

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 (Attigbe, 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

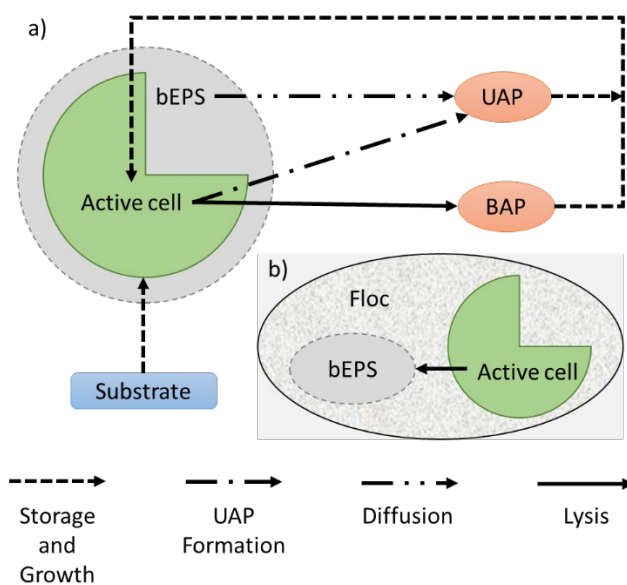
169 the UAP fraction could predominate when the substrate degradation rates were high, while the
170 BAP fraction could typically dominate over the UAP fraction at higher SRTs or under steady-
171 state conditions. Indeed, BAPs have been more assessed in the literature over the years due to
172 the lack 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

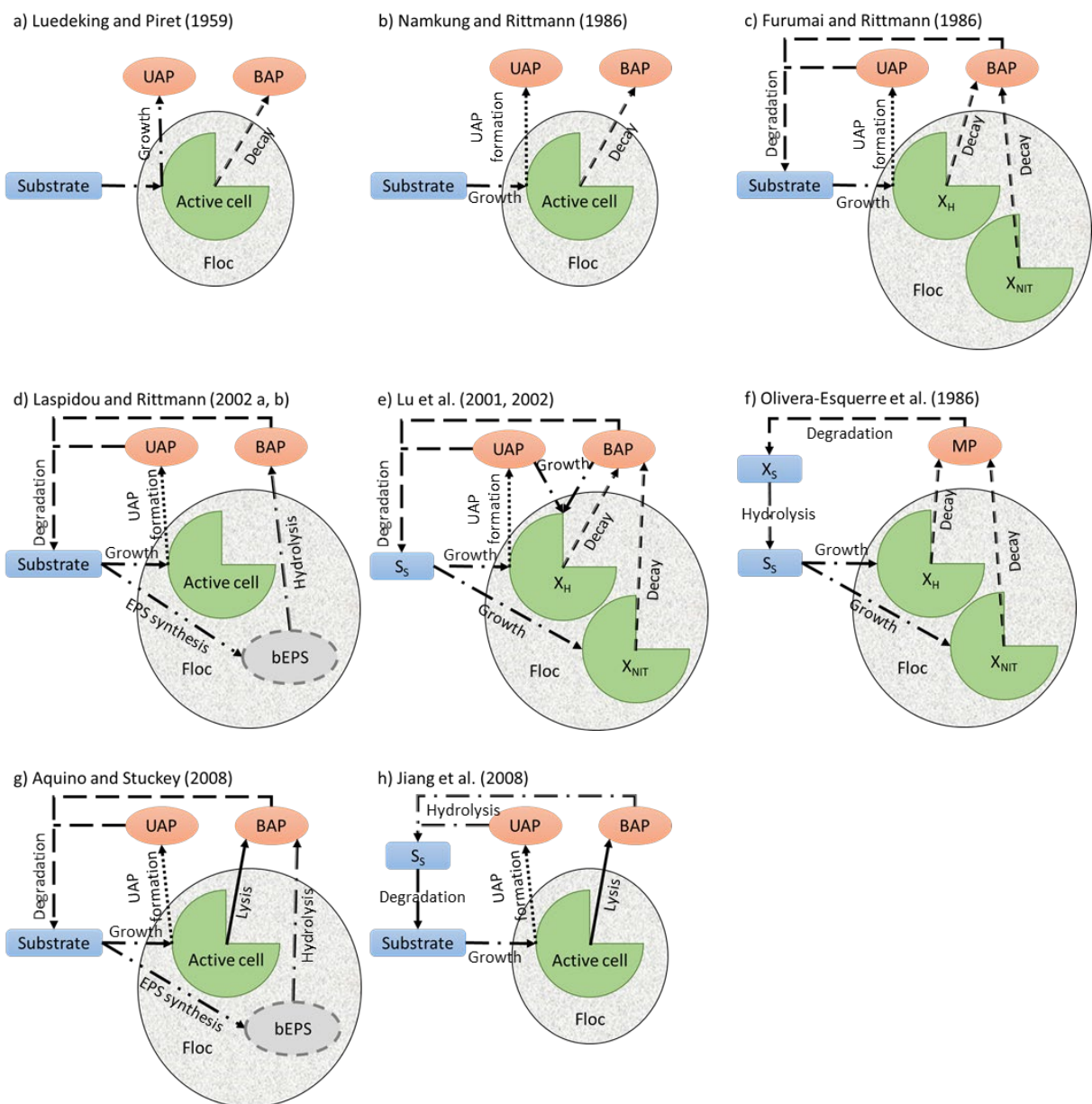
256 **3.1. Historical overview regarding SMP/EPS modelling**

