanding of different approaches to be used during the modeling exercise of membrane filtration processes within the MBR field, not only to enhance the comprehensibility of available filtration models, but also to help the comparison, implementation, and adaptation of available models and the comprehensive development of new ones.

1. Introduction

In recent years, membrane bioreactors (MBRs) have become a stable and advanced technological alternative for wastewater treatment, particularly for water resource recovery [\(Mannina](#page-20-0) et al., 2023). However, one of the persistent challenges of this technology is the phenomenon of membrane fouling. MBR operation below the so-called critical flux is commonly recommended for reducing membrane fouling propensity. Critical flux can be defined as the flow below which fouling theoretically does not occur (Field et al., [1995\)](#page-19-0) or the flux below which

there is theoretically no decrease in flux with time for a constant transmembrane pressure (TMP) ([Bacchin](#page-19-0) et al., 2006). From these general definitions, two different concepts have been described ([Bacchin](#page-19-0) et al., [2006\)](#page-19-0). In the "strong" concept, the critical flux is defined as the flux above which the membrane performance is not the same as the flux obtained when treating clean water under the same conditions. In the "weak" definition, the critical flux is the one below which the flux-TMP ratio is lower than the one obtained when treating pure water, i.e., the point at which there is no longer a linear relationship between them. However, bulk and membrane interactions are more complex, and these theoretical definitions are not commonly fulfilled. Indeed, a thorough

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comprehension of fouling is still essential for enhancing efficiency and developing effective mitigation and prevention strategies. The mechanisms, origin, and consequences of fouling still need to be fully understood, and there is a lack of consensus on those already examined. Significant efforts have been devoted to modeling membrane fouling. However, a diverse array of modeling approaches regarding fouling origin, mechanisms, process dynamics, and/or state variables can be found in the literature.

In terms of model types, it is possible to find mechanistic models (white-box models), semi-empirical models (grey-box models) and datadriven models (black-box models) (von [Sperling](#page-21-0) et al., 2020). Mechanistic models (e.g., [Broeckmann](#page-19-0) et al., 2006; [Busch](#page-19-0) et al., 2007) attempt to describe and predict the processes involved in membrane fouling formation through the laws of physics, chemistry, and biology. These models attempt to include most of the occurring phenomena and interactions, inducing a higher level of complexity and intricate detail. As such, mechanistic models are usually overparameterized, requiring more experimental data than what is typically available, which complicates their calibration and validation. Semi-empirical models (e.g., Charfi et al., [2018a](#page-19-0); [Sarioglu](#page-20-0) et al., 2012) combine physical, chemical, and biological principles of mechanistic models with empirical parameters or relationships. This approach simplifies the model and allows for greater flexibility, making it suitable when data is limited or a balance between detailed process interpretation and computational performance is required. Finally, data-driven models (Kaneko and [Funatsu,](#page-20-0) 2013; [Kim](#page-20-0) et al., [2011;](#page-20-0) Ren et al., [2023](#page-20-0)) are based on data collected and analyzed during system operation. They use data analysis techniques to predict membrane fouling behavior. These models can adapt to variations in operating conditions without requiring advanced knowledge of fouling mechanisms. Data-driven models are easier to calibrate, but their results could not be valid outside the operation range of the original data collection. A review of the literature reveals the emergence of recent

models developed through machine learning, grounded in data-driven learning processes for MBR optimization ([Galizia](#page-19-0) et al., 2024a). For example, [Schmitt](#page-20-0) et al. (2018) proposed the use of a radial basis function neural network (RBFNN) to study membrane permeability and identify membrane fouling. Liu et al. [\(2020\)](#page-20-0) employed a model based on support vector regression (SVR) to examine chemical oxygen demand (COD) removal, TMP, and total membrane resistance in an aerobic MBR process. Niu et al. [\(2023\)](#page-20-0) obtained successful predictions for membrane fouling in an anaerobic membrane bioreactor (AnMBR) through the utilization of operational parameters, biomass characteristics, and membrane properties as input variables. Nevertheless, despite the expansion of this category of models, it is important to acknowledge that the most prevalent are those based on the semi-empirical approach. Hence, independently from the modelling approach selected (white, grey, or black), it is worth to point out that each type of model presents specific advantages and limitations depending on the target of each modelling exercise. The selection of the appropriate model should be conditioned by factors such as data availability, filtration process complexity, or modelling objective.

For knowledge-based models, different model structures have been proposed to evaluate and predict membrane fouling within the different types of models discussed. On the one hand, there are models based on pore-blocking laws, such as [Hermia](#page-20-0) (1982), who proposed four models to describe fouling from a macroscopic point of view, without specifying the underlying mechanisms. On the other hand, models based on resistances-in-series define the total filtration resistance as the sum of the partial resistances that define the fouling (e.g., Li and [Wang,](#page-20-0) 2006). These models are the most unified, as their rationale of simultaneous fouling mechanisms is considered more realistic ([Robles](#page-20-0) et al., 2018a).

Most of the mathematical models based on RIS are semi-empirical models that differ in the degree of complexity considered. The degree of complexity depends on the state variables, fouling mechanisms and dynamic processes involved. Therefore, a thorough study is needed to analyze the main differences between existing models, focusing on how fouling is classified, which processes are considered, and which state variables are involved.

This work has been developed under the umbrella of the International Water Association (IWA) Task Group on Membrane Bioreactor Modeling and Control ([https://iwa-network.org/groups/membrane](https://iwa-network.org/groups/membrane-bioreactor-modelling-and-control/) [-bioreactor-modelling-and-control/](https://iwa-network.org/groups/membrane-bioreactor-modelling-and-control/)), which was formed to address the lack of consensus on modelling MBR systems within the scientific community. Since two of the objectives of this IWA Task Group are 1) to propose standardized criteria to integrate biological, filtration and energy models for modelling of MBR-based systems, and 2) to propose guidelines to apply appropriate models to be used for different purposes (e.g., academic research, or control and multi-criteria optimization of MBR systems), it is necessary to establish basic guidelines for adequately identifying key mechanisms and processes involved in fouling phenomena. These basic guidelines will help to 1) understand and model key mechanisms surrounding membrane fouling phenomena, and 2) assist the modelers on their choice of optimal model to use, depending on the purpose of the model. To this aim, this work reviews and critically analyzes different filtration process modelling exercises to establish the basis for a unified framework rooted in the fundamentals of membrane fouling, aiming to move towards good (RIS-based) modeling practices of membrane filtration process within the MBR field. Specifically, basic guidelines for fouling classification, and dynamic processes and state variables definition are proposed in this work. To this aim, a curated selection of 21 RIS-based "classical" filtration models used in MBR technology has been assessed, exploring the fouling classifications, process dynamics, and underlying processes used by each author for elucidating membrane fouling phenomena.

2. Membrane fouling in MBR technology

Membrane fouling in MBR is influenced by several factors, which can be categorized into four main groups: feed characteristics, bulk properties, operational conditions, and membrane and module design. Fig. 1 illustrates these factors and highlights the significant interactions between them. While some parameters directly impact membrane fouling,

others help to reduce the occurrence of this phenomenon. Membrane fouling and associated energy consumption (e.g., energy required for membrane scouring by air/gas sparging or crossflow velocity) are considered serious operational obstacles and challenges in the wider spread of the MBR technology (see, e.g., Jiménez-Benítez et al., 2023; [Krzeminski](#page-20-0) et al., 2017). In this respect, adequately modeling membrane filtration may significantly improve the understanding of fouling mechanisms. Moreover, suitable filtration models allow the development of energy-efficient fouling control strategies based on optimizing both membrane management (hydrodynamic conditions and physical cleaning procedures) and biological activity control.

