

Integrated benchmark simulation model of an immersed membrane bioreactor

Tomasz Janus*, Bogumil Ulanicki

Water Software Systems, De Montfort University, The Gateway, LE1 9BH Leicester, United Kingdom

Abstract

This paper presents a new integrated model of an immersed membrane bioreactor (iMBR) for wastewater treatment. The model is constructed out of three previously published submodels describing the bioreactor, the membrane, and the interface between them. The bioreactor submodel extends a conventional activated sludge model with soluble and bound biopolymers which have been found to cause irreversible and reversible fouling. The membrane model describes fouling as a function of biopolymer concentrations, permeate flow, and shear stresses on the membrane surface. The interface describes the dependency of oxygen transfer rate on suspended solids concentrations and calculates shear stresses on the membrane surface from air-scour rates. The paper serves three purposes. First, the integrated model is simulated on a plant layout of a previously published MBR benchmark model which did not consider any interactions between the submodels. Hence, this paper presents a new and upgraded MBR benchmark model. Secondly, the simulation results showcase how simulations with an integrated model can be used to optimise plant performance and minimise energy consumption. Finally, the paper introduces new measures of

*Corresponding author, Tel.: +44(0) 116 257 7070

Email addresses: tjanus@dmu.ac.uk (Tomasz Janus), bul@dmu.ac.uk (Bogumil Ulanicki)

fouling which can be used for benchmarking different MBR plant layouts and control strategies.

Keywords: benchmark model, biopolymers, EPS, fouling, MBR, SMP

Nomenclature

$AE_{\text{bioreactor}}$	energy demand for fine-bubble aeration (kWh d ⁻¹)
AE_{membrane}	energy demand for coarse-bubble aeration (kWh d ⁻¹)
AE_{total}	total energy demand for aeration (kWh d ⁻¹)
A_{mem}	total membrane area (m ²)
$BOD_{5,95}$	95%-ile of effluent biological oxygen demand (gO ₂ m ⁻³)
COD_{95}	95%-ile of effluent chemical oxygen demand (gO ₂ m ⁻³)
E.Q.	effluent quality index (kgPU d ⁻¹) - see Copp (2002) for definition
FI_i	Irreversible fouling index (m ⁻¹ L ⁻¹)
FI_r	Reversible fouling index (m ⁻¹ L ⁻¹)
$f_{EPS,dh}$	fraction of X_{EPS} produced during heterotrophic biomass decay (gO ₂ gO ₂ ⁻¹)
$f_{EPS,h}$	fraction of X_{EPS} produced during heterotrophic biomass growth (gO ₂ gO ₂ ⁻¹)
f_{EPS}^{inf}	extracellular polymeric substances (EPS) content in the influent biomass (-)
f_{nr}	fraction of S_{UAP} and S_{BAP} in the permeate (-)
f_{SMP}^{inf}	S_{BAP} content in the influent S_I (-)
g	gravity constant (9.81 m s ⁻²)
h_g	geometric head difference (m H ₂ O)
h_l	head loss due to friction (m H ₂ O)
i_{XB}^{inf}	N content of the influent biomass (-)
i_{XEPS}^{inf}	EPS content in the influent biomass (-)
i_{XBAP}^{inf}	N content in BAP (-)
I.Q.	influent quality index (kgPU d ⁻¹) - see Copp (2002) for definition
J	permeate flux (L m ⁻² h ⁻¹)
K_p	proportional gain (varies)
k_i	irreversible fouling strength (m kg ⁻¹)
k_r	cake detachment constant (kg m ⁻² s ⁻¹)
ME	energy for mixing anoxic tanks and aerobic tanks in case the amount of air provided is not sufficient for a thorough mixing of the tank contents (kWh d ⁻¹)
m_i	mass of irreversible foulant per membrane area (kg m ⁻²)
m_r	mass of reversible foulant per membrane area (kg m ⁻²)

\dot{m}_r^{back}	back-flux of reversible foulant per membrane area away from the membrane ($\text{kg m}^{-2} \text{d}^{-1}$)
OCI	operational cost index (-)
q_a	airflow rate ($\text{m}^3 \text{d}^{-1}$)
q_{ave}	average flow rate ($\text{m}^3 \text{d}^{-1}$)
$q_{a,1}$	airflow rate into the first aerobic tank ($\text{m}^3 \text{d}^{-1}$)
$q_{a,2}$	airflow rate into the second aerobic tank ($\text{m}^3 \text{d}^{-1}$)
$q_{a,3}$	airflow rate into the membrane tank ($\text{m}^3 \text{d}^{-1}$)
q_b	backflush flow ($\text{m}^3 \text{d}^{-1}$)
q_{eff}	effluent (permeate) flow rate ($\text{m}^3 \text{d}^{-1}$)
q_{inf}	influent flow rate ($\text{m}^3 \text{d}^{-1}$)
q_{ir}	internal recirculation flow rate ($\text{m}^3 \text{d}^{-1}$)
q_{ave}	average flow rate ($\text{m}^3 \text{d}^{-1}$)
q_{min}	minimum flow rate ($\text{m}^3 \text{d}^{-1}$)
q_{max}	maximum flow rate ($\text{m}^3 \text{d}^{-1}$)
q_{rec}	sludge recirculation flow rate ($\text{m}^3 \text{d}^{-1}$)
q_w	waste activated sludge flow rate ($\text{m}^3 \text{d}^{-1}$)
$PE_{permeate}$	energy associated with permeate pumping (kWh d^{-1})
$PE_{q_{back}}$	energy associated with back-flushing (kWh d^{-1})
$PE_{q_{eff}}$	energy associated with effluent pumping (kWh d^{-1})
$PE_{q_{int}}$	energy used on internal recirculation (kWh d^{-1})
PE_{q_r}	energy used on sludge recirculation (kWh d^{-1})
PE_{q_w}	energy used on WAS pumping (kWh d^{-1})
PE_{sludge}	energy associated with sludge pumping (kWh d^{-1})
PE_{total}	total pumping energy (kWh d^{-1})
R_i	resistance due to irreversible fouling (m^{-1})
R_m	clean membrane resistance (m^{-1})
R_r	resistance due to reversible fouling (m^{-1})
R_t	total membrane resistance (m^{-1})