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_{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 Lapidou 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 Lapidou 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; Lapidou 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**

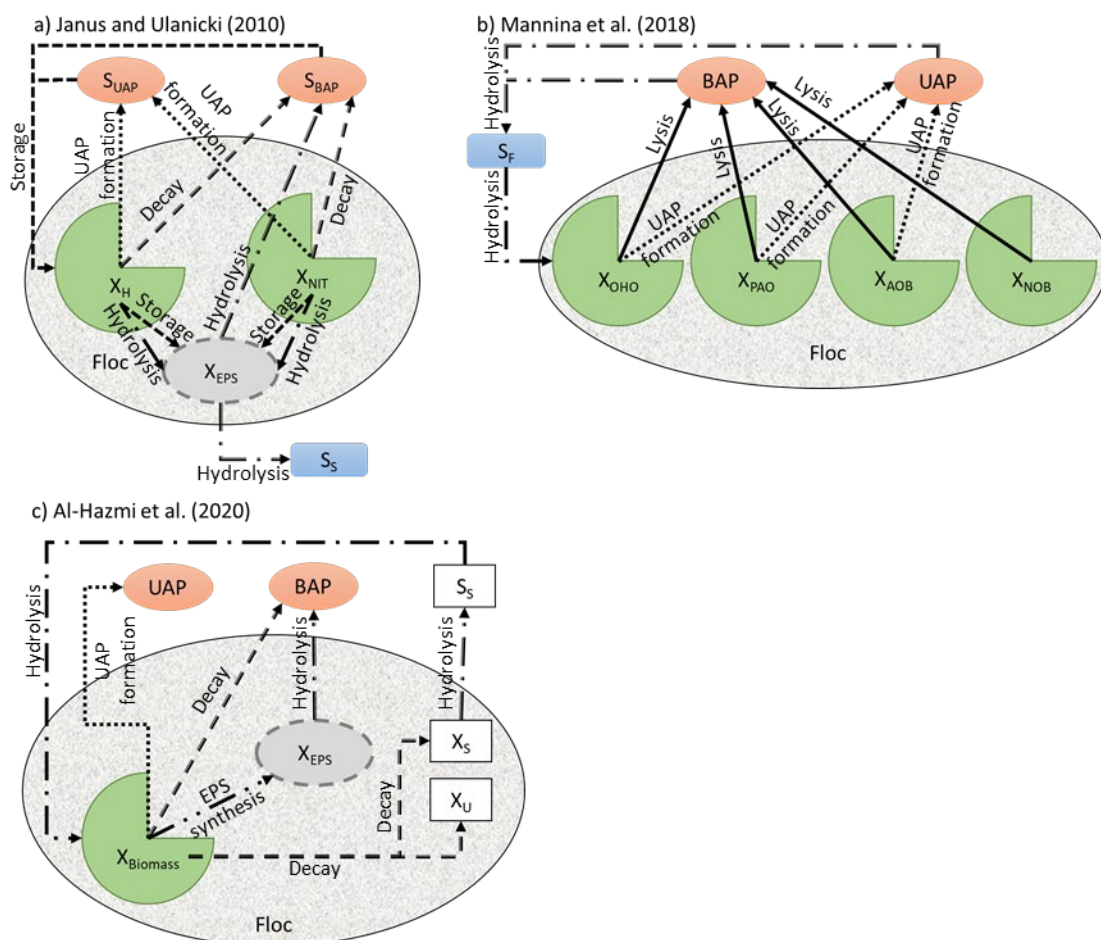
378 This section contains the most recent information regarding modelling SMP and EPS in MBR
379 systems during past ten years (Figure 3). The conceptual models, shown in Figure 3, are related
380 to the rate of formation and degradation of each process. For more details about the parameters
381 used 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.