2.1. Fouling classification

Various categories of fouling classification can be found in the literature. Most authors classify fouling according to the mechanisms involved in the process, while other authors (also) consider the type of foulant based on its chemical nature (e.g. Gul et al., [2021;](#page-20-0) [Hamedi](#page-20-0) et al., [2019\)](#page-20-0). To stablish a common framework, it is necessary to define the categories in which fouling can be classified. The literature review (e.g., Du et al., [2020;](#page-19-0) Guo et al., [2012](#page-20-0); [Hamedi](#page-20-0) et al., 2019; Judd and [Judd,](#page-20-0) [2011\)](#page-20-0) suggests classifying fouling based on fouling consolidation (the capability for permeability recovery by physical or chemical means), fouling mechanism, or foulant type (chemical or physical nature or origin). However, there is a lack of homogeneity in the types defined within each category. For example, Guo et al. [\(2012\)](#page-20-0) define organic adsorption as a mechanism, which is usually considered a classification based on the foulant type. Thus, it is important to clearly define the different classifications within the categories. To this end, various studies (e.g, Du et al., [2020](#page-19-0); Gul et al., [2021;](#page-20-0) Guo et al., [2012](#page-20-0); [Hamedi](#page-20-0) et al., [2019;](#page-20-0) [Iorhemen](#page-20-0) et al., 2016; Judd and [Judd,](#page-20-0) 2011; [Ladewig](#page-20-0) and [Al-Shaeli,](#page-20-0) 2017) were compared to propose a simple and clear classification.

Considering the cleaning strategy applied to recover permeability, fouling can be classified as follows (Du et al., [2020;](#page-19-0) Judd & [Judd,](#page-20-0) 2011):

• Reversible/temporary/removable: corresponding to the fouling that appears during filtration due to cake layer formation, which can be

Fig. 1. Main factors affecting fouling (adapted from Judd and [Judd,](#page-20-0) 2011).

removed by physical cleaning (e.g., membrane scouring by air/gas sparging or crossflow velocity). The cake layer formation depends on the filtration mode:

- Crossflow filtration or "pseudo" crossflow filtration: the flow moves tangentially across the membrane surface thanks to a feed pump or to gas sparging.
- Dead-end filtration: the pressure drop through the membrane length is uniform and perpendicular to the membrane surface. When other forces are not involved in the process, the thickness of the cake layer depends on the filtered volume.
- Residual reversible: corresponding to the persistent reversible fouling that requires enhanced or intensive physical cleaning (e.g., back-flushing).
- Irreversible: corresponding to the fouling that cannot be removed physically, requiring chemical cleaning protocols.
- Irrecoverable/irremovable: corresponding to fouling that cannot be removed, neither physically nor chemically from the membrane, i.e., permanent fouling.

Considering the classification above, different classical fouling control/removal strategies are usually applied [\(Hamedi](#page-20-0) et al., 2019; [Judd](#page-20-0) and [Judd,](#page-20-0) 2011; [Le-Clech](#page-20-0) et al., 2006; Min et al., [2024\)](#page-20-0).

- Physical cleaning:
	- Backwashing (see e.g., [Hwang](#page-20-0) et al., 2009; Liu et al., [2021;](#page-20-0) [Raffin](#page-20-0) et al., [2012\)](#page-20-0): consists in reversing the flow through the membrane to detach the cake accumulated on the membrane surface during filtration.
	- Membrane scouring by air/gas sparging (see e.g., [Galizia](#page-19-0) et al., [2024b](#page-19-0); [Monclús](#page-20-0) et al., 2015; [Robles](#page-20-0) et al., 2013a, [2013b;](#page-20-0) [Zhang](#page-21-0) et al., [2017\)](#page-21-0): consists in bubbling air/gas from the bottom of the system to apply turbulence in the membrane tank, making it more difficult for substances to be deposited on the membrane surface.
	- Membrane scouring by crossflow velocity (see e.g., [Martínez](#page-20-0) et al., [2021;](#page-20-0) Qin et al., [2024](#page-20-0)): consists in removing the material deposited on the membrane surface due to the shear forces generated by the tangential flow circulation.
	- Membrane flushing with water (ex-situ) or by using mechanical cleaning process (use of scouring media in-situ) (see e.g., [Zhang](#page-21-0) et al., [2022,](#page-21-0) [2021](#page-21-0)): consists in removing the material deposited that is not strongly attached onto the membrane surface.
- Chemical cleaning: when irreversible fouling appears, physical methods are not enough, thus chemical cleaning methods are required. Chemical cleaning uses chemical solutions (e.g., mineral/ organic acids such as citric acid, caustic soda, sodium hypochlorite, etc.) for removing the substances that have adhered to the membrane pores or onto the membrane surface.
	- Chemically enhanced backwashing (CEB) (see e.g., Lee et al., [2013](#page-20-0); Park et al., [2018\)](#page-20-0): consists in combining physical and chemical cleaning by adding chemical reagents at low concentrations into the backwash flow.
- Cleaning-in-place (CIP) (see e.g., Kim et al., [2022](#page-20-0); Wei et al., [2011](#page-21-0)): consists in a chemical cleaning in-situ. It is a maintenance cleaning, designed to maintain membrane permeability and to avoid ex-situ cleaning.
- Cleaning ex-situ (see e.g., Azis et al., [2019\)](#page-19-0): consists in intensive chemical cleaning ex-situ which requires the removal of the modules from the site and their immersion in a cleaning tank with the reagents.

Fig. 2 summarizes the relationship between the fouling types and the related fouling removal strategy.

Besides the classical fouling control strategies mentioned above, it is important to note that alternative techniques to address fouling issues are being developed (Min et al., [2024](#page-20-0)). However, the technical, economic and environmental feasibility of most of these techniques remains to be demonstrated. Moreover, although the combination of multiple strategies may hold potential for improved fouling control, special attention must be paid to several key aspects, such as the physical and chemical properties of the membranes (e.g., mechanical strength and chemical resistance) to safeguard membrane lifespan. Table 1 shows some examples of alternative fouling control strategies under study.

Considering fouling mechanisms, fouling can be classified as follows (see [Fig.](#page-4-0) 3) (Guo et al., [2012](#page-20-0); Judd and [Judd,](#page-20-0) 2011; [Ladewig](#page-20-0) and [Al-Shaeli,](#page-20-0) 2017):

- Pore plugging or complete pore blocking: particles with a diameter equal to the pore size of the membrane agglomerate in the pores and block them.
- Intermediate pore blocking: partial blockage of the pores occurs due to the deposition of some particles on the others already deposited. In this case, the particles are bigger than the membrane pore size.
- Pore narrowing or standard pore blocking: pores are narrowed or blocked due to the adsorption/retention of foulants (e.g., colloids, soluble microbial products (SMP), etc.) on their internal surfaces. In this case, the particles are smaller than the membrane pore size.

Alternative fouling control strategies (adapted from Min et al., [2024](#page-20-0)).

Fig. 2. Relationship between type of fouling type and related removal strategy.

Complete pore blocking

Intermediate pore blocking

Standard pore blocking

Particulate Colloidal

Fig. 3. Main fouling mechanisms.

• Cake/gel layer formation: a layer of cake or gel is formed on the membrane surface due to the deposition and accumulation of foulants, normally with a diameter larger than the membrane pore size.

It is possible to find different equations developed to model separately each of the mechanisms described above. Some authors describe fouling from a macroscopic point of view without specifying underlying models (e.g., [Charfi](#page-19-0) et al., 2012; Ho and [Sung,](#page-20-0) 2009; [Zheng](#page-21-0) et al., 2018). These models were normally developed to study the variation of TMP at constant permeate flux (J) or variation of J at constant TMP. On the other hand, [Hermia](#page-20-0) (1982) described a characteristic unified equation (see Eq. (1)) that can be developed to represent each one of the four

Table 2

Main fouling mechanisms used in models based on Hermia's pore blocking law (see, e.g., [Bolton](#page-19-0) et al., 2006; [Kirschner](#page-20-0) et al., 2019). J is the flux at constant TMP. TMP is the transmembrane pressure at constant J.

