

1 **Biological processes modelling for MBR systems: A review of the state-of-the-art**  
2 **focusing on SMP and EPS**

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25

26 **Abstract**

27 A mathematical correlation between biomass kinetic and membrane fouling can improve the  
28 understanding and spread of Membrane Bioreactor (MBR) technology, especially in solving  
29 the membrane fouling issues. On this behalf, this paper, produced by the International Water  
30 Association (IWA) Task Group on Membrane modelling and control, reviews the current state-  
31 of-the-art regarding the modelling of kinetic processes of biomass, focusing on modelling  
32 production and utilization of soluble microbial products (SMP) and extracellular polymeric  
33 substances (EPS). The key findings of this work show that the new conceptual approaches  
34 focus on the role of different bacterial groups in the formation and degradation of SMP/EPS.  
35 Even though several studies have been published regarding SMP modelling, there still needs  
36 to be more information due to the highly complicated SMP nature to facilitate the accurate  
37 modelling of membrane fouling. The EPS group has seldom been addressed in the literature,  
38 probably due to the knowledge deficiency concerning the triggers for production and  
39 degradation pathways in MBR systems, which require further efforts. Finally, the successful  
40 model applications showed that proper estimation of SMP and EPS by modelling approaches  
41 could optimise membrane fouling, which can influence the MBR energy consumption,  
42 operating costs, and greenhouse gas emissions.

43

44 **Keywords:** Biomass kinetic models, extracellular polymeric substances, membrane  
45 bioreactors, soluble microbial products.

46

## 47 **1. Introduction**

48 Membrane bioreactors (MBR) are widely known as reliable elements of water resource  
49 recovery facilities (WRRFs) in terms of effluent quality, compliance with strict regulation  
50 limits, low sludge production, well-arranged operation, and low spatial requirements (Zuthi et  
51 al., 2017; Zheng et al., 2018). Several studies were performed in the past years to ensure that  
52 MBR could become more mature and widespread (Bozkurt et al., 2016; Krzeminski et al.,  
53 2017). Indeed, their full-scale applications have been registered very often (Attiogbe, 2013;  
54 Xiao et al., 2014, Meng et al., 2017). However, managers and researchers still present  
55 membrane fouling issues, module blocking, high energy consumption, and, by a consequence,  
56 high operating costs as significant obstacles to an ever more spread application of this  
57 technology (Tang et al., 2022). Although practical examples show that significant reduction in  
58 energy consumption and a long membrane lifetime are possible (Tao et al., 2019; Brepols et  
59 al., 2020), still, finding solutions to the obstacles above demands comprehensive studies.

60

61 Studies focusing on experimental data can be complemented by others using mathematical  
62 modelling to obtain predictive possibilities with less time-consuming routines and lower cost  
63 of implementation (Sun et al., 2016; Charfi et al., 2017; Mannina et al., 2018). In the past years,  
64 several works have been developed in view of demonstrating how mathematical modelling  
65 could be applied to MBR systems (Naessens et al., 2012, Nadeem et al., 2022) and their  
66 utilisation has been contributing to updating the knowledge of the technology (Krzeminski et  
67 al., 2017; Robles et al, 2018). In particular, the activated sludge model (ASM) family (Henze  
68 et al., 2000), formerly developed for conventional activated sludge (CAS) systems, has been  
69 expanded to consider the specific biomass kinetics related to MBR bioprocesses. These models  
70 are known as biomass kinetic or hybrid models (Mannina et al. 2021).

71 The biomass kinetic models are modified versions of ASMs with the ability to account for the  
72 formation and degradation processes of soluble microbial products (SMP) and extracellular  
73 polymeric substances (EPS), either as stand-alone models or as part of the ASMs (Zuthi et al.,  
74 2012). The need for hybrid models is due to the particular characteristics of MBR systems, e.g.,  
75 higher concentration of mixed liquor suspended solids (MLSS) in the reactor and/or higher  
76 solids retention time (SRT), which contribute to the formation of microbial products in the  
77 MBR (Lu et al., 2001). These microbial products are known to cause membrane fouling, which  
78 has been one of the main constraints of MBR technology (Liu et al., 2018; Lin et al., 2014;  
79 Wang et al., 2022). The permeability of the membrane decreases due to fouling and leads to an  
80 increase in energy consumption caused by filtration and aeration (Juang et al., 2013). Mannina  
81 et al. (2017) showed the interlinkages between fouling, operational costs, and greenhouse gas  
82 emissions (GHG) from MBR systems. Fouling also increases chemical cleaning frequency  
83 (Wang et al., 2020). Therefore, minimising fouling would decrease energy and chemical  
84 consumption and eventually environmental footprint of the MBR system (Ioannou-Ttofa et al.,  
85 2016). Thus, considering the formation/degradation of SMP and EPS is a reasonable approach  
86 while assessing the biomass and bulk properties that influence the MBRs filtration performance  
87 (Lu et al., 2001). Indeed, these hybrid models are particularly important in developing an  
88 integrated MBR model (i.e., a combination of hybrid and physical models) to fully understand  
89 MBR behaviour from a modelling standpoint.

90

91 Several studies in the past (Lu et al., 2001; Zarragoitia-González et al., 2008; Janus and  
92 Ulanicki, 2010; Mannina et al., 2011-2021; Zuthi et al., 2012) have examined the bioprocesses  
93 related to MBR modelling, mainly focusing on the correlation between biomass kinetics and  
94 membrane fouling. This review aims to facilitate a re-evaluation of findings from past studies  
95 by providing a current state-of-the-art in biomass kinetic process modelling, with special

96 attention to the novel approaches to modelling SMP and EPS formation and degradation  
97 processes. Therefore, this work presents an overview of the concepts of SMP and EPS  
98 formation/degradation processes, followed by an overview of the biomass kinetic models.  
99 Then, the past and present applications of hybrid models to MBR are presented with a focus  
100 on updates related to bioprocesses. Finally, the main outlooks and conclusions retrieved from  
101 the review are presented.

102

## 103 **2. General characterisation and mechanisms of SMP/EPS formation and utilization in** 104 **MBR**

105 The SMP concept was first introduced by Luedeking and Piret (1959) by studying glucose  
106 metabolism. Two new components were introduced, including UAP for utilisation associated  
107 products (growth-associated products) and BAP for biomass associated products (by-products  
108 of cell lysis). The following equation was used to translate the dynamic approach where  $X_B$   
109 stands for active biomass.

$$\frac{dS_{SMP}}{dt} = \underbrace{\alpha \frac{dX_B}{dt}}_{S_{UAP}} + \underbrace{\beta X_B}_{S_{BAP}} \quad \text{Equation 1}$$

110

111 The existence of organic compounds generated by microbial cultures involved in wastewater  
112 treatment has been recognized in the 1960s (Barker and Stuckey, 1999). Nowadays, SMP and  
113 EPS are substances that cause fouling (Meng et al., 2017).

114

115 Prior to the presentation of SMP/EPS main concepts, some aspects must be introduced to  
116 ensure the full understanding of their formation and degradation processes. First, the organic  
117 substrates with high molecular weights (MW) are used by microorganisms for growth and  
118 become available due to a series of enzymatic reactions, collectively named hydrolysis. The

119 hydrolysis allows slowly particulate biodegradable compounds ( $X_S$ ) (with high molecular  
120 weight) to be converted into readily biodegradable substrates ( $S_S$ ). The hydrolysis reactions  
121 related to the formation/degradation processes of SMPs, may occur in aerobic, anaerobic, and  
122 anoxic conditions. In the biomass growth process, the readily biodegradable substrate is  
123 directly used for growth or stored for internal processes. On the other hand, biomass decay/lysis  
124 and floc dissolution/degradation processes occur during the treatment processes. Most of the  
125 processes above, that may release SMP/EPS as by-products, are described by kinetic rate  
126 expressions and are detailed in modelling approaches that can account for such compounds.