S_{ALK}	alkalinity ($\text{molHCO}_3^- \text{ m}^{-3}$)
S_{BAP}	concentration of biomass associated products (BAP) ($\text{gO}_2 \text{ m}^{-3}$)
S_{ND}	concentration of soluble organic nitrogen (gN m^{-3})
S_{NH}	concentration of ammoniacal nitrogen (gN m^{-3})
$S_{NH,95}$	95%-ile of effluent ammoniacal nitrogen concentration (gN m^{-3})
S_{NO}	concentration of nitrites and nitrates (gN m^{-3})
S_I	concentration of soluble inert organic matter ($\text{gO}_2 \text{ m}^{-3}$)
S_O	dissolved oxygen concentration ($\text{gO}_2 \text{ m}^{-3}$)
SP_{disp}	amount of sludge for disposal (kgTSS d^{-1})
SP_{tot}	total sludge production (kgTSS d^{-1})
S_S	concentration of readily biodegradable substrate ($\text{gO}_2 \text{ m}^{-3}$)
S_{SMP}	concentration of soluble microbial products ($\text{gO}_2 \text{ m}^{-3}$). $S_{SMP} = S_{UAP} + S_{BAP}$
S_{UAP}	concentration of utilisation associated products (UAP) ($\text{gO}_2 \text{ m}^{-3}$)
t_f	filtration cycle duration time (s)
t_I	integral time (d)
T_l	liquid temperature ($^{\circ}\text{C}$)
TN_{95}	95%-ile of effluent total nitrogen concentration (gN m^{-3})
t_{simu}	simulation time (d)
TSS_{95}	95%-ile of effluent total suspended solids concentration (gN m^{-3})
t_0	simulation start time (d)
v_{sg}	superficial gas velocity (cm s^{-1})
v_{sl}	superficial liquid velocity (cm s^{-1})
$V_{ax,1}$	first anoxic tank volume (m^3)
$V_{ax,2}$	second anoxic tank volume (m^3)
V_{mem}	membrane tank volume (m^3)
V_{eff}^{net}	net volume of permeate discharged from the plant (m^3)
$V_{ox,1}$	first aerobic tank volume (m^3)
$V_{ox,2}$	second aerobic tank volume (m^3)
X_A	concentration of autotrophic biomass ($\text{gO}_2 \text{ m}^{-3}$)

X_{EPS}	concentration of extracellular polymeric substances (EPS) ($\text{gO}_2 \text{ m}^{-3}$)
X_I	concentration of particulate inert organic matter ($\text{gO}_2 \text{ m}^{-3}$)
X_H	concentration of heterotrophic biomass ($\text{gO}_2 \text{ m}^{-3}$)
X_{MLSS}	concentration of mixed liquor suspended solids (MLSS) (g m^{-3})
X_{ND}	concentration of particulate organic nitrogen (gN m^{-3})
X_P	concentration of particulate products from biomass decay ($\text{gO}_2 \text{ m}^{-3}$)
X_S	concentration of slowly biodegradable organic substrate ($\text{gO}_2 \text{ m}^{-3}$)
X_{TSS}	concentration of total suspended solids (g m^{-3})
Y_{obs}	observed sludge yield ($\text{kgSS kg}^{-1}\text{BOD}_5$)
Y_{SMP}	yield coefficient for heterotrophic growth on S_{UAP} and S_{BAP} (-)
α	oxygen transfer coefficient (-)
α_c	specific cake resistance under field conditions (m kg^{-1})
$\alpha_{c,0}$	specific cake resistance at atmospheric pressure (m kg^{-1})
η	pumping efficiency (-)
μ_{BAP}	maximum specific heterotrophic growth rate on S_{BAP} (d^{-1})
ω	proportionality coefficient in the oxygen transfer coefficient equation (kg^{-1}TSS)
ρ_w	density of water (kg m^{-3})
τ_w	average shear stress on the fibre surface (Pa)

Abbreviations

ASM	activated sludge model
ASM1	Activated Sludge Model No. 1
ASP	activated sludge process
BAP	biomass associated products
BSM1	COST/IWA benchmark simulation model No.1
BSM-MBR	membrane bioreactor (MBR) benchmark simulation model
C	carbon
CASP	conventional activated sludge process
CES-ASM1	combined EPS and SMP production ASM1-based model
CFD	Computational Fluid Dynamics
COD	chemical oxygen demand
DO	dissolved oxygen
DWF	dry weather flow
EPS	extracellular polymeric substances
FSD	floc size distribution
HF	hollow fibre
IBMF-MBR	integrated bioreactor and membrane fouling MBR model
MBR	membrane bioreactor
MLSS	mixed liquor suspended solids
MWD	molecular weight distribution
N	nitrogen
NF	nanofiltration
NH ₄ ⁺ -N	ammoniacal nitrogen
NO ₃ ⁻ -N	nitrate nitrogen
P	phosphorus
PI	proportional integral
P&ID	piping and instrumentation diagram
PAC	powdered activated carbon
RAS	recirculated activated sludge

RO	reverse osmosis
SAD _m	specific aeration demand per membrane area
SMP	soluble microbial products
SRT	sludge retention time
TMP	trans-membrane pressure
TKN	total Kjeldahl nitrogen
TN	total nitrogen
UAP	utilisation associated products
UF	ultrafiltration
WAS	waste activated sludge
WWTP	wastewater treatment plant

1 **1. Introduction**

2 MBR systems are widely applied in municipal and industrial wastewater treat-
3 ment. The main three reasons for their popularity are: tightening effluent discharge
4 standards, rising water scarcity, and limited land availability for expansion of exist-
5 ing wastewater treatment plants (WWTPs). Under such circumstances membrane
6 bioreactors (MBRs) outperform traditional treatment systems thanks to superior ef-
7 fluent quality, better process stability and smaller footprint. The effluent is partly
8 disinfected and can be reused for non-drinking purposes or used as feed for further
9 treatment processes for recycling and water conservation. Despite of a widespread
10 use of MBRs in wastewater treatment the technology is currently missing bespoke dy-
11 namic process models that would allow simulation of MBR-based plants in commer-
12 cial WWTP simulation packages along with conventional processes such as activated
13 sludge reactors, trickling filters, or sedimentation tanks. None of the commercial
14 packages contain a MBR model which is able to predict bulk liquid concentrations