Mechanism	Expression	
Complete pore blocking	$J = J_0 \exp(-K \cdot t)$ $\mathit{TMP} = \frac{\mathit{TMP}_0}{1 - \frac{\alpha J}{P} (1 - \exp(-Bt))}$	(2)
Intermediate pore blocking	$J = \left(J_0^{-0.5} + K_I \cdot t\right)^{-2}$ $\mathit{TMP} = \frac{\mathit{IMP}_0}{\frac{1}{K} + \left(1 - \frac{1}{K} \right) \exp(-K_l B t)}$	(3)
Standard pore blocking	$J = (J_0^{-1} + K_S \cdot t)^{-1}$ $\mathit{TMP} = \frac{\mathit{TMP}_0}{\left(1 - K_s a_0 J t\right)^2}$	(4)
Cake/gel layer formation	$J = (J_0^{-2} + K_C \cdot t)^{-0.5}$ $TMP = TMP_0(1 + K_CJt)$	(5)
Combined cake filtration and intermediate blocking	$J = \frac{1}{K} ln \left(1 + \frac{K_I}{K_C I_0} \left(\left(1 + 2 K_C J_0^2 t \right)^{1/2} - 1 \right) \right)$ TMP_0 $TMP = \frac{IMP_0}{\exp(K_I J_0 t) \left(1 + \frac{K_C J_0}{K_I} (\exp(K_I J_0 t) - 1)\right)}$	(6)

K, a, α and B are model parameters.

above-mentioned mechanisms (see Table *2*).

$$
\frac{d^2t}{dV^2} = K \left(\frac{dt}{dV}\right)^n\tag{1a}
$$

$$
\frac{d^2t}{dP_t^2} = K \left(\frac{dt}{dP_t}\right)^n\tag{1b}
$$

where:

- *t* is the filtration time (s)
- $-$ *V* is the filtrate volume per unit of effective membrane area (m³⋅m⁻²)
- *K* is a constant model parameter with different dimensions and values for each type of mechanism
- $-P_t$ is the transmembrane pressure (Pa)
- *n* is a fouling index which can take different values depending on the dominant fouling mechanism ($n = 0$ for cake layer, $n = 1$ for intermediate blocking, $n = 1.5$ for standard blocking and $n = 2$ for complete pore blocking)

It should be noted that these models must be applied with an understanding of the assumptions being considered. These assumptions have limitations such as the fact that they consider ideal, straight, and cylindrical pores and they do not consider the effect of those mechanisms that occur simultaneously. Despite these drawbacks, this type of modeling approach has been widely applied to simulate fouling in MBRs (e.g., [Drews](#page-19-0) et al., 2009). However, although different models have been developed to address the main limitations of these models, this modeling approach remains less prevalent and less frequently implemented than RIS-based models. Indeed, in practice, the four "pure" fouling mechanism shown in Table 2 are superimposed, thus these models are not capable to fit the TMP jump. For this reason, some authors have proposed models combining these mechanisms (see, e.g., [Bolton](#page-19-0) et al., [2006;](#page-19-0) Eq. (6) in Table 2).

Considering foulant type according to their characteristics, behavior and origin, fouling can be classified as follows (see [Fig.](#page-5-0) 4) [\(Gul](#page-20-0) et al., [2021;](#page-20-0) [Iorhemen](#page-20-0) et al., 2016; Judd and [Judd,](#page-20-0) 2011; [Ladewig](#page-20-0) and [Al-Shaeli,](#page-20-0) 2017):

Particulate cake

Biofouling

Concentration polarization

Organic adsorption

Fig. 4. Main foulant types.

Inorganic precipitation

- Particulate cake: fouling is caused by the bulk particles that build-up a cake-layer on the membrane surface.
- Biofouling: fouling is caused by the accumulation of micro-organisms by adhesion, growth and metabolism of bacteria or flocs, which results in a layer/biofilm on the membrane surface.
- Concentration polarization: fouling is caused by the accumulation of contaminants near the membrane surface within the liquid phase. This phenomenon, known as concentration polarization, occurs due to specific (interconnected) factors at play:
	- Velocity and convective forces: near the membrane, the tangential velocity of the liquid is minimal. Simultaneously, the permeate flux creates convective forces perpendicular to the membrane. These opposing dynamics create a distinct region -the concentration boundary layer- where concentration gradients become significant.
	- Concentration gradient: the accumulation of foulants in the area adjacent to the membrane has an exponential trend with increasing flow. Additionally, the thickness of the boundary layer depends on the turbulence in the system. Thus, the higher the flux, the higher the accumulation at the interface, resulting in steeper concentration gradients. Consequently, the diffusion rate across the boundary layer increases.
	- Diffusion as dominant transport mode: within the concentration boundary layer the only mode of transport is diffusion. Compared to convective transport in the bulk, diffusion is slower.
	- Gel layer formation: when the concentration in the boundary layer becomes sufficiently high, a gel-like layer is formed. This layer introduces additional resistance to membrane flux, impacting overall filtration efficiency.
- Organic adsorption: fouling is caused by the adsorption of organic compounds on the membrane surface, e.g., SMP or natural organic matter (NOM) consisting of proteins, humic acids, hydrophobic substances, and polysaccharides. This mechanism forms a gel layer on the membrane surface.
- Inorganic precipitation or scaling: fouling is caused by precipitation of inorganic compounds on the membrane. After deposition, crystallization and crystal growth take place. Some of the foulants that can lead to this phenomenon are calcium carbonate (CaCO₃), barium sulfate (BaSO₄), silica (SiO₂) and calcium sulfate (CaSO₄), among others. Thus, the higher the ion strength of the medium, the higher the tendency to inorganic precipitation.

Table 3 illustrates the relationship between the fouling classifications based on foulant types, fouling mechanisms, and consolidation type.

Table 3

Relation between fouling classifications.

2.2. Fouling development

The evolution of fouling (represented by TMP increase when working at constant J mode) can be explained in three main steps that are related to the fouling mechanisms and foulant types (size, behavior, origin) explained above (Judd and [Judd,](#page-20-0) 2011; [Meng](#page-20-0) et al., 2009; [Wang](#page-21-0) et al., [2022\)](#page-21-0) and illustrated in [Fig.](#page-6-0) 5:

- *Stage 1 Conditioning fouling*: an initial increase in TMP occurs due to standard pore blocking or pore narrowing mechanism ([Zhang](#page-21-0) et al., [2006](#page-21-0)). Fouling is usually considered kind of negligeable compared to later stages, although irreversible [\(Ognier](#page-20-0) et al., 2002). SMPs and/or colloids (smaller than membrane pore size) adhere and accumulate into the membrane pores, thus narrowing them (complete blocking does not occur). SMPs and colloids mainly consist of hydrophilic proteins, polysaccharides and/or humic substances, but the specific nature is dependent on the type and concentration of the feed and the operating conditions ([Aslam](#page-19-0) et al., 2022; Liu et al., [2016\)](#page-20-0). SMP can be subdivided into utilization associated products (UAP), which are by-products resulting from substrate use and cell growth, and biomass associated products (BAP), which are by-products of endogenous respiration of the cell mass [\(Mannina](#page-20-0) et al., 2023). At this stage, foulants are subjected to a strong surface interaction of the inner walls of the pores, as their diameter is smaller than the membrane pore size ([Wang](#page-21-0) et al., 2020). In addition, the existence of sticky substances in the bulk enhances the adsorption of the contaminants inside the pores.
- *Stage 2 Slow/steady fouling*: a gradual linear or weakly exponential increase in TMP occurs mainly due to intermediate or complete pore blocking. Fouling propensity depends on the foulant size and