127

128 It is generally believed that SMP are primarily formed during substrate utilisation, biomass  
129 decay, and hydrolysis of EPS (Fenu et al., 2010). They are released during cell lysis, lost during  
130 synthesis, excreted for some purpose, or diffuse through the cell membrane (Laspidou and  
131 Rittmann, 2002a; Le-Clech et al., 2006). In other words, SMP could be defined as the pool of  
132 organic compounds that are released into the solution due to microbial metabolism during  
133 growth and decay of biomass (Barker and Stuckey, 1999). It is now widely accepted that the  
134 SMPs could be divided into two groups, as originally proposed by Namkung and Rittmann  
135 (1986), UAPs and BAPs. The differences between both groups rely upon their production  
136 mechanisms, i.e., the bacterial phase from which they are derived (Lu et al., 2001). The UAPs  
137 are produced during substrate metabolism and biomass growth, with a production rate  
138 proportional to substrate utilization (Namkung and Rittmann, 1986; Barker and Stuckey, 1999).  
139 On the other hand, BAP can be defined as a by-product of endogenous respiration of cell mass  
140 and its production is independent of the cell growth rate (Zuthi et al., 2012). Indeed, their  
141 production mechanisms include either decay of the active biomass, hydrolysis of bound EPS,  
142 turnover of intracellular components, or a combination of those processes (Zuthi et al., 2013a;  
143 Liu et al., 2018).

144

145 MW of microbial products is important since it affects the specific filtration resistance which  
146 is an index to represent the fouling propensity of a foulant (Teng et al., 2020). It is important  
147 to note that the chemical structure of microbial products is as essential as their MW. According  
148 to Meng et al. (2011), the primary component of the high-MW compounds (>100 kDa) found  
149 in both the sludge supernatant and the biofilm of an MBR was predominantly polysaccharides.  
150 The high tendency of polysaccharides to cause fouling is not only due to their large size but  
151 also because of their significant gelling properties (Meng et al., 2017). The presence of humic  
152 substances and proteins adds complexity to fouling in MBRs. Hydrophobic humic substances  
153 adsorb to membranes, reducing pore size and altering their surface properties that facilitate the  
154 accumulation of hydrophilic biomolecules, predominantly polysaccharides (Kimura et al.,  
155 2015). Furthermore, proteins and polysaccharides form non-covalent interactions, creating a  
156 network that promotes fouling (Neemann et al., 2013). Zhou et al. (2012) determined that the  
157 biopolymers that are associated with the fouling present in the biofilm were primarily  
158 comprised of slowly biodegradable polysaccharides, which originated from SMP. Schiener et  
159 al. (1998) showed that MW of SMP showed bimodal distribution with 30% >1 kDa and 25%>  
160 100 kDa. The SMP with low MW is associated with UAP and high MW is with BAP (Urban  
161 et al., 1998; Medina et al., 2020). Ni et al. (2011) showed that the UAPs exhibit the  
162 characteristics of carbonaceous compounds with a low MW (<290 kDa) compared to the BAPs  
163 (>290 kDa) which consist mainly of macromolecules. Jiang et al. (2008) distinguished two  
164 types of UAPs (with lower and higher MW) and their classification depends on the utilisation  
165 of storage associated products. Regardless of different MW, chemical composition, and degree  
166 of biodegradability, it is now generally accepted that both UAPs and BAPs are biodegradable  
167 and recycled to become a substrate for microbial growth (Lapidou and Rittmann, 2002; Jiang  
168 et al., 2008; Menniti and Morgenroth, 2010; Zuthi et al., 2013a). Fenu et al. (2010) noted that

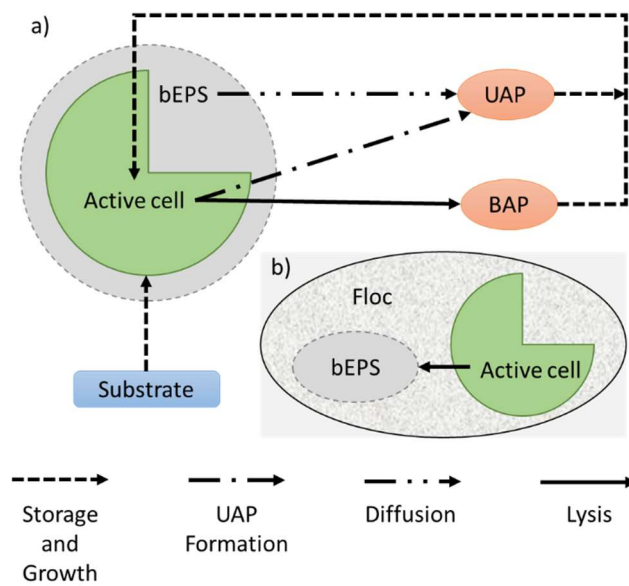
169 the UAP fraction could predominate when the substrate degradation rates were high, while the  
170 BAP fraction could typically dominate over the UAP fraction at higher SRTs or under steady-  
171 state conditions. Indeed, BAPs have been more assessed in the literature over the years due to  
172 the lack of consensus regarding their production and degradation mechanisms (Zuthi et al.,  
173 2012).

174  
175 EPS summarises numerous types of organic macromolecules, such as polysaccharides,  
176 proteins, nucleic acids, phospholipids, humic substances, and other polymeric compounds  
177 (Patsios and Karabelas, 2010; Gkotsis et al., 2014). They are usually bound at or outside the  
178 cell surface (regardless of the origin), surrounding cells and ensuring the stability and cohesion  
179 of the microbial aggregates, such as flocs, granules, and biofilms. The EPS provide a  
180 surrounding protection barrier, adhesion properties, and water retention around the bacteria  
181 (Laspidou and Rittmann, 2002a). The EPS can originate from several processes, e. g. active  
182 secretion, pouring of cell surface material, cell lysis, and adsorption from the mixed liquor  
183 suspended solids (MLSS) (Wingender et al., 1999). Polysaccharides in EPS have a higher  
184 fouling propensity compared to protein fractions when hydrophilic membranes are used,  
185 because the nature of proteins is hydrophobic and polysaccharides are hydrophilic (Li et al.,  
186 2012). Therefore, the protein-to-polysaccharide ratio in EPS is important for membrane  
187 fouling, particularly in cake layer formation in MBRs (Chang et al., 2002).

188  
189 The EPS can be divided into two fractions, including bound EPS (bEPS) and soluble EPS  
190 (sEPS). The bEPS are bound to the sludge flocs, whereas the sEPS can move freely between  
191 sludge flocs and the surrounding liquor. sEPS is often included as part of the SMP fraction,  
192 since it is difficult to distinguish from one another (Fenu et al., 2010; Judd, 2010). The major  
193 difference between SMP and EPS is that SMP is usually present as suspended in the



194 supernatant, while the EPS are bound to the floc (Drews, 2010; Zuthi et al., 2012). Moreover,  
 195 Ramesh et al. (2006) compared the physicochemical characteristics of SMP and sEPS from  
 196 different sludges. Their results did not support the hypothesis that SMP is identical to sEPS.  
 197 Modellers may assume that they are identical to simplify their models. Figure 1 presents a  
 198 schematic representation of the relation between SMP (UAP and BAP) and bEPS.  
 199



200  
 201 **Figure 1.** Schematic representation of the SMP and bEPS and their links, where a) represents  
 202 bEPS bound at the cell surface, while b) represents bEPS bound outside the cell surface.

203  
 204 SMP and bEPS are biological macromolecules with particular physical properties, such as a  
 205 three-dimensional structure, high porosity with an interconnected pore structure which provide  
 206 an appropriate surface structure for cell attachment, proliferation, and differentiation (Liu et  
 207 al., 2018). Recognising their existence and characteristics transformed the mathematical  
 208 modelling of MBRs since they play an important role in the initial and late fouling stages,  
 209 respectively (Meng et al., 2017). In particular, some studies had revealed that SMP exert a  
 210 significant influence before the jump of the transmembrane pressure (TMP) (Zhou et al., 2015;

211 Liu et al., 2019 b), while the bEPS originated from the deposited microbial cells contribute  
212 after the TMP jump (Luo et al., 2014; Zhou et al., 2015). These facts confirm that the inclusion  
213 of SMP and EPS (i.e., biomass biokinetics) in the assessment of MBR's bioprocesses is of  
214 utmost importance and leads to the development of biomass kinetic or hybrid models. Despite  
215 their importance in membrane fouling, it should be noted that the analytical determination of  
216 these compounds is challenging and often inaccurate. For example, Felz et al. (2019) showed  
217 that currently used colorimetric methods are not capable of accurately characterising EPS.