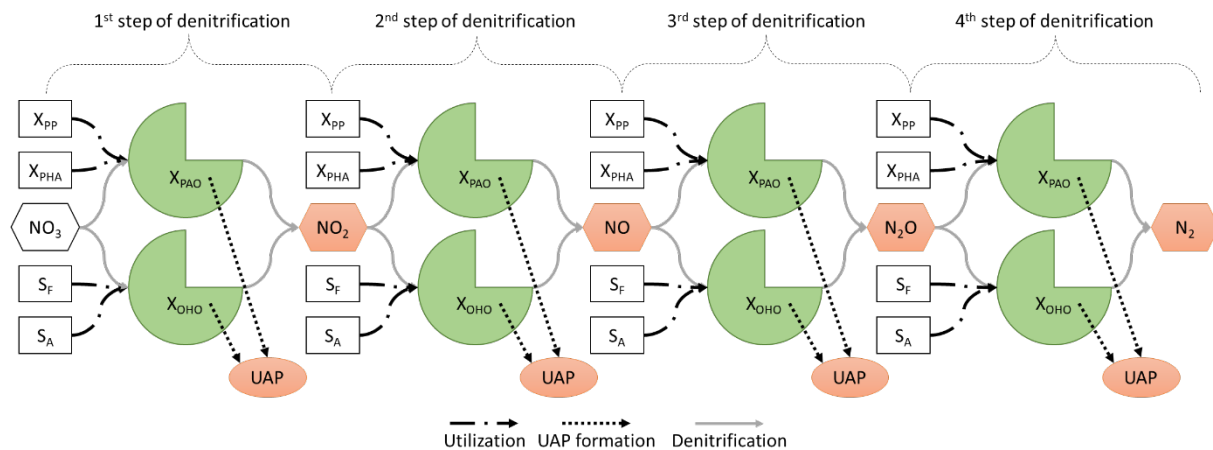
408

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

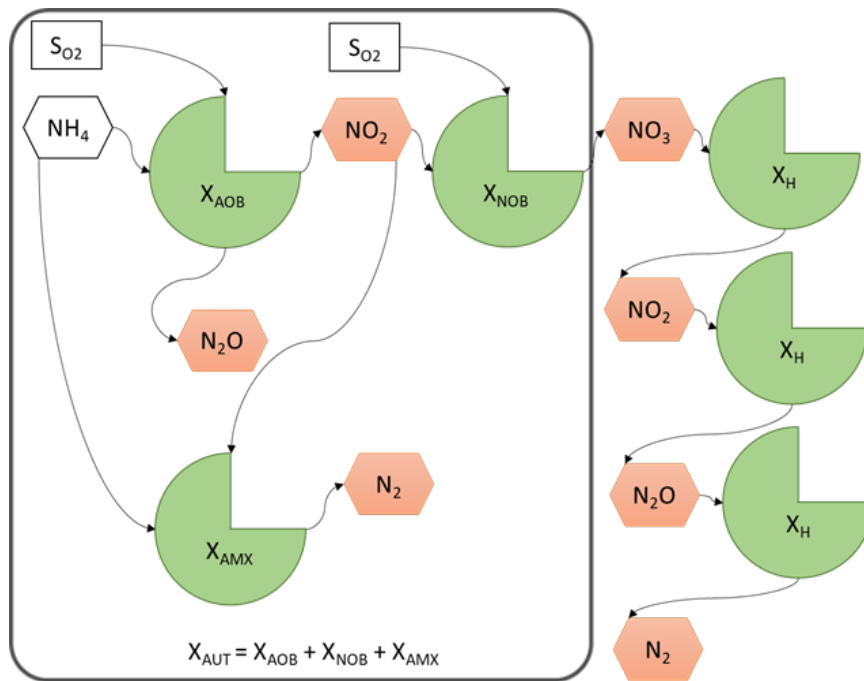
437 During step one, the NO_3^- is the main substrate of the processes and is reduced to nitrite (NO_2^-)
 438). In this step, the X_{PAO} stores polyphosphate (X_{PP}) and utilizes organic accumulating products
 439 (X_{PHA}), while X_{OHO} use organic fermentable products (S_{F}) and acetate (S_{A}) as a substrate. In
 440 step two, NO_2^- is reduced into nitric oxide (NO), then to N_2O in step three, and finally, to
 441 nitrogen gas (N_2) in step four. Both X_{PAO} and X_{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_s) was not only derived from the activity of anammox
 458 and heterotrophs, but also from both groups of nitrifiers (AOB and NOB). The S_s 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 α and β (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 α and β 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 (μ_{SMP}), UAP formation constant of heterotrophs ($\gamma_{UAP,H}$), and heterotrophic yield
491 coefficient from SMP (γ_{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 η_{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)
$\frac{k_1 \mu X + k_2 X}{k_{f,UAP} \frac{S_s}{K_S + S_s} X_b}$	UAP formation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$\frac{f_{UAP}(\mu_H X_H + \mu_A X_A)}{-k_{d,UAP} \frac{S_{UAP}}{K_{UAP} + S_{UAP}} X_b}$	UAP degradation	Lu et al. (2001) (Figure 2 e)
$\frac{-k_{d,SMP} \frac{S_{SMP}}{K_{SMP} + S_{SMP}} X_H}{k_{STO,UAP} \frac{S_{UAP}}{K_{UAP} + S_{UAP}} X_H}$		Lu et al. (2001) (Figure 2 e)