Fig. 5. Relationship between fouling stages, mechanisms, foulants, and TMP evolution.

membrane pore size. Fouling is related to extra-cellular polymer substances (EPS), SMP with large molecules, cellular debris, and colloidal substances of a size equivalent to the pore size [\(Chen](#page-19-0) et al., [2017](#page-19-0); [Stuckey,](#page-20-0) 2012). BAPs are larger in size than UAPs and are therefore attributed to be responsible for complete pore blockage; while UAPs are attributed to be responsible for intermediate pore blockage [\(Bolton](#page-19-0) et al., 2006; [Charfi](#page-19-0) et al., 2012; [Medina](#page-20-0) et al., 2020; Ni et al., [2011](#page-20-0)). Complete pore blocking of clean areas of the membrane is attributed to colloidal proteins and polysaccharides in EPS (Yu et al., [2021](#page-21-0)). Adsorption can also take place on the membrane surface; thus, different types of contaminants accumulate, including sludge flocs, gradually forming the cake layer. At this stage, fouling is mostly irreversible, thus the most effective mitigation strategies to be applied are based on chemical cleaning (see [Fig.](#page-3-0) 2).

• *Stage 3* – *TMP jump*: a jump in TMP occurs due to the accumulation of foulants on the membrane surface, i.e., foulants concentration reaches a critical point and fouling layers start to form and cover the whole membrane surface. This fouling can be considered partially reversible [\(Robles](#page-20-0) et al., 2018b). The key mechanism at this stage is cake/gel layer formation and compression, thus the foulant-foulant interactions are predominant (Xu et al., [2020](#page-21-0)). These interactions are complex because of the different nature of the mixed liquor components. Gel layers are formed from sticky proteins and polysaccharides in EPS, macromolecular SMPs and microbial colloids (Liu et al., [2019;](#page-20-0) [Maqbool](#page-20-0) et al., 2020; [Wang](#page-21-0) et al., 2014). A cake layer is mainly formed by the deposition of flocs and solids, microbial biomass, and humic substances [\(Aslam](#page-19-0) et al., 2022; Xu et al., [2020](#page-21-0); Yu et al., [2021](#page-21-0)). This jump in TMP is also attributed to the loss of area, exceeding the critical flux due to preferential flux paths through membrane areas less affected by fouling. At this stage, the most effective mitigation strategies to be applied are based on physical cleaning, such as backwashing or air/gas sparging (see [Fig.](#page-3-0) 2), as the fouling present is largely reversible.

2.3. Main dynamic processes: shear stress integration, and reversible and irreversible fouling formation

Adequately defining the dynamic processes involved in fouling formation and removal is essential for successfully modelling filtration process performance, thus properly linking fouling type and mechanisms to possible remedial fouling actions.

- Cake layer attachment: during the filtration phase, colloidal and particulate contaminants are carried along by the permeate flow and accumulate on the surface of the membrane, gradually forming the cake layer.
- Cake layer detachment by scouring: this cake detachment may be due to biogas/air sparging and/or crossflow velocity.
	- Mitigation by air/gas sparging: air/gas sparging generates complex local phenomena ([Braak](#page-19-0) et al. 2011) that interact in the mitigation of the formation of the cake layer, such as turbulence and back-transport, fibers movement, aeration shear stress on membrane surface and on biomass. This makes it difficult for substances to deposit on the membrane surface and promotes the detachment of the cake layer.
	- Detachment by crossflow velocity: it involves the removal of the foulants deposited on the membrane surface because of the shear forces produced by the tangential flow circulation.
- Cake layer detachment by backwashing: the flow throughout the membrane is reversed and the flow force itself allows the reversible fouling accumulated on the membrane surface to be carried away and detached. At this stage, residual reversible fouling can be also removed.
- Cake compressibility and slackening: during the filtration process, TMP compresses the cake. The pressure of the fluid against the cake matrix exerts a compressive effect on its structure. This compression is reflected in an increased flow resistance through the cake. During pressure relaxation, the structure of the cake matrix releases, and this resistance decreases.
- Irreversible fouling consolidation: as filtration progresses, irreversible fouling intensifies, primarily caused by the accumulation of foulants on the membrane surface or into the membrane pores, which cannot be removed by physical means.

3. Filtration process modeling

3.1. Historical evolution of MBR filtration modeling

To progress on filtration process modeling, it is important to analyze what advances and proposals have been made over time. [Table](#page-8-0) 4 shows a relation of the main historical milestones that have led to most advances on (RIS) filtration process modeling within the MBR field.

During the 1980s, modeling began with the development of a basic filtration equation for microfiltration (not specific to MBR) based on Darcy's law and the composition of the foulants. Later, the definition of the calculation of the specific resistance of the cake and the phenomenon of concentration by polarization was defined. In the late 1980s and 1990s the study of crossflow conditions and the effect of colloidal components on the filtration process gained traction. In addition, the existence of the mechanisms of pore blocking and cake layer formation as the responsible for fouling was raised. In the 2000s, special emphasis was given to the consideration of the impact of particle distribution and membrane pore diameters and the adhesion between particles and membrane surface, considering some properties of MBR sludge and operating. In addition, mass and force balances are jointly applied to model the cake layer and the effect of cake compression was considered. The concepts of fouling under subcritical and supercritical conditions were introduced and the MBR system geometry and hydrodynamics were studied. In the 2010s, the specific resistance of the cake was proposed as variable and dependent on parameters such as sludge concentration. It was also attempted to control the effect of solids removal in the cake mass calculation by defining a switching function and a semisaturation coefficient. Furthermore, the cake layer was studied as a layered structure of different porosity. The impact of fluidized media on filtration and the effect of cake layer formation on the pore blocking mechanism were modelled. The blocked and released filtration area were also evaluated.

3.2. Fundamentals

A few approaches have been proposed to study the impact of different mechanisms on membrane permeability. Darcy's Law and the Kozeny-Carman equations are the most generically used and are related to the concept of RIS modeling.

3.2.1. Darcy's law

In filtration process modeling, it is common practice to use Darcy's Law of filtration to represent the flow through different media in series (Eq. (7)). This law provides the theoretical basis for understanding and predicting the behavior of flow through a porous medium. It can therefore be used to characterize and design filtration processes such as MBR, representing the basis of RIS-based modeling.

In this law, the permeate volume (V_P) is driven through each media by a difference in TMP. Thus, the flow is directly proportional to the pressure gradient and inversely proportional to the viscosity of the fluid. It is possible to calculate the total resistance to filtration (R_T) from the combination of the partial resistances that are associated with the different fouling types.

$$
J = \frac{1}{A} \frac{dV_P}{dt} = \frac{TMP}{\mu R_T} \tag{7}
$$

where:

- *J* is the permeate flux $(m^3 \cdot s^{-1} \cdot m^{-2})$
- *A* is the membrane area (m^2)
- V_P is the permeate volume (m^3)
- *TMP* is the transmembrane pressure (Pa)
- *μ* is the permeate viscosity (Pa⋅s)
- R_T is the total resistance (m^{-1})

Although the original statement of Darcy's Law did not define the conditions of application, it is worth noting that the law is based on simplifications and assumptions such as a saturated, homogeneous, and isotropic medium and a laminar, continuous flow.