218

### 219 **3. Conceptual models of SMP/EPS formation and utilization**

220 The biomass kinetic or hybrid models can be defined as expanded versions of the ASMs, in  
221 which the formation and degradation of SMP and EPS are inserted (Zuthi et al., 2012). The  
222 need to expand the ASM for application in MBRs is based on two rationales: (i) the ASMs  
223 were originally designed to address issues related to CAS systems, considering their specific  
224 features (e.g., lower SRT and low organic load compared to MBR); (ii) they were based on the  
225 Monod equations, which predict that the effluent concentration of the rate-limiting substrate  
226 should be independent of the influent substrate concentration (Barker and Stuckey, 1999). In  
227 the latter case, studies have demonstrated that soluble materials in the effluent were  
228 proportional to those in the influent. Thus, there was a demand for a new model that could  
229 describe the bioprocess complexity and account for the biomass characteristics that can affect  
230 membrane filtration performance (Patsios and Karabelas, 2010). According to Zuthi et al.  
231 (2012), a basic model of biomass kinetics in MBR should at least provide estimations of EPS  
232 concentration in the activated sludge flocs and SMP concentrations outside the flocs, which is  
233 not addressed by the original ASMs.

234 Fenu et al. (2010) recommended the use of ASM extensions with the EPS/SMP concepts in  
235 three cases, specifically when (i) linking biology with membrane fouling, (ii) predicting soluble

236 COD, (iii) modelling systems with long SRTs. Additionally, this approach can be applied in  
237 modelling systems where heterotrophic activity is observed despite the absence of organic  
238 carbon in the influent. For example, Mehrani et al. (2022) modelled heterotrophic  
239 denitrification on SMP to describe the dominant abundance of heterotrophs in a system fed  
240 only with inorganic carbon and trace elements.

241

242 The first application of the original ASMs to model an MBR (Chaize and Huyard, 1991) was  
243 unsuccessful since the kinetics considered by the ASMs did not fully represent the reality of  
244 the MBR under assessment. The kinetics considered in an MBR model must be adapted to  
245 specific sludge characteristics that are influenced by different operating conditions (high SRT  
246 and MLSS concentration), which have a significant impact on the biomass metabolic pathways  
247 such as microbial product formation (Furumai and Rittmann, 1992). In this case, considering  
248 SMP and EPS formation avoids over-parametrization and overestimating biomass growth rates,  
249 which could lead to a severe error in predicting the effluent COD (Jiang et al., 2008).  
250 Neglecting SMP and EPS may thus lead to erroneous estimations of membrane fouling. On  
251 this behalf, several hybrid models have been developed and described in the literature over the  
252 years (Barker and Stuckey, 1999; Zuthi et al., 2012; 2013a). For this reason, a brief historical  
253 review of their conceptual approaches is presented in the following section, with a particular  
254 attention to the latest progress.

255

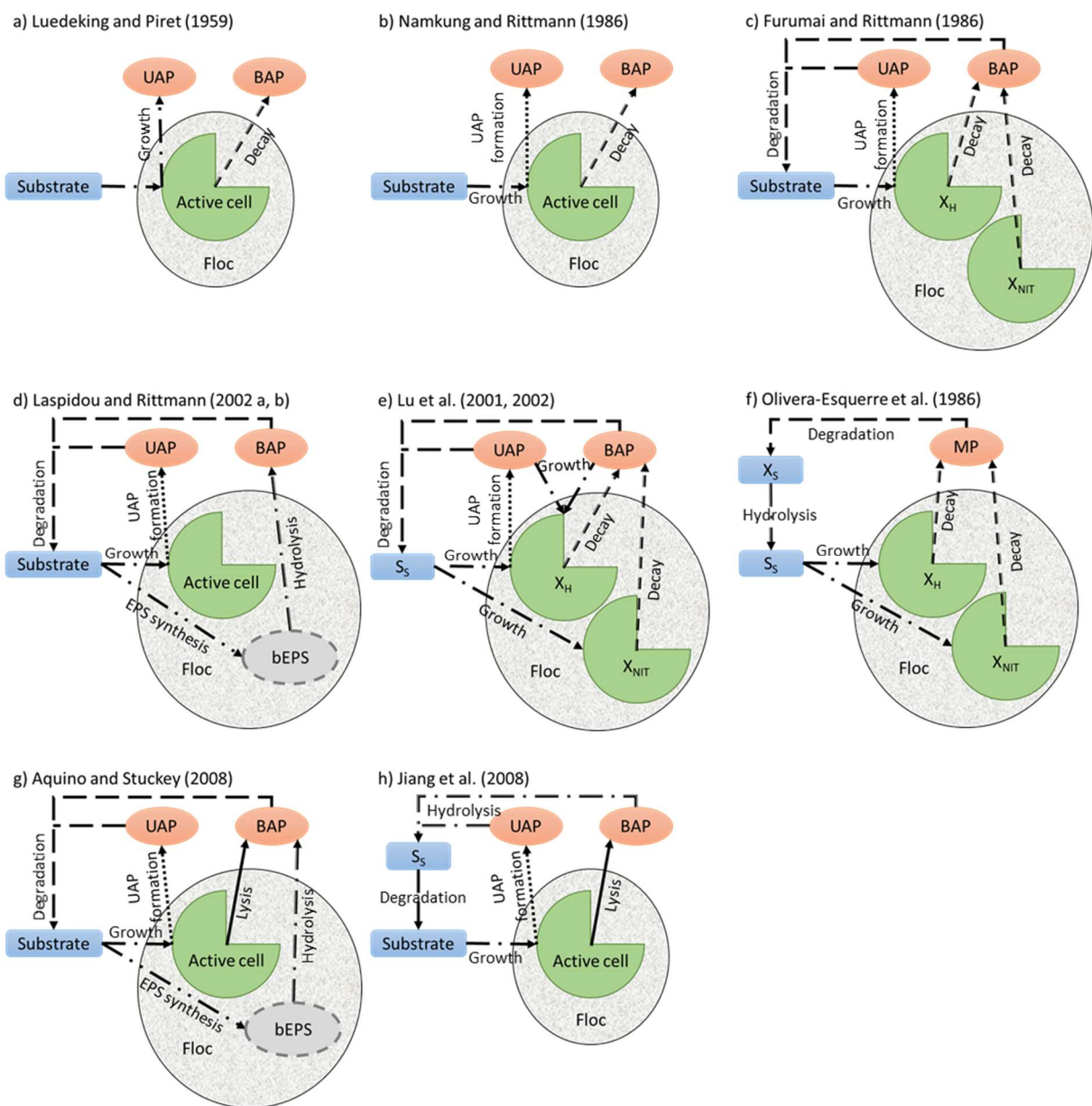
### 256 **3.1. Historical overview regarding SMP/EPS modelling**

257 Different concepts have been developed for the formation and degradation of SMP/EPS over  
258 the past few decades, summarized in Figure 2.

259 The first modelling attempt to estimate SMP was proposed by Luedeking and Piret (1959)  
260 (Figure 2a). The purpose was to define the relationship between lactic acid formation and

261 biomass growth in lactic acid fermentation. They observed that the lactic acid formation rate  
 262 correlates with the biomass growth rate and amount. Baskir and Hansford (1980), considering  
 263 the lactic acid in Luedeking and Piret's (1959) study is SMP, concluded that SMP are related  
 264 to (a) UAP that is proportional to the rate of biomass growth and (b) BAP that are not associated  
 265 with growth but proportional to the concentration of biomass (associated with cell autoxidation  
 266 or degradation).

267



268

269 **Figure 2.** Conceptual models of the formation and degradation of SMPs used in typical  
270 modelling studies - partially adapted and modified from Zuthi et al. (2013a). The acronyms are  
271 detailed in the text.

272

273 The modelling SMP accumulation gained attention, especially in determining the source of  
274 effluent organic matter (EfOM), and several models have been proposed by different  
275 researchers (Baskir and Hansford, 1980; Namkung and Rittmann, 1986; Furumai and  
276 Rittmann, 1992; de Silva and Rittmann, 2000). Baskir and Hansford (1980) incorporated the  
277 Luedeking and Piret (1959) model into suspended activated sludge and showed that by-  
278 products of biological activity contribute to organic effluent concentration. Namkung and  
279 Rittmann (1986) presented a model for SMP growth in biofilm reactors to describe the fraction  
280 of SMP in the soluble EfOM. In the Baskir and Hansford (1980) and Namkung and Rittmann  
281 (1986) models, the UAP formation is correlated with the substrate utilization rate and the UAP  
282 consists of the direct by-products of substrate utilisation and microbial growth (Figure 2b). On  
283 the other hand, the BAP formation is independent of microbial growth, and the formation rate  
284 is proportional to the concentration of active biomass. However, the formation rate of BAPs  
285 may be proportional to the biomass decay rate with a stoichiometric coefficient, since BAPs  
286 are considered decay products of the overall active biomass (Jiang et al., 2008). The model  
287 proposed by Namkung and Rittmann (1986) is still considered a reference for modelling SMP  
288 formation. Before that work, only SMP production was studied in activated sludge systems, as  
289 it was believed to be inevitable due to its production from biomass decay and low  
290 biodegradability (Gaudy and Blachly, 1985).