$\frac{k_{EPS} X_{EPS}}{k_h X_S + k_{h,EPS} X_{EPS}}$	BAP formation	Janus and Ulanicki (2010) (Figure 3 a)
$\frac{f_{BAP}(b_H X_H + b_{PAO} X_{PAO} + b_{AUT} X_{AUT})}{f_{BAP} b X + (1 - f_s) k_{h,EPS} X_{EPS}}$		Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$\frac{-k_{d,BAP} \frac{S_{BAP}}{K_{BAP} + S_{BAP}} X_b}{-k'_{d,BAP} \frac{S_{BAP}}{K_{BAP} + S_{BAP}} X_H}$	BAP degradation	Aquino and Sruckey (2008) (Figure 2 g)
$\frac{k_{STO,BAP} \frac{S_{BAP}}{K_{BAP} + S_{BAP}} X_H}{f_{p,EPS} r_s}$		Jiang et al. (2008) (Figure 2 h)
$\frac{f_{p,EPS} r_s}{k'_{EPS} X_B}$	EPS formation	Janus and Ulanicki (2010) (Figure 3 a)
$\frac{-k_{h,EPS} X_{EPS}}{f_{p,EPS} \mu X}$	EPS degradation	Laspidou and Rittmann (2002 a, b) (Figure 2 d)
$\frac{f_{p,EPS} r_s}{-k_{h,EPS} X_{EPS}}$	EPS hydrolysis/dissolution	Aquino and Sruckey (2008) (Figure 2 g)
		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 X_{EPS} 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; α (k₁): Formation coefficient for UAP; β (k₂): Formation coefficient for BAP; μ (μ_H): Maximum growth rate for heterotrophs; μ_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)
UAP						
$k_{f,UAP}$	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		
BAP						
$k_{d,BAP}$	BAP degradation rate constant (Monod equation)	$\frac{\text{mg COD}_{BAP}}{\text{mg COD}_{\text{cell}} \cdot \text{d}}$	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	$\frac{\text{mg COD}_{BAP}}{\text{mg COD}_{\text{cell}} \cdot \text{d}}$			0.03	