3.2.2. Kozeny-Carman equation

The Kozeny-Carman equation $(Eq. (8))$ allows widening the applicability of Darcy's Law since it can be used to estimate the specific resistance of different in-series media. However, it should be noted that the Kozeny-Carman equation requires some work to correctly determine the specific characteristics of the filter media. Specifically, the Kozeny-Carman equation relates the permeability to the structure of a porous medium, describing the pressure loss proportionally to the laminar fluid flow passing through the medium. This fundament highlights the link between the Kozeny-Carman equation and Darcy's Law.

$$
\frac{dP}{dx} = \frac{180\mu}{\phi_s^2 d_p^2} \frac{(1-\varepsilon)^2}{\varepsilon^3} \nu
$$
\n(8)

where:

- $-\phi_s$ is the sphericity of the particles (-)
- *dp* is the pore diameter (m)
- *ε* is the porosity (-)
- *v* is the superficial velocity $(m \cdot m^{-2} \cdot s^{-1})$
- $\frac{dP}{dx}$ is the pressure loss (Pa⋅m⁻¹)</sup>

3.2.3. Resistance-in-series concept

As can be seen from the explanation of Darcy's law, the total resistance to filtration (R_T) , can be calculated from the sum of different partial resistances (*Ri*) (Eq. (9)).

$$
R_T = R_i + R_{ii} + \dots + R_n \tag{9}
$$

Different partial resistances can be found in the literature, which define fouling based on the classifications described before (fouling consolidation, fouling mechanism, and type of foulant), such as:

- ⋅ Intrinsic membrane resistance
- ⋅ Reversible, irreversible, and irrecoverable fouling resistances
- ⋅ Cake layer, standard pore blocking, complete pore blocking, and intermediate pore blocking resistances
- ⋅ Dynamic sludge film, stable sludge, and thin layer resistances
- ⋅ Concentration polarization, scaling, and biofilm resistance

It should be noted that, besides the intrinsic membrane resistance that can be experimentally measured using pure water, estimating/ determining the magnitude of each individual resistance represents a complex task due to the interactions of the different substances present in the bulk. Indeed, experimental procedures (see, e.g., [Sanchis-Perucho](#page-20-0) et al., [2023](#page-20-0)) only allow to estimate specific fouling resistance at a given time. Therefore, individual models might be required to dynamically predict the behavior of the key fouling mechanisms affecting membrane performance.

Table 4

Key milestones achieved during the evolution of MBR filtration models.

Selected models assessed in this work, ordered by year of publication. AFMBR: Fluidized AnMBR; GAC; Granular Activated Carbon; MF: microfiltration; PET: Polyethylene Terephthalate.

3.2.4. Complementary empirical approaches

In RIS models, if the cake layer is assumed to be uniform and homogeneous, it is possible to calculate the layer thickness (*δ*) by Eq. (10).

$$
\delta_i = \frac{m_i}{\rho_i (1 - \varepsilon) A} \tag{10}
$$

where:

- m_i is the dry mass of the reference component i of the layer (kg)

- ρ_i is the component density, mass of dry matter of component i per layer volume (kg⋅m⁻³)
- A is the area of the cake (m^2)
- ϵ is the porosity (-) $=$ $\frac{Total\ powers\ volume}{Total\ porous\ median}$

It is also possible to estimate the specific dry mass per membrane area, ω_i (kg⋅m⁻²), from the coefficient m_i/A . This variable represents the mass of the component i deposited per membrane area and allows to redefine the cake layer thickness equation (Eq. (10)) shown in Eq. (11) :

$$
\delta_i = \frac{\omega_i}{\rho_i \cdot (1 - \varepsilon)}\tag{11}
$$

On the other hand, the cake layer resistance (R_C) can be calculated by combining the cake layer thickness equation (Eq. (10)) and the Kozeny-Carman equation $(Eq. (8))$ $(Eq. (8))$ $(Eq. (8))$ in the following way:

$$
R_C = 180 \frac{(1 - \varepsilon) \cdot \omega_C}{\varepsilon^3 \cdot d_P^2 \cdot \rho_C} \tag{12}
$$

where:

- ω_C is the mass of cake deposited per membrane area (kg⋅m⁻²)
- ρ_C is the cake density, mass of dry matter per layer volume (kg⋅m⁻³)

Other modeling methods introduced the concept of the average specific resistance, α_i (m⋅kg $^{-1}$), for a particular reference layer component. Thus, it is possible to define the calculation of a partial resistance (R_i) as shown in Eq. (13):

$$
R_i = \omega_i \cdot \alpha_i \tag{13}
$$

From Eq. (12) it is possible to define the average specific cake resistance α_C (Eq. (14)) and, finally, R_C can be expressed as the product of *ω^C* and *α^C* (Eq. (15)).

$$
a_C = \frac{180 \cdot (1 - \varepsilon)}{\varepsilon^3 \cdot d_p^2 \cdot \rho_C} \tag{14}
$$

$$
R_C = \omega_C \cdot \alpha_C \tag{15}
$$

Hence, combining [Eq.](#page-7-0) (7), Eq. (9) and Eq. [\(13\),](#page-8-0) the dynamic evolution of TMP in RIS models can be empirically expressed as shown in Eq. (16).

$$
TMP(t) = J \cdot \mu \cdot (\omega_i \cdot \alpha_i + \omega_{ii} \cdot \alpha_{ii} + \dots + \omega_n \cdot \alpha_n)
$$
\n(16)

The assessment of partial resistances using specific resistances (Eq. (13)) allows to reduce the effort to determine the specific characteristics of the filter medium necessary to apply the Kozeny-Carman equation. Therefore, the use of this approach could minimize the number of model parameters to be calculated and calibrated.

4. RIS-based filtration models

A critical analysis on "classical" RIS-based filtration models used in both MBR and AnMBR applications has been performed based on a collection of models selected from the literature [\(Table](#page-9-0) 5). From all available models, the selection was made to representatively cover different modeling approaches entailing diverse fouling classification (foulant, mechanism, and consolidation types), dynamic processes, and state variables. Other aspects were also considered within the selection process, such as which models were the most frequently cited or applied in other studies, what new features they presented, or the complexity they involved. Specifically, 21 "classical" models are in-detail analyzed in this work: 1 model developed using a microfiltration (MF) membrane treating synthetic media (microspheres and BSA), 4 models developed/ proposed for AnMBRs, and 16 models developed/proposed for conventional MBRs. Although the MF model (Choi et al., [2000\)](#page-19-0) was not developed in an MBR system, it is evaluated in this work since it represents the basis of several MBR models developed by other authors.

Choi et al. [\(2000\)](#page-19-0) proposed a RIS model based on the cake layer filtration theory. The model considers the resistance offered by the membrane, by the cake layer, and by the internal fouling of the pores, since there are small materials that can penetrate the membrane and be adsorbed by the pores. Lee et al. [\(2002\)](#page-20-0) did not consider the effect of particle adsorption in the pores. On the other hand, their model defined the resistance offered by the cake layer differently from the previous model because it introduced the effect of crossflow filtration. [Wintgens](#page-21-0) et al. [\(2003\)](#page-21-0) characterized the TMP by considering hydrostatic pressure,

suction pressure, and axial pressure loss. They defined an expression equivalent to the one proposed by Choi et al. [\(2000\)](#page-19-0) considering the fouling resistance. However, [Wintgens](#page-21-0) et al. (2003) modelled the cake layer resistance as a function of the mixed liquor concentration on the membrane surface.