291

292 Furumai and Rittmann (1992) focused on the interaction between heterotrophs and nitrifiers in  
293 terms of the exchange of organic matter and modelled SMP produced by nitrifiers ( $X_{\text{NIT}}$ ) as an

294 energy and carbon source for heterotrophs ( $X_H$ ) (Figure 2c). The degradation of SMP was  
295 studied later by Noguera et al. (1994), who developed a model using experimental results from  
296 a glucose-fed anaerobic chemostat. The results of Noguera et al. (1994) has validated by  
297 Aquino and Stuckey (2008) showing that most of the SMP accumulation corresponded to BAP  
298 and presented that BAP have slower degradation rates compared to UAP, suggesting that the  
299 decrease in acidogenic biomass was due to SMP formation rather than oxidation to carbon  
300 dioxide. It is important to note that quantitative formation of SMP may differ between  
301 anaerobic and aerobic systems and distinguishing SMP from fermentation products (volatile  
302 fatty acids (VFAs) is crucial (Mesquita et al., 2010). However, Ni et al. (2011) indicated that  
303 SMP/EPS modelling theories developed for aerobic systems are valid for anaerobic systems.  
304 Noguera et al. (1994) also proposed Monod constants for the storage of BAP and UAP from  
305 the growth kinetics of SMP as a substrate (Janus and Ulanicki, 2010).

306

307 In the meantime, an attempt to model SMP and EPS kinetics in activated sludge systems was  
308 made by Hsieh et al. (1994a, b), who proposed a simple biokinetic model in which EPS and  
309 SMP production were measured in a single bacterial culture. That work was later tested and  
310 validated by Laspidou and Rittmann (2002a, b), who used the prior works as a foundation for  
311 their model. In this regard, Laspidou and Rittmann (2002a, b) differentiated bEPS from the  
312 active biomass and EPS hydrolysis as the sole mechanism of BAP formation, while no SMPs  
313 were assumed to be formed from the decay of the active biomass (Figure 2d). They also  
314 hypothesised in their “unified theory” that SMP and soluble EPS are identical in systems where  
315 particle organics are not important, the growth-associated part of soluble EPS is identical to  
316 UAP, soluble EPS polymerizes to bEPS, the formation of bEPS is growth-associated and in  
317 direct proportion to substrate utilisation.

318

319 The simple concepts of SMPs concepts were incorporated into the ASMs by including non-  
320 biodegradable soluble products (equivalent to BAPs) produced during hydrolysis of slowly  
321 biodegradable organic compounds ( $X_S$ ) (Orhon et al., 1989) and UAPs (Artan et al., 1990).  
322 However, ASM extensions incorporating SMP/EPS concepts became more common than the  
323 SMP/EPS stand-alone models since Lu et al. (2001, 2002) proposed the combination for  
324 MBRs. Lu et al (2001, 2002) were the first to combine the concepts of SMP presented by  
325 Namkung and Rittmann (1986) with the ASMs for MBR studies. They highlighted that since  
326 biomass concentration and SRT are high and the F/M ratio is low, microbial products in MBR  
327 cannot be ignored. They initially modified the ASM1 (Lu et al., 2001) and then the ASM3 (Lu  
328 et al., 2002). Consequently, the overall active biomass was differentiated into  $X_H$  and  
329 autotrophic ( $X_{AUT}$ ) biomass (Figure 2e). In the modified ASM1, the UAPs are formed directly  
330 by the metabolism of readily biodegradable substrate ( $S_S$ ). The soluble biodegradable organic  
331 compounds, derived from biomass decay, are classified as the BAPs. Both UAPs and BAPs  
332 can be reused directly by heterotrophs for their growth. Although the simulation results agreed  
333 with the experimental data, the model was subsequently questioned regarding COD and charge  
334 imbalances (Jiang et al., 2008). Oliveira-Esquerre et al. (2006) proposed a modification of  
335 ASM3 (ASM3-MP) by lumping the UAPs and BAPs together into a general term MP  
336 (microbial product), for which only the decay products of the biomass were considered (Figure  
337 2f). Active biomass was considered by Furumai and Rittmann (1992) (i.e.,  $X_H$  and  $X_{NIT}$ ), and  
338 their growth was based on the prior hydrolysis of the slowly biodegradable substrate ( $X_S$ ) into  
339 the readily biodegradable substrate ( $S_S$ ). They also pointed out that the link between MPs and  
340 the fouling process must be evaluated.

341

342 Moving forward, Aquino and Stuckey (2008) disagreed with the unified theory proposed by  
343 Laspidou and Rittmann (2002a, b) that soluble EPS and UAP are identical since Ramesh et al.

344 (2006) demonstrated that the physicochemical characteristics of these components are  
345 different. They proposed a new approach to model EPS formation under anaerobic conditions  
346 as a non-growth associated process (Figure 2g), while EPS degradation was modelled similarly  
347 to Namkung and Rittmann (1986). Differently from Laspidou and Rittmann (2002a, b), they  
348 assumed that soluble EPS is not UAP and soluble EPS and cell decay products are the sources  
349 of BAP (Table 1). Concerning BAP formation, the model combined the approaches of the  
350 previous two models, where both decay of active biomass and hydrolysis of the bound EPS are  
351 the sources of BAP (Figure 2g). Unlike Laspidou and Rittmann (2002a, b), the EPS formation  
352 was considered as a mechanism independent of the microbial growth rate but related to biomass  
353 concentration and described by a first-order equation for the active biomass concentration  
354 (Table 1). Aquino and Stuckey (2008) emphasized that incorporating the SMP formation  
355 mechanism from the decay of the active biomass was a significant advantage in capturing SMP  
356 kinetics over a wide range of operational conditions (specifically SRTs) in the studied MBR,  
357 similar to Lu et al. (2001, 2002). Zuthi et al. (2013b) further confirmed that the model was  
358 flexible enough to predict the dynamic changes in bEPS and SMP production. Distinguishing  
359 soluble EPS and SMP formation in MBR models can be useful when testing different fouling  
360 control strategies since they have other factors that can affect their production and  
361 accumulation on the membrane surface.

362

363 Meanwhile, Jiang et al. (2008) criticized the SMP modelling effort of Lu et al. (2001-2002)  
364 because of its complexity and over-parameterization. Additionally, they modelled BAP  
365 degradation not as a direct process (e.g. Lu et al., 2001; Lu et al., 2002; Laspidou and Rittmann,  
366 2002a, b; Oliveira-Esquerre et al., 2006; Aquino and Stuckey, 2008) but after the hydrolysis  
367 process yielding  $S_s$  (Figure 2h). The rationale of that approach was based on the experimental  
368 observation that most BAP had an MW larger than 20 kDa and such large molecules would not



369 be able to pass the cell membranes directly. That approach was adopted in future studies by  
370 Fenu et al. (2011) and Mannina et al. (2011, 2018). Jiang et al. (2008) also argued that previous  
371 SMP modelling studies were lacking proper calibration due to limited measurements and the  
372 validity of these models were questionable. They collected BAP and SMP data separately in  
373 their modelling study and validated their model with independent MBR steady-state  
374 measurements. The following section addresses the novel approaches presented by these  
375 works.