15 of the most dominant biofoulants, i.e. soluble microbial products (SMP) and extra-
16 cellular polymeric substances (EPS) despite the fact that SMP and EPS are indis-
17 pensable for integration of the biological and filtration models as these substances
18 have been found to have a direct impact on the rates of different membrane foul-
19 ing mechanisms such as pore constriction, pore blocking, and cake filtration (Hoa
20 et al., 2003; Broeckmann et al., 2006; Nuengjamnong, 2006; Wang et al., 2009). Ad-
21 ditionally, MBR models in commercial software packages do not provide a detailed
22 mechanistic description of membrane fouling and fouling control mechanisms. As
23 long as the mathematical models for MBR systems do not become richer and the
24 main interactions between the bioreactor and the membrane are not described, tasks
25 such as simulation-based process design, process and energy optimisation, diagnosis,
26 risk-analysis, or control strategy development, which can be carried out using com-
27 mercial simulation packages on conventional treatment processes such as activated
28 sludge process or anaerobic digestion, will not be able to be performed on MBR
29 systems.

30 Luckily, recent years have seen a number of dynamic mathematical models of
31 membrane bioreactors described in the scientific literature. These publications are
32 briefly summarised in Janus and Ulanicki (2014, 2015c). Although the MBR model
33 described in this paper has some similarities with these earlier published works,
34 it is also significantly different. The biological model used in this study is set to
35 predict the concentrations of soluble and bound polymers contrary to the majority
36 of biological models developed in the earlier studies which only consider soluble
37 biopolymer kinetics - see Janus and Ulanicki (2015c). It was also ascertained that
38 the biological model obeys mass and charge balance equations which were violated in
39 the activated sludge model of Lu et al. (2001) - the biological model of choice in the
40 studies of Zarragoitia-González et al. (2008) and Di Bella et al. (2008). As shall be

41 seen later in this paper, our biological model additionally produces similar outputs
42 to the widely accepted Activated Sludge Model No. 1 (ASM1), hence allowing easy
43 comparison of results with BSM1 (Copp, 2002) and BSM-MBR (Maere et al., 2011)
44 benchmark models. The fouling model has a simple structure and a small number
45 of parameters which are easy to identify with a ‘pen and ruler’ approach using flux
46 and pressure data from flux stepping experiments - see Janus and Ulanicki (2015b).
47 Our MBR model also considers the role of both soluble and insoluble biopolymers on
48 reversible and irreversible fouling, contrary to the previously published models which
49 generally only consider the role of SMP in cake filtration (reversible fouling) rather
50 than pore constriction (irreversible fouling), whilst neglecting the effects of EPS on
51 fouling in general. In our model irreversible fouling is assumed to be caused by SMP
52 whilst reversible fouling is accelerated by EPS content in mixed liquor suspended
53 solids (MLSS) which leads to an increase in the specific cake resistance. The cake
54 detachment rate is calculated as a function of air-scour intensity with a formula
55 obtained from the results of a steady-state slug flow model of Zaisha and Dukler
56 (1993) solved on the hollow fibre (HF) membrane module geometry of Busch et al.
57 (2007). These additional interactions between the bioreactor and the membrane
58 described in our integrated MBR model will allow a better process integration and
59 more realistic simulation results, thus increasing our ability to optimise the process,
60 energy, and develop better control strategies. Some of the results from this model
61 have already been, albeit briefly, described in an earlier conference publication of
62 Janus and Ulanicki (2014). The purpose of this earlier publication was to briefly
63 outline the benefits of model integration while the current paper describes in detail
64 the simulation results of the benchmark model and compares these results with the
65 earlier simulation benchmark models of Copp (2002) and Maere et al. (2011).

66 This paper starts with a formulation of modelling hypotheses and then proposes

67 a model structure built around them. Next, this integrated model is simulated on a
68 plant layout of the MBR benchmark simulation model (BSM-MBR) by Maere et al.
69 (2011), albeit, as shall be described later, with minor changes to the tank volumes.
70 Simulations are performed with inputs and simulation scenarios defined in Copp
71 (2002) and later adopted in Maere et al. (2011). Hence, this paper presents a new
72 MBR benchmark simulation model which extends the BSM-MBR with biopolymer
73 kinetics and fouling. It shall be later referred to as integrated bioreactor and mem-
74 brane fouling MBR model (IBMF-MBR) as it integrates the biological process with
75 membrane fouling by providing mechanisms of bi-directional interaction between
76 these two parts of an MBR. In order to show the similarities and the differences
77 between both benchmarks the simulation results obtained from IBMF-MBR and
78 BSM-MBR are compared and presented in a tabular form adhering to the conven-
79 tion adopted in Copp (2002) and Maere et al. (2011). To quantify and compare the
80 level of fouling accumulated over the simulation period of each benchmark scenario
81 the paper also introduces a new measure of fouling which is applied separately to
82 irreversible and reversible fouling. The irreversible fouling index FI_i describes the
83 amount of irreversible resistance, R_i , accumulated in the last 7 days of dynamic
84 simulation divided by the net volume of permeate discharged from the plant V_{eff}^{net} ,
85 i.e. the volume of permeate produced minus the volume of permeate used for back-
86 flushing. The reversible fouling index FI_r describes the average amount of reversible
87 resistance R_r accumulated in one filtration cycle over the last 7 days of dynamic sim-
88 ulation divided by V_{eff}^{net} . Both fouling indices can be used as yet another parameter
89 for the comparison of operating strategies in a benchmark model as well as for the
90 calculation of operational expenditures (OPEX) associated with fouling mitigation.
91 Finally, by demonstrating the outputs of the integrated benchmark model under var-
92 ious control strategies, the paper presents how the model can be used to optimise

93 the process and minimise the energy consumption.