[Broeckmann](#page-19-0) et al. (2006) considered two new phenomena affecting cake and pore resistance: i) the distribution of particles and membrane pore diameters, and ii) the adhesion between particles and membrane surface. Hence, this can be regarded as the first model that considers the effect of pore and particle size distribution on pore blockage resistance modeling. This model also considered membrane resistance, cake layer resistance, and irreversible fouling resistance. The irreversible fouling resistance was defined using the expression proposed by [Wintgens](#page-21-0) et al. [\(2003\),](#page-21-0) while for the formation of the cake layer, a forces balance was assumed together with both a mass balance and the Blake-Kozeny equation. The model also considers the effect of backwashing on cake layer removal. Li and Wang [\(2006\)](#page-20-0) proposed a sectional approach to the membrane surface since the turbulence force of aeration is not uniformly distributed, thus resulting in the heterogeneity of the cake and its consequent irregular flux. They also used, for the first time, a term to define the probability of a particle being deposited on the membrane surface. This model involves the intrinsic resistance of the membrane, the pore blocking, and the resistance offered by the cake layer. In addition, within the cake layer formation, the model differentiates between the dynamic sludge layer, which is the layer of sludge that temporarily adheres to the membrane during the filtration phase, and the stable cake layer, which is the one that remains after the cleaning period.

Giraldo and [LeChevallier](#page-19-0) (2006) introduced the concept of subcritical and supercritical fouling into their model. This model can be regarded as one of the first models where the role of SMPs in internal fouling is discussed, although it is not explicitly considered in the model equations. The authors proposed a mass balance for the formation of the cake layer and considered the compressibility of the cake layer in the specific resistance.

Busch et al. [\(2007\)](#page-19-0) included three sub-models describing the geometry and hydrodynamics inside and outside the membrane fibers, which implies a higher degree of complexity in the modeling task. As per [Wintgens](#page-21-0) et al. (2003), the TMP was described in terms of two components: the pressure inside and outside the fibers. Concerning resistances, besides pore blockage and cake layer, which were proposed as in [Broeckmann](#page-19-0) et al. (2006), three new parameters appear in the model: the resistance due to biological fouling or biofouling, the resistance due to concentration polarization, and the resistance due to scaling. Nonetheless, the last two resistances were disregarded and finally not considered in the model. [Broeckmann](#page-19-0) et al. (2006) and [Busch](#page-19-0) et al. [\(2007\)](#page-19-0) represent a clear example of the complexity of working with models based on physical laws aiming to study fouling in a greater detail. In both cases, the description of the geometry and the study of the particle distribution results in a significant increase of model complexity.

[Zarragoitia-Gonz](#page-21-0)ález et al. (2008) proposed modifications to the model of Li and Wang [\(2006\).](#page-20-0) The former highlighted that the specific resistances of the dynamic and stable sludge cake layers should not be considered constant, and they are assumed to be equal. For its calculation, the model considers the concentration of both SMP and total suspended solids (TSS). Khan et al. [\(2009\)](#page-20-0) mainly focused on modeling the specific resistance of the cake, proposing a relationship between specific resistance and shear intensity. [Ludwig](#page-20-0) et al. (2012), as per [Wintgens](#page-21-0) et al. [\(2003\),](#page-21-0) defined the TMP from the suction pressure. Unlike previous models, [Ludwig](#page-20-0) et al. (2012) did not calculate the cake layer resistance from the specific resistance but applied an integral-type equation with calibration-adjusted parameters. This model considered the same resistances as Choi et al. [\(2000\),](#page-19-0) defining the fouling resistances in the same way as [Wintgens](#page-21-0) et al. (2003).

[Mannina](#page-20-0) et al. (2011) proposed a model based on Li and [Wang](#page-20-0)

 (2006) and Zarragoitia-González et al. (2008) . Therefore, this model has unified parameters for the forces balance, the probability of particle deposition on the membrane surface, and the specific mass of both stable cake and dynamic sludge. By considering the cake layer to act as a filter at depth, the model includes an equation for calculating the mass concentration on the membrane surface. The model of Wu et al. [\(2012\)](#page-21-0) was also based on the one proposed by Li and Wang [\(2006\)](#page-20-0) but accounts for the role of soluble and colloidal components. This model considered several layers of filter cake acting as filters stacked in the thickness direction. It described pore fouling by soluble material and colloidal compounds in the membrane and in these layers.

The model of [Sarioglu](#page-20-0) et al. (2012) was characterized by considering the cake layer as homogeneous, thus calculating the resistance offered by the cake layer from a state variable referring to the dry mass of the cake. A dynamic mass balance was proposed for this state variable, which considered the following processes: formation of cake layer during filtration, detachment of cake layer by backwashing, and removal of solids by crossflow aeration. The resistance offered by the cake layer was given without reference to the concept of specific resistance and the fouling resistance was given as in Choi et al. [\(2000\).](#page-19-0) [Robles](#page-20-0) et al. [\(2013b\)](#page-20-0) modelled the dynamic variation of both reversible and irreversible fouling dry mass by two mass balances, including two specific resistances for calculating the resistance to filtration of reversible and irreversible fouling, being the specific cake layer resistance affected by cake compression. The following processes were considered: cake layer formation during filtration, membrane cleaning by biogas bubbling, cake layer removal by backwashing, and consolidation of irreversible fouling. As per [Sarioglu](#page-20-0) et al. (2012), this model considered the cake layer to be homogeneous. Importantly, the model considered the influence of subcritical fouling on the specific strength offered by the cake layer. In addition, an inhibition function for the modeling of the biogas bubbling cleaning process was proposed to consider the impact of working at supercritical and subcritical conditions.

Charfi et al. [\(2014\)](#page-19-0) considered fouling to be caused by the accumulation of particles on the surface of the membrane. The authors considered the resistance offered by the membrane and by cake layer formation. In this model, the calculation of a specific cake layer resistance was not detailed. The cake mass balance proposed by the authors can be considered a simplification from Li and Wang [\(2006\)](#page-20-0). Later, Charfi et al. [\(2015\)](#page-19-0) included SMP for modeling cake layer formation and pore blocking. SMPs were considered to be retained within the formed cake, leading to an increase in the specific cake layer resistance and to an accumulation on the membrane surface, so that the pores are blocked, and a thin layer is formed. Pore blocking resistance was not considered as it was argued to be negligible compared to the resistance of the cake layer, but the influence of the thin layer on the resistance was proposed. The mass balance to the specific dry mass of cake (kg per $m²$ of membrane area) was modified from Charfi et al. [\(2014\)](#page-19-0) to include the soluble part and the thin layer.

Zuthi et al. [\(2017\)](#page-21-0) considered the mechanisms of pore blocking due to adsorption of soluble compounds and cake layer formation. Unlike previous models, pore blocking resistance was related to the reduction of pore radius and effective membrane porosity. Based on the approach proposed by Giraldo and [LeChevallier](#page-19-0) (2006), a mass balance was proposed for the particles around the membrane that cause a porosity decrease. This model also included a differential expression to consider the effect of the decrease in pore size due to the adsorption of soluble components. As per Robles et al. [\(2013b\)](#page-20-0), the cake was considered compressible, but the model also proposes a dynamic process for modeling the thickness of the cake layer.

Charfi et al. [\(2017b\)](#page-19-0) modelled cake layer formation introducing soluble components in an AnMBR. In contrast to other models (e.g., Zuthi et al., [2017\)](#page-21-0), despite including soluble components, the authors did not model their relationship with pore blocking resistance. [Charfi](#page-19-0) et al. [\(2017a\)](#page-19-0) described fouling analysis based on media fluidization using granular activated carbon particles. The aim of this approach was

to quantify the effect of fluidized media on the decrease in filtration resistance, thus modeling the effect of cake layer formation on pore blocking. Charfi et al. [\(2018a\)](#page-19-0) introduced the novelty of assessing the effect of fluidized media on the mitigation of different fouling mechanisms, besides the cake layer formation presented in [Charfi](#page-19-0) et al. [\(2017a\).](#page-19-0) The model considered the effect on the removal of gel layers produced by soluble compounds. Moreover, they considered the effective membrane filtration area to be dynamic due to i) the blockage caused by the deposition of SMP and ii) the released/recovery due to gas bubbling. The model also assessed fouling propensity from the increase in TMP due to pore blocking and cake layer formation. Similarly, [Charfi](#page-19-0) et al. [\(2018b\)](#page-19-0) modelled the effect of polyethylene terephthalate (PET) beads fluidization on fouling mitigation, considering cake layer formation and pore blocking as main mechanisms. There are similarities between this model and Charfi et al. [\(2018a\)](#page-19-0) regarding the variation of membrane area. Specific mass balances were proposed for solids and SMP concentration.