376

### 377 **3.2. New development of conceptual approaches regarding SMP/EPS modelling**

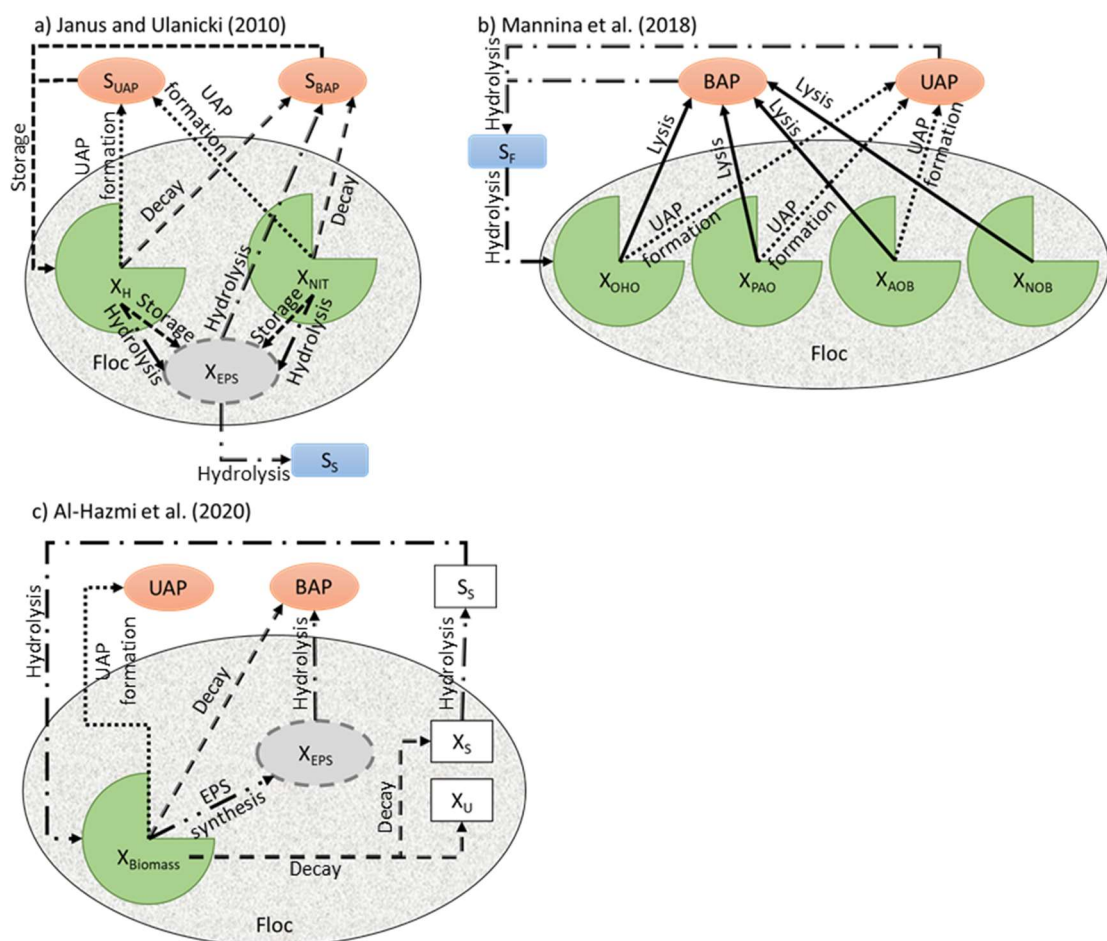
378 This section contains the most recent information regarding modelling SMP and EPS in MBR  
379 systems during past ten years (Figure 3). The conceptual models, shown in Figure 3, are related  
380 to the rate of formation and degradation of each process. For more details about the parameters  
381 used in the model, readers can refer to the publications (Janus and Ulanicki, 2010; Mannina et  
382 al., 2018, Al-Hazmi et al., 2020).

383

384 Zuthi et al. (2013b; 2015) proposed a novel approach for estimating SMP and bEPS from an  
385 MBR system. They argued that there was no unambiguous SMP/EPS measurement method to  
386 characterize the biomass and that the biomass viability could provide a better estimate of these  
387 components. They assumed that SMP affects biomass viability and serves as the binding sites  
388 for cake formation on the membrane surface, based on observations by Lee et al. (2003) and  
389 Rojas et al. (2005). They used the specific oxygen uptake rate (SOUR) as a reference to explain  
390 quantitatively the correlation between the SMP or bEPS and the biomass viability based on the  
391 trace of soluble or colloidal components (soluble or colloidal COD) in the effluent. They  
392 calibrated their model with 50-day of operating data for the results of SOUR and the

393 concentrations of MLSS, its volatile fraction (MLVSS), SMP, and EPS, and later tested the  
 394 model validity with another data set.  
 395  
 396 Janus and Ulanicki (2010; 2015) began modelling SMP and EPS from MBRs around 2010, and  
 397 their work provided novel aspects until recent days. Initially, they were looking for the best  
 398 approach to model SMP/EPS formation and degradation to propose an integrated MBR model.  
 399 In particular, they presented ASM-based models that could account for the formation of SMP  
 400 and EPS. They applied the unified SMP/EPS approach provided by Laspidou and Rittmann  
 401 (2002b) to ASM-based models. UAP was considered as the fraction produced as a by-product  
 402 of substrate utilisation and cell growth. BAP was assumed to originate from biomass decay and  
 403 hydrolysis/dissolution of bEPS (Figure 3 a).

404



405

406 **Figure 3.** Conceptual models of the formation and degradation of SMPs used in recent  
407 modelling studies. The acronyms are detailed in the text.

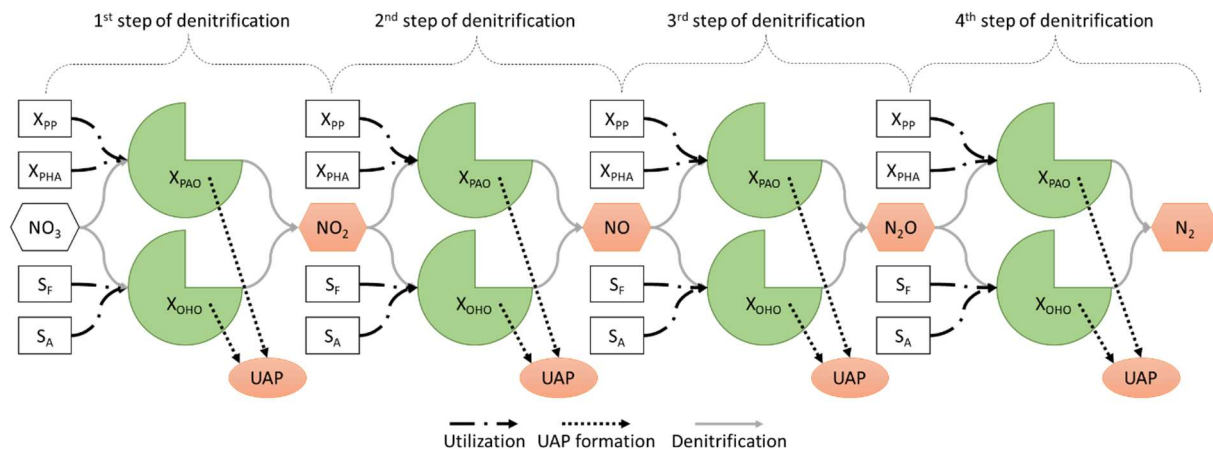
408

409 The model has been calibrated manually with data from biopolymer production from pure  
410 culture (Hsieh et al., 1994a, b) and SMP/EPS production from a pilot scale MBR system (Yiğit  
411 et al., 2008). However, it needs to be validated with a different set of data to confirm the extent  
412 to which it accurately describes them. They also highlighted the SMP and EPS modelling  
413 limitations: (i) although SMP is divided into UAP and BAP based on their metabolic origin,  
414 the chemical compositions of UAP and BAP are important from a fouling perspective; (ii) apart  
415 from SMP and EPS, floc size distribution also affects fouling; (iii) SMP and EPS production  
416 are affected by parameters that the models do not consider, such as temperature and salinity.

417

418 The works of Janus and Ulanicki (2010; 2015) inspired a new model proposal by Mannina et  
419 al. (2018), which presented a comprehensive integrated MBR model to assess the organic  
420 matter, nitrogen and phosphorus biological removal, and greenhouse gas (GHG) formation.  
421 The model considers SMP formation and degradation (dividing SMP into BAP and UAP) and  
422 MLSS concentration as interactions between the biological and physical processes. In that  
423 model, the heterotrophic biomass was divided in phosphorus accumulating organisms (PAO)  
424 ( $X_{PAO}$ ), ordinary heterotrophic organisms ( $X_{OHO}$ ), while the autotrophic biomass was divided  
425 into ammonia-oxidizing bacteria ( $X_{AOB}$ ) and nitrite-oxidizing bacteria ( $X_{NOB}$ ). As shown in  
426 Figure 3 b, UAP and BAP are utilised by heterotrophic biomass for storage, growth, and  
427 respiration. The production of BAP is proportional to biomass decay and its reduction is related  
428 to the hydrolysis process. On the other hand, the production of UAP is related to biomass  
429 growth (except the  $X_{AOB}$ ). Mannina et al. (2018) also considered the denitrification process to  
430 be responsible for the release of UAP, which in the model is performed by  $X_{PAO}$  and  $X_{OHO}$

431 following the four-step denitrification approach of Hyatt and Grady (2008). It should be noted  
432 that Hyatt and Grady (2008) did not consider  $X_{PAO}$  in their work. Figure 4 shows the four-step  
433 denitrification with the release of UAP.