94 **2. Modelling hypotheses and model structure**

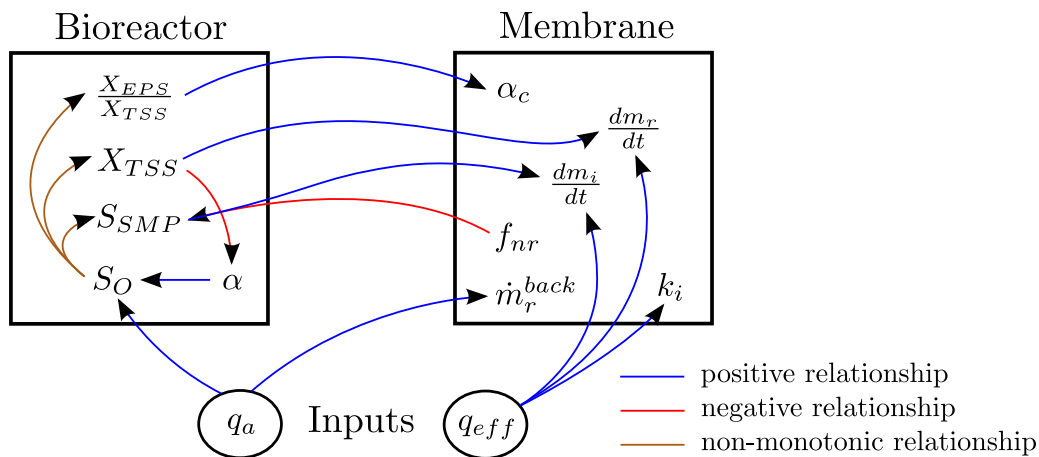


Figure 1: Graphical representation of the links existing between the biological and the filtration part of the IBMF-MBR model.

95 As earlier explained in Janus and Ulanicki (2015c) the bioreactor is modelled with
 96 the combined EPS and SMP production ASM1-based model (CES-ASM1) while the
 97 membrane is described with a behavioural fouling model based on the modelling
 98 concept of Liang et al. (2006) who divided fouling into two processes based on their
 99 intrinsic time constants and reversibility. These two processes, namely irreversible
 100 and reversible fouling collectively contribute to the loss of membrane permeability
 101 over time. As CES-ASM1 is similar in structure to ASM1 which forms the back-
 102 bone of BSM1 and BSM-MBR, it is easy to compare the simulation results from
 103 IBMF-MBR with the results from the two above earlier simulation benchmark mod-
 104 els. Behavioural fouling model was chosen over other more complicated fouling mod-
 105 els available in the literature for its simplicity and ease of calibration. Both parts
 106 of the system and the links between them are graphically presented in Figure 1. A

107 detailed description of CES-ASM1 and the fouling model can be found in Janus and
108 Ulanicki (2015a) and Janus and Ulanicki (2015b) respectively.

109 CES-ASM1 predicts the concentrations of various constituents of activated sludge,
110 including bound biopolymers EPS and soluble biopolymers SMP. The EPS fraction
111 in activated sludge $\left(\frac{X_{EPS}}{X_{TSS}}\right)$ determines the value of specific cake resistance α_c ac-
112 cording to the modified model of Ahmed et al. (2007). Total solids concentration
113 (X_{TSS}) affects the reversible fouling rate $\left(\frac{dm_r}{dt}\right)$ whilst SMP in the bulk liquid affects
114 the rate of irreversible fouling $\left(\frac{dm_i}{dt}\right)$. SMP concentration in the bioreactor (S_{SMP})
115 depends on SMP production and utilisation kinetics in the bioreactor as well as the
116 retentive properties of the membrane. Membrane retention is modelled here with
117 parameter f_{nr} representing the fraction of SMP ending up in the permeate.

118 The rate of cake back-transport from membrane surface depends on coarse-bubble
119 aeration rate q_a . The air bubbles which move upward in the vicinity of the membrane
120 create shear stresses τ_w on the membrane surface leading to detachment of deposited
121 solid particles and preventing new particles to come into contact with the membrane.
122 The relationship between q_a and τ_w is represented with a quadratic polynomial ob-
123 tained through nonlinear regression on the data points obtained from a solution of a
124 two-phase slug flow model (Janus and Ulanicki, 2015c). The shear stresses are linked
125 to the cake detachment constant k_r accordingly to the model of Nagaoka et al. (1998).
126 Moreover, coarse bubble aeration leads to an increase in oxygen concentration (S_O)
127 in the membrane tank as a result of mass transfer of oxygen from air bubbles to the
128 bulk liquid. The oxygen mass transfer coefficient α is hindered by suspended solids
129 and is described with an empirical relationship $\alpha = e^{-\omega X_{TSS}}$ in which α decreases
130 exponentially with X_{TSS} .

131 The rates of reversible $\left(\frac{dm_r}{dt}\right)$ and irreversible $\left(\frac{dm_i}{dt}\right)$ fouling depend on the per-
132 meate flux J and hence the permeate flow rate q_{eff} . Whilst $\frac{dm_r}{dt} \propto q_{eff}$, $\frac{dm_i}{dt}$ is

133 in a non-linear relationship with q_{eff} because the proportionality constant k_i in the
134 irreversible fouling equation is itself dependent on permeate flux J and hence the
135 permeate flow rate (Janus and Ulanicki, 2015b). The form of this equation, particu-
136 larly its nonlinearity with respect to flux and linearity with respect to S_{SMP} , has a
137 direct impact on the final simulation results with the IBMF-MBR model which, as
138 shall be explained later, show that irreversible fouling is more sensitive to flux than
139 to bulk liquid SMP concentrations. The membrane is assumed to be ‘backflushable’,
140 hence the operation of the membrane is assumed to be comprised of filtration and
141 backflush cycles, whilst idle/relaxation cycles are not modelled. The block diagram
142 of the MBR model structure showing the links between the three separate interacting
143 subsystems, i.e. the Bioreactor (Subsystem 1), the Membrane (Subsystem 2) and
144 the Interface (Subsystem 3) can be found in Janus and Ulanicki (2015c) or an earlier
145 publication of Janus and Ulanicki (2014).

146 **3. Plant model description**

147 *3.1. Process and instrumentation diagram*

148 The plant layout, simulation scenarios, inputs and control schemes used in the
149 simulations are based on the BSM-MBR simulation benchmark of Maere et al. (2011).
150 However, compared to BSM-MBR, the airflow rates, sludge wastage rates and tank
151 volumes in IBMF-MBR were altered in order to take into consideration the differ-
152 ences in ASM1 and CES-ASM1 model kinetics. The individual reactor volumes are
153 respectively 1,800 m³ for anoxic tanks $V_{ax,1}$ and $V_{ax,2}$ and 1,300 m³ for aerobic tanks
154 $V_{ox,1}$, $V_{ox,2}$ and the membrane tank V_{mem} . Recirculation, sludge wastage and airflow
155 rates in open-loop simulations and controller setpoints and gains in closed-loop sce-
156 narios are provided further down in Section 3.2. The IBMF-MBR simulation model

157 also features a new nitrate control loop, as shown in the piping and instrumentation
 158 diagram (P&ID) in Figure 2.