Considering the set of models evaluated, it is possible to conclude that filtration process modeling is characterized by significant heterogeneity within the available models. Moreover, cross comparison among different models is a complex task due to a lack of standardized nomenclature and fouling classifications, among others. Hence, it is necessary that the filtration process modeling community advance towards the development of a unified framework aimed to standardize not only filtration process modeling notation (kinetics, state variables, etc.), but also fouling classification (foulant, mechanism, and consolidation types).

4.1. Model variables

[Table](#page-12-0) 6 shows a selection of model inputs and outputs considered in the models evaluated in this work, including model parameters, state variables and derived calculated variables. These have been grouped here into compounds (colloidal, soluble and suspended), TMP, filtration area, thickness, mass (dry and specific) and resistance (absolute and specific) variables. Nevertheless, it is important to emphasize that other variables and parameters are also considered within the different models by different authors, which must be considered for a proper modeling of filtration in the MBR field, such as bulk characteristics (e.g., sludge viscosity or EPS, both of which affect the stickiness of the sludge and the cake layer formation rate). In addition, special attention must be also paid to the importance of design and operation conditions, as shown in [Fig.](#page-2-0) 1.

As [Table](#page-12-0) 6 illustrates, model's structure ranges from simple ones with few variables to more complex with many, being TMP and resistances the most general and common variables used within RIS-based modelling, defined as both state variables or calculated variables from other states. Increasing the number of parameters and variables in a model enhances its intrinsic complexity but also its ability to predict simultaneous or complex phenomena occurring in the system. The selection of one model among other may be based on the target of each specific modelling exercise, e.g., selecting a detailed mathematical model to be used for academic research, or a simplified one that can be embedded in system/plant-wide models allowing environmental and economic sustainability assessment and control and multi-criteria optimization of MBR systems.

4.2. RIS classification

Given the importance of resistance as state variable, [Table](#page-14-0) 7 compiles the filtration resistances included in each RIS model evaluated in this work, according to the definitions and considerations of each author. As this table shows, all models contemplate the intrinsic membrane resistance (*Rm*) as expected. Cake layer resistance (*Rc*) was involved in most of the evaluated models, followed by pore blocking (*Rp*) and irreversible fouling resistance (*Rirr*), but in a lesser extent.

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Selection of model inputs and outputs considered in the evaluated models.

The first noteworthy aspect observed in [Table](#page-14-0) 7 is the diversity when modeling the resistance offered by the cake layer. While most authors propose a single resistance, other authors (e.g., Li and [Wang,](#page-20-0) 2006 ; [Mannina](#page-20-0) et al., 2011; Zarragoitia-González et al., 2008) define two resistances to differentiate between the dynamic cake layer (*Rdc*) that forms during each filtration phase and the stable cake layer (*Rsc*) that remains after the detachment processes. However, [Mannina](#page-20-0) et al. (2011) stated that the sum of both resistances is considered equivalent to *Rc* , which is included in other models. On the other hand, [Charfi](#page-19-0) et al. [\(2015\)](#page-19-0) defined the resistance offered by a first thin cake layer (*Rs*) although an equivalence with the dynamic sludge layer resistance defined by Li and Wang [\(2006\)](#page-20-0) is observed when evaluating the definition and dynamics of this thin cake layer. Busch et al. [\(2007\)](#page-19-0) also defined polarization concentration and scaling resistances, although the related model processes were not finally considered since their impact on total filtration resistance were assumed negligible.

[Table](#page-15-0) 8 shows the resistances defined in each model along with the associated fouling types (fouling consolidation, mechanism type and foulant type), as it has been deduced from each proposed modeling approach. It is important to highlight that the association between foulant types and resistances has been conducted here with the aim of enhancing the comprehensibility and implementation of RIS-type modeling in general, and each evaluated model in particular. Since this association is not explicitly stated in all the works examined, it has been deduced by carefully analyzing the description of each studied model.

For example, Choi et al. [\(2000\)](#page-19-0) defined *Rc* involving: 1) reversible fouling caused by cake layer formation and derived from particulate foulants, 2) polarization concentration, and 3) organic adsorption. These authors considered *Rirr* to be caused by pore blockage, but not defining associated foulants to it. On the other hand, [Sarioglu](#page-20-0) et al. [\(2012\)](#page-20-0) associated *Rc* with the reversible fouling caused by the cake layer formation and derived from particulate foulants, while considering *Rirr* as per Choi et al. [\(2000\)](#page-19-0) . Thus, this table also demonstrates the different features that each author can consider when describing similar resistances, emphasizing heterogeneity within filtration process modeling.

4.3. Dynamic processes involved in fouling layer generation and removal

The link between the resistances and the dynamic processes of fouling generation and removal considered by each author has also been analyzed. These processes have been classified into cake/gel layer formation (cake/gel layer attachment, cake/gel layer detachment by scouring, cake/gel layer detachment by backwashing, and cake compressibility) and irreversible fouling consolidation. In general, cake layer, biofilm, stable cake layer, dynamic sludge layer, concentration polarization, and first thin cake layer resistances have been classified as cake/gel layer formation processes, whereas irreversible and pore blocking resistances have been classified as irreversible fouling consolidation processes. The corresponding classification for each evaluated work is shown in [Table](#page-16-0) 9 . When modeling cake/gel layer attachment, different state variables are defined within the set of evaluated models (see, e.g., Choi et al., [2000](#page-19-0) ; Li and [Wang,](#page-20-0) 2006 ; [Sarioglu](#page-20-0) et al., 2012), such as cake thickness, cake dry mass, or specific cake dry mass. Some models combine cake attachment and detachment processes by incorporating a parameter representing the membrane scouring effect (e.g., Khan et al., [2009](#page-20-0) ; [Wintgens](#page-21-0) et al., 2003). On the other hand, other models consider independent model processes to represent cake detachment: air/biogas scouring (e.g., [Robles](#page-20-0) et al., 2013b), crossflow operation (e.g., Lee et al., [2002](#page-20-0)), or backwashing (e.g., [Broeckmann](#page-19-0) et al., [2006\)](#page-19-0). When modeling irreversible fouling consolidation, many authors use the expression proposed by [Wintgens](#page-21-0) et al. (2003) . However, it can be observed that other authors defined a specific mass balance for irreversible fouling (e.g., dry mass of irreversible fouling) or even modelled the dynamics on the blocked filtration area due to pore blocking mechanism. Finally, the compressibility of the cake is usually

Resistances included in the evaluated models (*Defined but not modelled).

modelled by including a specific parameter or by modeling the effect of TMP on the specific resistance of the cake layer.