434

435 **Figure 4.** Four steps of denitrification process considered by Mannina et al. (2018).

436

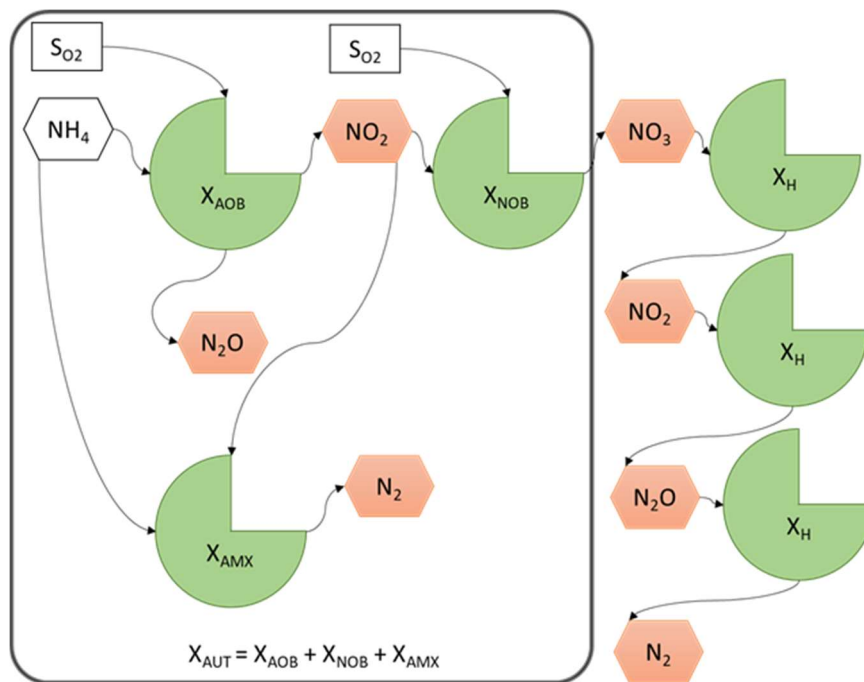
437 During step one, the  $\text{NO}_3^-$  is the main substrate of the processes and is reduced to nitrite ( $\text{NO}_2^-$ )  
 438 ). In this step, the  $X_{\text{PAO}}$  stores polyphosphate ( $X_{\text{PP}}$ ) and utilizes organic accumulating products  
 439 ( $X_{\text{PHA}}$ ), while  $X_{\text{OHO}}$  use organic fermentable products ( $S_{\text{F}}$ ) and acetate ( $S_{\text{A}}$ ) as a substrate. In  
 440 step two,  $\text{NO}_2^-$  is reduced into nitric oxide ( $\text{NO}$ ), then to  $\text{N}_2\text{O}$  in step three, and finally, to  
 441 nitrogen gas ( $\text{N}_2$ ) in step four. Both  $X_{\text{PAO}}$  and  $X_{\text{OHO}}$  release UAP during the denitrification, and  
 442 all related-processes are included in the model. The calibrated simulation results were  
 443 compared to the data from an existing pilot plant treating real wastewater, which adds to the  
 444 reliability and applicability of the integrated approach used by the authors.

445

446 This link between denitrification and SMP production was also found regarding the significant  
 447 heterotrophic growth that takes place in anammox and deammonification systems (fed with no  
 448 organic carbon). In this case, the SMPs were found to be the sole organic carbon and energy  
 449 source for denitrifying heterotrophs. With this regard, Liu et al. (2016) developed a theoretical  
 450 model for the biological processes occurring in an anammox biofilm system and they validated  
 451 their model with experimental data. Organic carbon for the growth of the heterotrophic bacteria  
 452 was exclusively derived from three internal sources: anammox/heterotrophic growth (UAP),

453 biomass decay (cell decay products and BAP), and hydrolysis of EPS (BAP). Subsequently,  
 454 Lu et al. (2018) and Al-Hazmi et al. (2020) adopted the concept of Liu et al. (2016) to expand  
 455 the ASM1 in view of predicting aerobic/anoxic growth of heterotrophic biomass from a  
 456 laboratory-scale deammonification system. In both studies, it was assumed that the formation  
 457 of microbial products (UAP, BAP, and S<sub>s</sub>) was not only derived from the activity of anammox  
 458 and heterotrophs, but also from both groups of nitrifiers (AOB and NOB). The S<sub>s</sub> utilization  
 459 and BAP/UAP degradation were exclusively attributed to the growth of heterotrophs (Figure 3  
 460 c). Liu et al. (2016) applied a stepwise calibration procedure including sensitivity and  
 461 uncertainty analysis and model validation. The conceptual deammonification model of Al-  
 462 Hazmi et al. (2020) is presented in Figure 5.

463



464

465 **Figure 5.** The conceptual model of a deammonification system fed with inorganic substrates  
 466 (Al-Hazmi et al., 2020)

467

468 All the three models emphasised the significant role of autotrophic and heterotrophic bacteria  
469 on SMP formation. For further details, the reader is referred to Liu et al. (2016), Lu et al. (2018),  
470 and Al-Hazmi et al. (2020).

471

#### 472 **4. Kinetic models for the formation and utilization of SMP/EPS**

473 Table 1 summarises the expressions for the SMP/EPS formation and degradation in selected  
474 models. The terms  $\alpha$  and  $\beta$  (Equation 1) represent the formation coefficients for UAP and BAP,  
475 respectively (Luedeking and Piret, 1959). According to Janus (2013), different values can be  
476 assigned to  $\alpha$  and  $\beta$  due to different kinetic dynamics present in mixed bacterial cultures (e.g.  
477 Berry et al., 2004). SMP/EPS dissolution was not considered due to the simplicity of the model.

478

479 In the Laspidou and Rittmann (2002a, b) model (Figure 2 d), the UAP and bound EPS  
480 formation rates are described by the Monod-type equations. The rate of bounded EPS  
481 degradation due to hydrolysis is described by a first-order relationship with respect to the EPS  
482 concentration ( $X_{EPS}$ ). The UAP and BAP degradation rates are described by similar Monod-  
483 type equations. However, the subsequent experimental observations revealed that the  
484 hypothesis of BAP formation only related to EPS hydrolysis was weak for two reasons (Fenu  
485 et al., 2010; Zuthi et al., 2013a). First, the BAP/UAP kinetics were not flexible enough,  
486 especially for predicting dynamic changes of the bound EPS to BAP. Secondly, the  
487 physicochemical properties of the hydrolysed (soluble) EPS and BAP were different. Laspidou  
488 and Rittmann (2002b) calibrated, Lu et al. (2001) calibrated and applied sensitivity analysis to  
489 model parameters. Lu et al. (2001) found that the maximum specific growth rate of SMP for  
490 heterotrophs ( $\mu_{SMP}$ ), UAP formation constant of heterotrophs ( $\gamma_{UAP,H}$ ), and heterotrophic yield  
491 coefficient from SMP ( $\gamma_{SMP}$ ) were sensitive to effluent COD and TN concentrations.

492

493 Jiang et al. (2008) defined the stoichiometric parameter  $f_{BAP}$  as a fraction of BAP generated as  
494 a product of cell ( $X_H$ ,  $X_{PAO}$ ,  $X_{AUT}$ ) lysis. Janus and Ulanicki (2010) defined BAP is originated  
495 from biomass decay and hydrolysis of EPS. They also defined processes for aerobic and anoxic  
496 storage of UAP and BAP. They added a limiting factor  $\eta_{NO}$  for anoxic storage of UAP and  
497 BAP.  
498



499 **Table 1.** Expressions for the formation and degradation of UAP, BAP, and EPS in selected  
500 models – adapted and modified from Fenu et al. (2010) and Zuthi et al. (2013a).