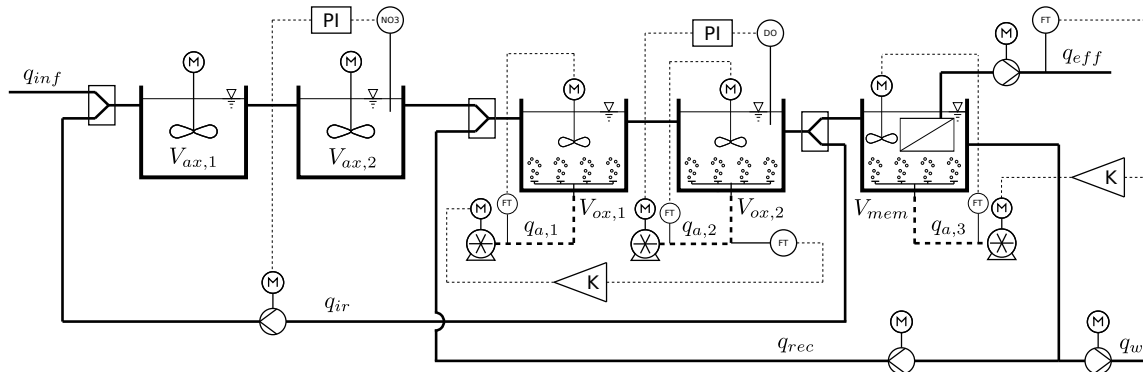


Figure 2: Process and instrumentation diagram of the IBMF-MBR simulation benchmark scheme.

159 Air supply to the first aerobic tank, the second aerobic tank and the membrane
 160 tank is facilitated by three separate air blowers. Mixing of anoxic tanks is carried
 161 out with mechanical mixers operating constantly with an assumed energy input of
 162 0.008 kW m^{-3} . Both aerobic tanks and the membrane tank are assumed to be fully
 163 mixed if the aeration rate per m^2 of ground surface area in each tank is higher than
 164 $2.2 \text{ Nm}^3 \text{ h}^{-1} \text{ m}^{-2}$. In times when the actual unit aeration rate in the tank is lower
 165 than $2.2 \text{ Nm}^3 \text{ h}^{-1} \text{ m}^{-2}$, the tank is assumed to be instead mixed mechanically with
 166 the same unit energy demand as the anoxic tanks.

167 IBMF-MBR simulations are carried out in the same way as described in Copp
 168 (2002), i.e. initially under constant flow-averaged inputs for a period of, in our
 169 case, 300 days which was found sufficient to reach steady-state for all states in the
 170 system, then under time-varying inputs with three different 14-day weather sce-
 171 narios: dry weather, rain event, and storm event. Each simulation sequence, i.e.
 172 steady-state \rightarrow dry weather \rightarrow dry weather, steady-state \rightarrow dry weather \rightarrow rain event,
 173 and steady-state \rightarrow dry weather \rightarrow storm event is performed at four levels of pro-

174 cess control: (a) open-loop, (b) closed-loop with dissolved oxygen (DO) control,
175 (c) closed-loop with DO and nitrate nitrogen (NO_3^- -N) control, and (d) closed-loop
176 with DO, NO_3^- -N and specific aeration demand per membrane area (SAD_m) con-
177 trol. All simulations have been performed in SIMBA[®] v.5.0 software running on
178 MATLAB[®] R2010.

179 The three closed-loop control strategies described above are not meant to indi-
180 cate the most adequate strategies for this particular system, but serve the purpose
181 of demonstrating how different control strategies can be compared using benchmark
182 models such as BSM-MBR or IBMF-MBR. The IBMF-MBR benchmark model de-
183 veloped here adopts the same control strategies as BSM-MBR in order to demonstrate
184 the similarities and the differences between both models under different operating
185 conditions. In all simulations it is assumed that all actuators and sensors are ideal,
186 i.e. without any noise and delay.

187 3.2. Process control scenarios

188 In all four process control variants the return activated sludge flow rate, q_{rec} , is
189 set to a constant value of $55,338 \text{ m}^3 \text{ d}^{-1}$ which is equivalent to 3 times the rate of
190 dry weather flow (DWF). Sludge wastage rate, q_w , is assigned a constant value of
191 $160 \text{ m}^3 \text{ d}^{-1}$ which guarantees a steady-state MLSS concentration in the membrane
192 tank of $\sim 10 \text{ kg m}^{-3}$. q_w in IBMF-MBR is lower from the $200 \text{ m}^3 \text{ d}^{-1}$ setpoint
193 used in BSM-MBR due to alteration of the flow of organic substrates in CES-ASM1
194 as a side-effect of addition of biopolymer kinetics. This resulted in $\sim 18.5\%$ lower
195 predicted sludge yields in CES-ASM1 compared to ASM1 as shall be later explained
196 in Sections 5.1 and 5.2.

197 In the open-loop simulation, internal recirculation, q_{ir} , is kept at a constant
198 rate of $55,338 \text{ m}^3 \text{ d}^{-1}$ equal to the return activated sludge flow rate q_{rec} . Fine-

199 bubble aeration flow rates, $q_{a,1}$, and $q_{a,2}$, are maintained at $3,440 \text{ Nm}^3 \text{ d}^{-1}$ and
 200 $3,360 \text{ Nm}^3 \text{ d}^{-1}$ respectively. Total fine bubble aeration flow rate is thus equal to
 201 $6,800 \text{ Nm}^3 \text{ d}^{-1}$, which is $300 \text{ Nm}^3 \text{ d}^{-1}$ higher than in the BSM-MBR benchmark
 202 model. Although the difference in total airflow is minimal, the flow split between both
 203 aeration tanks is very different. Whilst the airflow in BSM-MBR was split between
 204 $V_{ox,1}$ and $V_{ox,2}$ at $1.89 : 1$ ratio, the flow split in CES-ASM1 is near $1 : 1$ in open-loop
 205 simulations and has been assigned a value of $1.3 : 1$ in closed-loop simulations with
 206 DO control. Coarse-bubble aeration flow rate, $q_{a,3}$, is kept at $20,025 \text{ Nm}^3 \text{ d}^{-1}$ which
 207 corresponds to SAD_m of $0.3 \text{ Nm}^3 \text{ h}^{-1} \text{ m}^{-2}$ based on the total membrane area, A_{mem} ,
 208 of $66,750 \text{ m}^2$. A_{mem} in BSM-MBR is slightly smaller than $71,500 \text{ m}^2$ used in Maere
 209 et al. (2011) due to reduction of the membrane tank volume, V_{mem} , from $1,500 \text{ m}^3$
 210 to $1,300 \text{ m}^3$.