[Table](#page-16-0) 9 illustrates a strong heterogeneity within available RIS-based filtration models applied to MBR technology. This heterogeneity arises from both differences in underlying processes and similar processes due to variation in fouling phenomena considered. Additionally, distinct state variables and their corresponding dynamics are employed across these models. These disparities contribute to the complexity of understanding and applying filtration models in practice. To address this complexity, it is crucial to establish a common basic framework for membrane fouling classification that would help to conduct good modeling practices, which would facilitate modeling practices and enhance the ability to compare and evaluate different models. Researchers can collectively advance in the field and promote better modeling practices by adhering to a standardized membrane fouling classification. Indeed, a unified and widely followed membrane classification framework, jointly with a standardizing RIS-based filtration modeling methodology, will facilitate future modeling exercises within the field. Moreover, this will also make it possible to unify the additional measurements or tools to be carried out: deposit thickness, accumulated mass, chemical composition, transient TPM/J monitoring, cake compressibility, among others. Finally, the analysis conducted in this study provides a deeper understanding of the perspectives offered within the available filtration models, aiming to facilitate the comparison, implementation, and adaptation of existing models.

5. Basic guidelines towards good modeling practices

After conducting a comprehensive literature review, it is possible to

discern the fundamental aspects of membrane fouling. This involves considering classifications, dynamics, and underlying processes to develop a mathematical model approach for effective fouling modeling. [Fig.](#page-18-0) 6 illustrates the key foulants, dynamic processes and filtration resistances to be considered when modelling a filtration process within the MBR field, while [Fig.](#page-18-0) 7 summarizes the critical elements that must be identified and categorized before conducting a membrane fouling modeling exercise.

Primarily, it is essential to properly identify/categorize fouling phenomena within the three categories before stablished, i.e., foulant type, mechanism type, and consolidation type, considering the existing relationships among each other. These relationships illustrate that the identification and classification of fouling could be more straightforward when referring to a unified definition of categories and specific associated characteristics. This categorization represents a fundamental step for adequately selecting the processes and state variables to be considered in the model structure.

Secondly, for each filtration resistance associated to each fouling category identified, the main processes and state variables involved in the formation and removal of fouling can be selected. Specifically, aiming to meet a compromise between model complexity and accuracy, 5 model processes are proposed in this work for modelling membrane filtration within the MBR field. The first three phenomena, relating to the construction and control of the deposit, are classic, while the last two reflect the rapid evolution of the TMP (TMP jump):

- Cake layer attachment
- Cake layer detachment by scouring
- Cake layer detachment by backwashing

Relationship between the resistances defined by each author and fouling types with the abbreviations introduced in [Table](#page-14-0) 7.

- Cake layer compressibility and slackening

- Irreversible fouling consolidation

Based on these processes, the following partial resistances are proposed to be considered as state variables of the model:

- Intrinsic membrane (*Rm*)
- Cake layer (R_c) , which could be divided into dynamic cake layer (R_{dc}) and stable cake layer (R_{sc}) when differences on fouling removal by scouring and backwashing may be estimated, related to reversible and residual fouling, respectively
- Irreversible fouling (*Rirr*) or pore blocking (*Rp*)

Simplification of model structure may be considered depending on system configuration, operation mode, available data, modeling target, and/or prediction time horizon. In addition, it should be noted that a systematic analysis of the dominant phenomena is recommended as a preliminary step to the development of a new MBR models.

6. Future perspectives

The literature review described and discussed in the previous sections reveals a strong heterogeneity in the modeling of MBR fouling. Although this work focuses on RIS models, it is important to consider the accelerated growth in the use of machine learning and other artificial intelligence techniques. As mentioned in previous sections, many models based on artificial neural network or another machine learning techniques have been presented and studied in recent years. Indeed, this preliminary work on data-driven models will facilitate the development of hybrid MBR models that integrate machine learning techniques with semi-empirical models such as RIS-based models. This study, therefore, provides the fundamental aspects that will advance the integration of MBR models.

Nevertheless, within the RIS-based modeling approach discussed in this paper, which is the most prevalent in the modeling of MBR filtration, there are still issues that require further attention. One such issue is the need to differentiate between the mechanisms of cake layer and gel layer formation, despite their distinguishable natures. It is crucial that future mathematical models acknowledge the distinction between these mechanisms to accurately assess the accumulation of SMP in gel layer formation. Additionally, due to the lack of uniformity in MBR modeling, creating a widely accepted standardized framework for notation (e.g., Corominas et al., 2010; Brepols et al., 2020) is required. This framework will represent a useful tool when communicating future modelling results or when developing new models, thereby advancing the understanding and optimization of membrane-based filtration systems in the wastewater treatment field.

The need for experimental data from full-scale (or demo-scale) plants is also critical to validating MBR models. Although laboratory and pilotscale studies provide important insights, they could be not enough to represent the complexity and variability found in real-world conditions. Full-scale operational data allows for a more accurate assessment of MBR system performance and reliability. Therefore, data collection is also essential to improve model validation.

Integrated models, which combine biological and physical models, are also receiving much attention for describing MBR performance. This modeling approach leads to achieve a better comprehensive prediction of the systems' behavior in view of a global optimization. In this respect,

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Water

(*continued on next page*)

Table 9 (*continued*)

Fig. 6. Schematic representation of the critical elements to be considered for membrane filtration modelling in MBR systems.

further progress in integrated MBR modeling is needed to address the many outstanding issues in field modeling.

The findings of this study might contribute to the development of more effective modelling techniques for minimizing MBR fouling. The literature review allows for an examination of methodologies that minimize fouling, including an analysis of physical and chemical cleaning strategies. Consequently, if more accurate modelling of these methodologies can be achieved, it would be possible to study their effects on fouling development. This will result in the identification of the optimal strategy for reducing fouling.

Fig. 7. Framework proposal for membrane fouling classification.

Finally, since there are advantages and disadvantages intrinsically associated to each modelling approach (e.g., semi-empirical and datadriven models, integrated models, etc.), it is important to point out that depending on the objective of the modelling exercise, it is necessary to find a balance between complexity, simplicity and accuracy of the model.

7. Conclusions

This work critically reviews the state-of-the-art of RIS-based filtration models applied to MBR technology, revealing a strong heterogeneity among available models. Filtration models' heterogeneity is depicted by the diverse nomenclature or state variables and fouling formation and removal processes considered, which is directly affected by the dissimilar and interrelated criteria used to classify membrane fouling.

An identification of the filtration resistances and model processes associated with each fouling classification is conducted, which will help to quickly and easily understand and analyze available filtration models. To this aim, the basis for stablishing a unified framework rooted in the fundamentals of membrane fouling classification is defined in this work, encompassing a set of general model processes and state variables to be applied for filtration process modelling within the MBR field, which is directly linked with each fouling category (fouling consolidation, foulant types, and fouling mechanisms) but also, and above all, linked to the design of the scouring system.

CRediT authorship contribution statement

V. Sandoval-García: Writing – original draft, Visualization, Methodology, Investigation, Conceptualization. **M.V. Ruano:** Writing – review & editing, Validation, Supervision, Methodology, Formal analysis, Conceptualization. **M. Alliet:** Writing – review & editing, Visualization, Validation, Formal analysis, Conceptualization. **C. Brepols:** Writing – review & editing, Validation, Supervision, Formal analysis, Conceptualization. **J. Comas:** Writing – review & editing, Visualization, Validation, Formal analysis, Conceptualization. **J. Harmand:** Writing – review & editing, Visualization, Validation, Formal analysis, Conceptualization. **M. Heran:** Writing – review & editing, Visualization, Validation, Formal analysis, Conceptualization. **G. Mannina:** Writing – review & editing, Validation, Supervision, Formal analysis, Conceptualization. **I. Rodriguez-Roda:** Writing – review & editing, Visualization, Validation, Formal analysis, Conceptualization. **I. Smets:** Writing – review & editing, Visualization, Validation, Formal analysis, Conceptualization. **A. Robles:** Writing – review & editing, Validation, Supervision, Methodology, Funding acquisition, Formal analysis, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Data availability

No data was used for the research described in the article.

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