Equation*	Process	Reference
$\alpha \frac{UAP}{dt} + \beta \frac{BAP}{dt}$	SMP production	Luedeking and Piret (1959) (Figure 2 a)
$k_1\mu X + k_2X$		
$k_{f,UAP} \frac{S_s}{K_S + S_s} X_b$	UAP formation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$f_{UAP}(\mu_H X_H + \mu_A X_A)$		Lu et al. (2001) (Figure 2 e)
$-k_{d,UAP} \frac{S_{UAP}}{K_{UAP} + S_{UAP}} X_b$	UAP degradation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$-k_{d,SMP} \frac{S_{SMP}}{K_{SMP} + S_{SMP}} X_H$		Lu et al. (2001) (Figure 2 e)
$k_{STO,UAP} \frac{S_{UAP}}{K_{UAP} + S_{UAP}} X_H$		Janus and Ulanicki (2010) (Figure 3 a)
$k_{EPS} X_{EPS}$	BAP formation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$k_h X_S + k_{h,EPS} X_{EPS}$		Aquino and Sruckey (2008) (Figure 2 g)
$f_{BAP}(b_H X_H + b_{PAO} X_{PAO} + b_{AUT} X_{AUT})$		Jiang et al. (2008) (Figure 2 h)
$f_{BAP} bX + (1 - f_s) k_{h,EPS} X_{EPS}$		Janus and Ulanicki (2010) (Figure 3 a)
$-k_{d,BAP} \frac{S_{BAP}}{K_{BAP} + S_{BAP}} X_b$	BAP degradation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$-k'_{d,BAP} S_{BAP} X_H$		Jiang et al. (2008) (Figure 2 h)
$k_{STO,BAP} \frac{S_{BAP}}{K_{BAP} + S_{BAP}} X_H$		Janus and Ulanicki (2010) (Figure 3 a)
$f_{p,EPS} r_s$	EPS formation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)

$k'_{EPS}X_B$		Aquino and Sruckey (2008) (Figure 2 g)
$-k_{h,EPS}X_{EPS}$	EPS degradation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$f_{p,EPS} \mu X$		Aquino and Sruckey (2008) (Figure 2 g)
$f_{p,EPS}r_s$		Janus and Ulanicki (2010) (Figure 3 a)
$-k_{h,EPS}X_{EPS}$	EPS hydrolysis/dissolution	Janus and Ulanicki (2010) (Figure 3 a)

\* Monod terms for nutrients and electron acceptors are not shown in the table

( $b$  ( $b_H$ ): Lysis rate constant for heterotrophs;  $b_{AUT}$ : Lysis rate constant for autotrophs;  $b_{PAO}$ : Lysis rate constant for PAOs;  $f_{BAP}$ : Fraction of BAP generated as a product of cell lysis;  $f_{p,EPS}$ : Part of the substrate electrons shunted to EPS formation;  $f_s$ : Fraction of SS produced from XEPS hydrolysis;  $f_{UAP}$ : UAP formation yield;  $K_{BAP}$ : BAP affinity constant;  $k_{d,BAP}$ : BAP degradation rate constant;  $k_{d,SMP}$ : SMP degradation rate constant;  $k_{d,UAP}$ : UAP degradation rate constant;  $k_{EPS}$ : EPS formation rate constant;  $k_{f,UAP}$ : UAP formation rate constant;  $k_{h,EPS}$ : EPS hydrolysis rate constant;  $k_h$ : Hydrolysis rate constant;  $K_S$ : Substrate affinity constant;  $K_{SMP}$ : SMP affinity constant;  $k_{STO,BAP}$ : BAP storage rate constant;  $k_{STO,UAP}$ : UAP storage rate constant;  $K_{UAP}$ : UAP affinity constant;  $r_s$ : Substrate utilization rate;  $S_{BAP}$ : BAP concentration;  $S_{SMP}$ : SMP concentration;  $S_{UAP}$ : UAP concentration;  $X_A$  ( $X_{AUT}$ ): Active autotrophic biomass;  $X_b$  ( $X_H$ ): Active heterotrophic biomass;  $X_{EPS}$ : EPS concentration;  $\alpha$  ( $k_1$ ): Formation coefficient for UAP;  $\beta$  ( $k_2$ ): Formation coefficient for BAP;  $\mu$  ( $\mu_H$ ): Maximum growth rate for heterotrophs;  $\mu_A$ : Maximum growth rate for autotrophs)

## 502 **5. SMP/EPS model applications and kinetic parameter values in MBRs**

503 The previously discussed works represent some of the most recent approaches to estimate SMP  
504 and EPS production in MBR systems. However, other recent modelling applications have also  
505 correlated bioprocesses (i.e., SMP and EPS) with MBRs. For physical model, the resistance-  
506 in-series model is usually used as it simulates fouling process with an increase in  
507 transmembrane pressure (TMP) due to the accumulation of deposited material on both the  
508 membrane surface and inside the membrane pores (Wintgens et al., 2003). Lee et al. (2002)  
509 combined SMP production/degradation model of Lu et al. (2001) with a physical model  
510 (resistance-in-series) to simulate fouling. However, Lee et al. (2002) did not calibrate their  
511 model by experimental data. Zarragoitia-González (2008) integrated the unified theory of  
512 Laspidou and Rittmann (2002a) (as SMP model) and physical model. Their model predicted  
513 system performance under different MLSS concentrations, filtration cycles, and aeration  
514 strategies. However, it overlooks the possible influence of the dynamic deep-bed filtration  
515 which acts as a secondary filter, of cake on the organic removal (Mannina et al., 2011). Later,  
516 Di Bella et al. (2008) implemented the deep-bed theory to their physical processes in their  
517 integrated model for MBR systems. They applied their model on a pilot-scale MBR system and  
518 showed the linkage between SMP and fouling. The downside of their modelling study is the  
519 assumption of uniform distribution of the cake deposition on the membrane surface which is  
520 not the case in real situations. Gabarrón et al. (2015) used a dynamic ASM2d-based model to  
521 test optimisation strategies to an MBR system in terms of effluent quality, energy, and cost.  
522 Then they applied the optimum operation strategy that was determined from the modelling  
523 study (dissolved oxygen concentration at 0.8 mg/L) to a full-scale plant and monitored sludge  
524 characteristics. They find out that there were no significant changes in SMP/EPS production.  
525 Zuthi et al. (2017) applied a simplified integrated modelling approach to a lab-scale sponge-  
526 submerged membrane bioreactor (SSMBR) to account for pore blocking and cake formation

527 by taking into consideration the combination of aeration and backwashing effects. The  
528 integrated MBR model used SMP and MLSS concentration as a link between biological and  
529 physical models, mainly considering SMP as a cause of pore blocking. The model described  
530 the effect of pore size reduction due to the adsorption of particles within the pores. According  
531 to the authors, the model could predict fouling development well, but the further assessment of  
532 the model is required by operating MBR systems under different MLSS concentrations and at  
533 different operating conditions.

534

535 Despite the significant results provided by these works regarding MBR performance and  
536 optimisation in both laboratory- and full-scale, the use of site-specific data hampers the  
537 replicability of such model approaches in future works, as no relationship between plant  
538 performance and SMP and EPS was provided. This hindrance may be observed in the number  
539 of model applications in the literature that applied comprehensive MBR models without  
540 coupling the conceptual expressions for the formation/degradation of SMP and EPS.

541

542 To address this issue, Mannina et al. (2020) proposed a process-based plant-wide model to  
543 assess a semi-hypothetical MBR plant in terms of effluent quality, energy consumption, and  
544 GHG emissions. In this model, the SMP concentration inside the MBR was considered a by-  
545 product of biological processes and estimated using a mathematical relationship obtained from  
546 Mannina et al. (2018). The relationship between SMP concentration and SRT was obtained by  
547 performing 2,000 Monte Carlo simulations varying the SRT (Mannina et al., 2020). In spite of  
548 the fact that this model application was based on a semi-hypothetical MBR case study, the  
549 correlation applied was based on a comprehensive dynamic model based on the ASM-family  
550 with a significant data set as a baseline. Results of the model application showed a direct  
551 correlation between SMP concentrations and fouling, which also contributed to an increase in

552 the energy consumption and, consequently, an increase in the GHG emissions. In other words,  
 553 for that specific case, one may say that the SMP represented a significant influence over the  
 554 model outputs that are considered the main obstacles to the spread of MBR as a wastewater  
 555 treatment technology (Capodici et al., 2015; Qin et al., 2018). However, it is worth mentioning  
 556 that the relationship between SMP concentration and fouling depends on multiple parameters  
 557 such as SRT, organic loading rate (OLR), and F/M ratio of the system and MLSS and dissolved  
 558 oxygen concentrations in the reactor (Drews, 2010).