211 In the closed-loop simulation scenario with DO control DO concentration in the
 212 second aerobic tank is kept at $1.5 \text{ mgO}_2 \text{ L}^{-1}$ by a proportional integral (PI) controller
 213 set to adjust $q_{a,2}$ based on the signal received from the DO probe positioned in the
 214 same tank. $q_{a,1}$ is adjusted in proportion to $q_{a,2}$ at a $1.3 : 1$ ratio. The PI controller
 215 has been assigned the same gains as in the BSM-MBR benchmark model of Maere
 216 et al. (2011), i.e. $K_p = 500 \text{ Nm}^3 \text{ h}^{-1}$ per $\text{mgO}_2 \text{ L}^{-1}$ and $t_I = 0.002 \text{ d}$.

217 In the closed-loop simulation scenario with DO and nitrate control, denitrifica-
 218 tion is additionally controlled via a PI controller which is set to keep the nitrate
 219 concentration in the second anoxic tank at a constant setpoint of $1.0 \text{ mgNO}_3^- \text{ L}^{-1}$ by
 220 adjusting the nitrate recycle rate q_{ir} . The controller receives a $\text{NO}_3^- \text{-N}$ concentration
 221 signal from the nitrate probe located in the second anoxic tank and has a propor-
 222 tional gain $K_p = 15,000 \text{ m}^3 \text{ d}^{-1}$ per $\text{mgNO}_3^- \text{ L}^{-1}$ and integral time $t_I = 0.05 \text{ d}$. q_{ir}
 223 is capped at $92,230 \text{ m}^3 \text{ d}^{-1}$, i.e. $5 \times \text{DWF}$.

224 In the closed-loop simulation scenario with DO, nitrate, and SAD_m control,

225 coarse-bubble aeration in the membrane tank is additionally adjusted in proportion
 226 to the permeate flux rate J , as described in Maere et al. (2011). The P controller
 227 receives the permeate flow rate signal from the flow transmitter positioned on the
 228 discharge side of the permeate suction pump, calculates the value of the permeate
 229 flux and adjusts the SAD_m rate in proportion to J . The controller's proportional
 230 gain K_p is equal $0.015 \text{ Nm}^3 \text{ h}^{-1} \text{ m}^{-2}$ per Lmh. SAD_m is capped from the top and
 231 the bottom at $SAD_m^{\min} = 0.15 \text{ Nm}^3 \text{ h}^{-1} \text{ m}^{-2}$ and $SAD_m^{\max} = 0.30 \text{ Nm}^3 \text{ h}^{-1} \text{ m}^{-2}$ which
 232 correspond to permeate fluxes of 10 Lmh and 20 Lmh, respectively.

233 3.3. Pumping and aeration

234 The aeration model implemented in IBMF-MBR and its parameters are identical
 235 to the aeration model of Maere et al. (2011) implemented in BSM-MBR, however the
 236 energy consumption for pumping is calculated differently to both BSM-MBR and the
 237 COST/IWA benchmark simulation model No.1 (BSM1). Instead of using pumping
 238 energy factors representing energy consumption per m^3 of pumped liquid, as used
 239 in the earlier benchmarks, pumping energy is calculated with Equation 1 describing
 240 the amount of work required to raise a given volume of liquid to a required height.

$$PE = \frac{60 \rho_w g}{1000 t_{simu}} \sum_{i=1}^{i=5} \frac{h_g^i + h_l^i}{\eta_i} \int_{t_0}^{t_0+t_{simu}} q_i(t) dt \quad (1)$$

241 where $i = 1$ for waste activated sludge (WAS) flow, $i = 2$ for internal recycle flow,
 242 $i = 3$ for recirculated activated sludge (RAS) flow, $i = 4$ for pumped permeate flow
 243 and $i = 5$ for backflush flow. The parameters characterising each pumped stream
 244 are provided in Table 3.

Table 3: Values of the parameters used for pumping energy calculations with Equation 1 - Reprinted from Janus and Ulanicki (2014).

Parameter	Symbol	Unit	Flow				
			q_w	q_{int}	q_r	q_{eff}	q_b
Geometric height	h_g	m	7.0	0.50	0.50	calc	calc
Sum of losses	h_l	m	2.17	1.42	1.42	0.5	0.5
Efficiency	η	–	0.5	0.7	0.7	0.7	0.7

245 3.4. Fouling indices

246 In order to compare the operating strategies in our benchmark model with respect
 247 to fouling we introduced two new measures of fouling which describe the increase
 248 of irreversible and reversible membrane resistance per net unit volume of permeate
 249 within a given time period. The irreversible fouling index FI_i describes the amount
 250 of irreversible resistance R_i accumulated in the last 7 days of dynamic simulation
 251 divided by the net volume of permeate discharged from the plant (see Equation 2).

$$FI_i = \frac{R_i^{14d} - R_i^{7d}}{1000 \int_{7d}^{14d} (q_{eff} - q_b) dt} = \frac{\Delta R_i}{1000 V_{eff}^{net}} \quad (2)$$

252 Here, V_{eff}^{net} denotes the volume of permeate produced minus the volume of permeate
 253 used for backflushing. The reversible fouling index FI_r describes the average amount
 254 of reversible resistance R_r accumulated in one filtration cycle over the last 7 days of
 255 dynamic simulation divided by V_{eff}^{net} (see Equation 3).