562

563 **6. Discussion and perspectives**

564 The main outcomes of this review highlighted the modelling 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 summarized. 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 is a gap in the 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 are not being
584 accounted for in the current modelling approaches. Additionally, the relationship between their
585 nature (e.g., protein or carbohydrates) and the effects over formation, degradation, fouling and
586 many other aspects from a modelling point of view is still lacking in the literature. Moreover,
587 depending on the objectives of the model development, changes in model structures are not

588 anodyne: for instance, in (Benyahia et al., 2013) it was shown that introducing SMP in simple
589 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 the pathways of their formation. According to Scholes et al. (2016), the
594 lack of consensus on the causes of EPS production in the scientific literature is unsurprising
595 given the variation in wastewater influent and microbial populations. The authors also
596 emphasized that each MBR may have its own triggers (SRT, OLR, F/M ratio etc.) for EPS
597 production, which could influence membrane fouling in various ways. For this reason, the
598 establishment of modelling approaches is necessary to encourage new findings and increase
599 knowledge about 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 should be calibrated and validated on the basis of data
604 retrieved from full-scale WRRFs treating real wastewater in order to consider their real
605 response to dynamic changes in influent composition and operating conditions. Finally, the
606 influence of these components on MBR optimization can appropriately be validated by
607 correlating them with optimization outputs (e.g., membrane fouling, energy consumption,
608 operating costs, GHG emissions), during model simulations. The successful applications
609 endorse the importance of including conceptual SMP/EPS approaches to model simulations
610 since optimization of an MBR system could be better assessed by the use of more accurate
611 SMP and EPS estimations.

612

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

625

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

633

634 **Conclusions**

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

- 636 ● Accurate estimation of SMP and EPS can contribute to optimizing membrane fouling
637 results, which directly influence energy consumption, operating costs, and GHG
638 emissions.
- 639 ● AI models accurately predict TMP increase from fouling in MBRs but struggle to
640 correlate permeate quality with TMP. This emphasizes the ongoing importance of
641 mathematical modeling to understand SMP production and its impact on permeate
642 quality.
- 643 ● Although many studies have been published concerning SMPs, there are still gaps in
644 the literature due to their complex nature and multiple origins.
- 645 ● Only a few studies have focused on the estimation of EPS due to a lack of information
646 on the triggers for their production.
- 647 ● The physicochemical properties of SMP/EPS such as protein and carbohydrate contents
648 or MW have been neglected in most modelling studies.
- 649 ● Most of the data used for modelling SMP and EPS have been retrieved from
650 experimental estimation, which may limit replicability since such information does not
651 represent the dynamic changes in influent composition and operating conditions.
- 652 ● The novel conceptual approaches presented in this work primarily focus on biomass-
653 related processes and the role of different bacterial groups in the release of SMP.
654 However, these studies did not consider the direct influence of SMP and EPS on
655 membrane fouling, presenting opportunities for future developments.

656

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660 [network.org/groups/membrane-bioreactor-modelling-and-control/](http://www.iwa-network.org/groups/membrane-bioreactor-modelling-and-control/)).

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