559

560 **Table 2.** Values of the kinetic and stoichiometric parameters in the expressions presented in

561 Table 1

Symbol	Definition	Unit	Laspidou and Rittmann (2002 a, b)	Lu et al. (2001)	Aquino and Sruckey (2008)	Jiang et al. (2008)
<b>UAP</b>						
$k_{f,UAP}$	UAP formation rate constant	$\frac{\text{mg COD}_{UAP}}{\text{mg COD}_{\text{cell}} \cdot \text{d}}$	0.05			
$k_{d,UAP}$	UAP degradation rate constant	$\frac{\text{mg COD}_{UAP}}{\text{mg COD}_{\text{cell}} \cdot \text{d}}$	1.27			
$K_{UAP}$	UAP affinity constant	$\frac{\text{mg COD}}{\text{L}}$	100			
$f_{UAP}$	UAP formation yield	$\frac{\text{mg COD}_{UAP}}{\text{mg COD}_{\text{cell}} \cdot \text{d}}$		0.3		
$k_{d,SMP}$	SMP degradation rate constant	$\frac{\text{mg COD}_{SMP}}{\text{mg COD}_{\text{cell}} \cdot \text{d}}$		4.2		

$K_{SMP}$	SMP affinity constant	$\frac{\text{mg COD}_{SMP}}{\text{L}}$	60	
<b>BAP</b>				
$k_{d,BAP}$	BAP degradation rate constant (Monod equation)	$\frac{\text{mg COD}_{BAP}}{\text{mg COD}_{cell} \cdot \text{d}}$	0.07	
$K_{BAP}$	BAP affinity constant	$\frac{\text{mg COD}_{BAP}}{\text{L}}$	85	
$k'_{d,BAP}$	BAP degradation rate constant (First order equation)	$\frac{\text{mg COD}_{SMP}}{\text{L}}$		$7.1 \cdot 10^{-7}$
$k_h$	BAP formation rate constant from biomass decay	$\frac{\text{mg COD}_{BAP}}{\text{mg COD}_{cell} \cdot \text{d}}$		0.03

562

## 563 6. Discussion and perspectives

564 The main outcomes of this review highlighted the modelling of SMP and EPS in MBR systems  
565 under a common frame. Indeed, SMP-based models are spread in the literature and have been  
566 improved and updated since the late 1950s until the present day. In this section, the  
567 improvement of and updates on SMP and EPS models and the strengths and weaknesses of  
568 these models in MBR systems are summarised. Furthermore, suggestions to improve MBR  
569 models have been given.

570

571 Concerning the novel conceptual approaches hereby presented, Liu et al. (2016), Al-Hazmi et  
572 al. (2020), and Mannina et al. (2018) proposed modelling approaches that can be considered

573 an evolution of those represented in Figure 2, except for Namkung and Rittmann (1986) which  
574 did not attribute the formation of SMPs to the biomass. For this reason, their work could be  
575 applied to other MBR-related studies, even though Liu et al. (2016) and Al-Hazmi et al. (2020)  
576 did not direct the model efforts to MBR systems. As far as the authors are aware, the recent  
577 model applications to anammox-MBR systems (Tao and Hamouda, 2019; Wisniewski et al.,  
578 2019; Liu et al., 2019 a) did not consider the role of the bioprocesses over membrane fouling  
579 issues, which is a very important issue to be addressed in future works.

580

581 Regardless of the numerous published data, there needs to be more knowledge concerning SMP  
582 kinetics due to their multiple origins and highly complicated nature. The major issue is related  
583 to the fact that their kinetics are dependent on many different factors that need to be accounted  
584 for in the current modelling approaches. Additionally, the relationship between their nature  
585 (e.g., protein or carbohydrates) and the effects over formation, degradation, fouling and many  
586 other aspects from a modelling point of view still needs to be improved in the literature.  
587 Moreover, depending on the objectives of the model development, changes in model structures  
588 are not anodyne: for instance, (Benyahia et al., 2013) it was shown that introducing SMP in  
589 simple an-MBR models used for control resulted in significant changes in their mathematical  
590 properties (notably in the number and stability of their steady states).

591

592 The estimation of EPS has not received much attention in the literature, likely due to the lack  
593 of understanding of their formation pathways. According to Scholes et al. (2016), the lack of  
594 consensus on the causes of EPS production in the scientific literature is unsurprising given the  
595 variation in wastewater influent and microbial populations. The authors also emphasised that  
596 each MBR may have its own triggers (SRT, OLR, F/M ratio etc.) for EPS production, which  
597 could influence membrane fouling in various ways. For this reason, the establishment of

598 modelling approaches is necessary to encourage new findings and increase knowledge about  
599 EPS formation/degradation.

600

601 Another serious issue is that most of the data used for modelling SMP and EPS have been  
602 obtained from experimental estimation (Scholes et al., 2016; Park et al., 2018). Therefore, it is  
603 recommended that MBR models be calibrated and validated on the basis of data retrieved from  
604 full-scale WRRFs treating real wastewater to consider their real response to dynamic changes  
605 in influent composition and operating conditions. Finally, the influence of these components  
606 on MBR optimisation can appropriately be validated by correlating them with optimization  
607 outputs (e.g., membrane fouling, energy consumption, operating costs, GHG emissions),  
608 during model simulations. The successful applications endorse the importance of including  
609 conceptual SMP/EPS approaches to model simulations since optimisation of an MBR system  
610 could be better assessed by the use of more accurate SMP and EPS estimations.

611

612 Given the number of publications that have used the modelling of SMP and EPS formation and  
613 degradation to estimate membrane filter performance and energy consumption it seems that  
614 these approaches are convincing and, although the models can be complex, they tend to give a  
615 monocausal explanation for membrane fouling and MBR behaviour. In practical MBR  
616 operations, multiple factors may inflict membrane performance, which can be eventually  
617 mistakenly attributed to genuine fouling, but actually may have causes that lie outside the scope  
618 of a model (e.g. Hai et al., 2019). Other adverse effects on membrane performance (e.g. coarse  
619 fouling, module blocking, filter integrity, uneven flow distribution etc.), which are common at  
620 full-scale installations, may lead to an overestimation of the role of EPS and SMPs in a model.  
621 Thus, these modelling approaches have to be used with caution and uncertainties at all stages



622 of the model formulation, data collection, set-up, calibration and validation should be taken  
623 into account while applying good modelling practices.

624

625 In addition to empirical and mathematical models, the application of artificial intelligence (AI)  
626 in membrane fouling modelling has been a subject of research for the past two decades (Niu et  
627 al., 2022). While these AI models have effectively predicted the increase in TMP resulting  
628 from membrane fouling, they have struggled to establish a correlation between permeate  
629 quality and TMP (Schmitt et al., 2018; Hamed et al., 2019). This highlights the ongoing  
630 significance of mathematical modelling studies focused on understanding the production of  
631 SMP, which directly impact the quality of the permeate.

632

### 633 **Conclusions**

634 The key findings identified from this state-of-the-art review are listed below:

- 635 ● Accurate estimation of SMP and EPS can contribute to optimising membrane fouling  
636 results, which directly influence energy consumption, operating costs, and GHG  
637 emissions.
- 638 ● AI models accurately predict TMP increase from fouling in MBRs but struggle to  
639 correlate permeate quality with TMP. This emphasizes the ongoing importance of  
640 mathematical modelling to understand SMP production and its impact on permeate  
641 quality.
- 642 ● Although many studies have been published concerning SMPs, there are still gaps in  
643 the literature due to their complex nature and multiple origins.
- 644 ● Only a few studies have focused on the estimation of EPS due to a need for more  
645 information on the triggers for their production.

- 646 ● Most modelling studies have neglected the physicochemical properties of SMP/EPS  
647 such as protein and carbohydrate contents or MW.
- 648 ● Most of the data used for modelling SMP and EPS have been retrieved from  
649 experimental estimation, which may limit replicability since such information does not  
650 represent the dynamic changes in influent composition and operating conditions.
- 651 ● The novel conceptual approaches presented in this work primarily focus on biomass-  
652 related processes and the role of different bacterial groups in the release of SMP.  
653 However, these studies did not consider the direct influence of SMP and EPS on  
654 membrane fouling, presenting opportunities for future developments.

655

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