$$FI_r = \frac{\sum_{j=1}^N \left(R_r^{7d+(t_f+t_b)(j-1)+t_f} - R_r^{7d+(t_f+t_b)(j-1)} \right)}{1000 N \int_{7d}^{14d} (q_{eff} - q_b) dt} = \frac{\sum_{j=1}^N \Delta R_r^j}{1000 N V_{eff}^{net}} \quad (3)$$

256 Both fouling indices can be used to calculate the fouling cost indices FCI_i and

257 FCI_r describing the operational expenditures associated with mitigation of, respec-
 258 tively, irreversible fouling (Equation 4) and reversible fouling (Equation 5).

$$FCI_i = FI_i \cdot c_i + \frac{PE_{q_{eff}}^i \cdot 7 \text{ d}}{V_{eff}^{net}} p_{kWh} \quad (4)$$

$$FCI_r = \frac{\left(PE_{q_{eff}}^r + PE_{q_{back}} + AE_{membrane} \right) \cdot 7 \text{ d}}{V_{eff}^{net}} p_{kWh} \quad (5)$$

259 where c_i , (€ m) denotes the financial effort required to recover 1m^{-1} of irreversible
 260 membrane resistance, $PE_{q_{eff}}^i$ and $PE_{q_{eff}}^r$ (kWh d^{-1}) represent daily pumping energy
 261 requirements for permeate pumping incurred due to, respectively, irreversible and
 262 reversible fouling, and p_{kWh} (€ kWh^{-1}) is the unit price of electrical energy. Since
 263 the financial costs are not compared in our benchmark model nor in BSM-MBR,
 264 FCI_i and FCI_r calculations are not included in this paper, however the equations
 265 are still provided for further reference and for future applications of the IBMF-MBR
 266 benchmark model.

267 3.5. Kinetic parameters

268 The kinetic and stoichiometric parameters of the biological model are assigned
 269 the default values provided in Janus and Ulanicki (2015a) except 3 biopolymer ki-
 270 netic and stoichiometric parameters: $f_{EPS,h}$, $f_{EPS,dh}$, and μ_{BAP} . $f_{EPS,h}$ and $f_{EPS,dh}$
 271 were decreased, respectively from 0.18 to 0.10 $\text{g}X_{EPS} \text{g}^{-1} X_H$ and from 0.045 to 0.025
 272 $\text{g}X_{EPS} \text{g}^{-1} X_H$ to reduce the production of EPS and bring the bulk liquid EPS con-
 273 centrations closer to the values reported by Ahmed et al. (2007). μ_{BAP} was increased
 274 from 0.05 d^{-1} to 0.15 d^{-1} in order to lessen the dominance of biomass associated
 275 products (BAP) production over utilisation associated products (UAP) production.
 276 Simulations were performed at the same temperatures as used in BSM-MBR, i.e.

277 wastewater temperature T of 15°C and air temperature T_{air} of 20°C.

278 3.6. Membrane filtration

279 The membrane module is modelled with a hollow fibre module geometry of Busch
 280 et al. (2007) and with geometric dimensions provided in Janus and Ulanicki (2015c).
 281 The module is assumed to cover 100% of the tank’s floor plan area. The resulting
 282 membrane packing density is equal to 49.4 m² m⁻³ which is slightly higher from the
 283 packing density of 46.2 m² m⁻³ featured in Maere et al. (2011).

284 The membrane is operating with 10-minute filtration periods followed by a 1-
 285 minute backflush. The module is aerated during filtration, however the aeration is
 286 switched off during backflush periods. Other membrane and fouling-specific param-
 287 eters of the membrane filtration model used in the simulations are listed in Table 4.

Table 4: Parameters of the membrane filtration and fouling model applied in IBMF-MBR.

Symbol	Value	Unit	Description
R_m	3.0×10^{12}	m ⁻¹	Clean membrane resistance
ΔP_{crit}	30	kPa	Threshold pressure below which no cake compression occurs
n_α	0.25	–	Dimensionless cake compressibility factor
b	6.8×10^{-2}	–	Dimensionless proportionality coefficient
k_i	1.0×10^{11}	m kg ⁻¹	Irreversible fouling strength factor
γ_m	1500	d ⁻¹ Pa ⁻¹	Proportionality constant
λ_m	2.0×10^{-6}	–	Static friction coefficient

288 4. Model inputs

289 Input files from BSM1 and BSM-MBR simulation benchmarks have been modified
 290 to take into account three new state variables, i.e. X_{EPS} , S_{UAP} , and S_{BAP} featured in
 291 IBMF-MBR. It is assumed that the influent wastewater does not contain any UAP,
 292 hence $S_{UAP} = 0$, whilst S_{BAP} makes up 70% of the influent soluble inert substrates,
 293 S_I , in BSM1 and BSM-MBR benchmarks. Influent X_{EPS} is assumed to constitute

Table 5: Flow proportionally averaged influent composition for the IBMF-MBR simulation model.

Compound	Unit	Dry weather	Rain weather	Storm weather
S_I	$\text{gO}_2 \text{ m}^{-3}$	9.00	7.78	8.41
S_S	$\text{gO}_2 \text{ m}^{-3}$	69.50	60.13	64.93
X_I	$\text{gO}_2 \text{ m}^{-3}$	51.20	44.30	51.92
X_S	$\text{gO}_2 \text{ m}^{-3}$	202.32	175.05	193.32
X_H	$\text{gO}_2 \text{ m}^{-3}$	26.76	23.15	25.89
X_A	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00
X_{EPS}	$\text{gO}_2 \text{ m}^{-3}$	1.41	1.22	1.36
S_{UAP}	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00
S_{BAP}	$\text{gO}_2 \text{ m}^{-3}$	21.00	18.17	19.62
X_P	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00
S_O	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00
S_{NO}	gN m^{-3}	0.00	0.00	0.00
S_{NH}	gN m^{-3}	31.56	27.30	29.48
S_{ND}	gN m^{-3}	6.95	6.01	6.49
X_{ND}	gN m^{-3}	9.37	8.10	9.10
S_{ALK}	$\text{molHCO}_3^- \text{ m}^{-3}$	7.00	7.00	7.00
q_{ave}	$\text{m}^3 \text{ d}^{-1}$	18446.33	21319.75	19744.72
q_{min}	$\text{m}^3 \text{ d}^{-1}$	10000.00	10000.00	10000.00
q_{max}	$\text{m}^3 \text{ d}^{-1}$	32180.00	52126.00	60000.00

310 model for all three weather scenarios are presented in Table 5. These concentra-
311 tions along with the average flows were used as inputs to the benchmark model to
312 obtain a steady-state condition and produce steady-state outputs presented in Sec-
313 tion 5.1. In reality, all three weather scenarios exhibit a diurnal flow and load pattern
314 as a result of changes in human activity over the course of the day. Additionally,
315 rain and storm events include, respectively, diluting effects of rain water on wastew-
316 ater constituents and increase of particulate wastewater constituents during the first
317 storm event as a results of sediment washout from the sewer. Extensive description
318 of these time-series data can be found in Copp (2002). These time-series data, orig-
319 inally used for the ASM1 model have been converted to suit the CES-ASM1 model
320 using Equation 6.

321 **5. Simulation results**

322 *5.1. Steady-state results*

Table 6: Steady state concentrations in all reactor zones, membrane permeate and retentate stream from dry-weather open-loop simulations.

	Inf	R.1	R.2	R.3	R.4	R.5	Perm	Ret
S_I	9.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00
S_S	69.50	4.53	4.24	2.91	2.51	1.90	1.90	1.90
X_I	51.20	3342.24	3342.24	4439.27	4439.27	5901.99	0.00	5901.99
X_S	202.32	64.46	60.04	34.81	27.33	24.32	0.00	24.32
X_H	26.76	1298.25	1292.43	1716.50	1716.94	2277.89	0.00	2277.89
X_A	0.00	119.73	119.29	159.87	160.18	212.86	0.00	212.86
X_{EPS}	1.41	550.59	550.32	732.31	732.56	974.03	0.00	974.03
S_{UAP}	0.00	10.31	11.10	11.65	11.59	11.97	5.99	11.97
S_{BAP}	21.00	25.81	26.54	27.64	27.29	29.92	14.96	29.92
X_P	0.00	2161.24	2162.84	2878.66	2879.53	3831.03	0.00	3831.03
S_O	0.00	0.01	0.00	1.34	1.81	7.08	7.08	7.08
S_{NO}	0.00	3.44	0.60	8.37	10.487	12.43	12.43	12.43
S_{NH}	31.56	9.50	10.23	3.18	1.248	0.23	0.23	0.23
S_{ND}	6.95	1.15	0.77	0.98	0.990	0.88	0.88	0.88
X_{ND}	9.37	4.04	4.13	2.63	2.157	2.05	0.00	2.05
S_{ALK}	7.00	5.18	5.43	4.38	4.086	3.87	3.87	3.87
X_{TSS}	211.27	5652.38	5645.37	7471.06	7466.85	9916.58	0.000	9916.58
Q	18446.33	73784.33	73784.33	129122.33	129122.33	129122.33	18286.33	55498.00

323 Steady-state simulation results from IBMF-MBR model in open-loop configura-
324 tion and closed-loop configuration with DO, NO_3^- -N and SAD_m control are listed
325 in Tables 6 and 7, where Inf denotes the influent stream, R.1, R.2, R.3, R.4, and
326 R.5 denote the individual bioreactors, Perm denotes the permeate stream and Ret
327 is the retentate stream. The effluent quality in open-loop and closed-loop simula-
328 tions is similar but, as shall be shown later, the treatment costs are different. SMP
329 concentration in the membrane tank is found to be around $42 \text{ mgO}_2 \text{ L}^{-1}$ while the
330 EPS/MLSS ratio is equal to $\sim 98.2 \text{ mgO}_2 \text{ g}^{-1} \text{ TSS}$. The plant produces a relatively
331 low steady state nitrate concentration S_{NO} of about 12 mgN L^{-1} and a very low

Table 7: Steady state concentrations in all reactor zones, membrane permeate and retentate stream from dry-weather closed-loop simulations with DO, SAD_m and NO₃⁻-N control.

	Inf	R.1	R.2	R.3	R.4	R.5	Perm	Ret
S_I	9.00	9.00	9.00	9.00	9.00	9.00	9.00	9.00
S_S	69.50	4.35	3.34	2.90	2.55	1.94	1.94	1.9
X_I	51.20	3466.97	3466.97	4439.76	4439.76	5902.64	0.00	5902.64
X_S	202.32	61.27	58.01	35.09	28.01	24.78	0.00	24.78
X_{BH}	26.76	1329.57	1324.45	1696.30	1696.77	2251.41	0.00	2251.41
X_{BA}	0.00	122.84	122.44	158.02	158.30	210.37	0.00	210.37
X_{EPS}	1.41	565.27	565.04	724.74	724.98	963.97	0.00	963.97
S_{UAP}	0.00	10.22	10.71	11.35	11.35	11.83	5.91	11.83
S_{BAP}	21.00	25.61	26.08	27.11	26.82	29.46	14.73	29.46
X_P	0.00	2248.04	2249.49	2885.59	2886.39	3840.12	0.000	3840.12
S_O	0.00	0.01	0.00	1.69	1.50	4.49	4.49	4.49
S_{NO}	0.00	3.661	1.000	7.900	9.77	11.670	11.670	11.67
S_{NH}	31.56	8.616	9.258	3.018	1.29	0.240	0.240	0.24
S_{ND}	6.95	1.129	0.762	0.985	1.00	0.889	0.889	0.89
X_{ND}	9.37	3.886	4.008	2.648	2.20	2.081	0.000	2.08
S_{ALK}	7.00	5.100	5.336	4.397	4.14	3.930	3.930	3.93
X_{TSS}	211.27	5845.47	5839.80	7454.62	7450.66	9894.97	0.00	9894.97
Q	18446.33	83217.50	83217.50	138555.50	138555.50	129122.33	18286.33	55498.00

332 ammoniacal N concentration of ~ 0.25 mgN L⁻¹. The biomass is not uniformly dis-
333 tributed in the bioreactor but instead exhibits an upward gradient with lower MLSS
334 concentrations of around 6 kgSS m⁻³ in the anoxic tanks and higher MLSS concen-
335 trations in the aerobic tanks and the membrane tank of, respectively ~ 7.5 kgSS m⁻³
336 and ~ 10 kgSS m⁻³. What this MLSS concentration gradient along the bioreactor
337 implies is that despite allowing a large volumetric anoxic fraction $V_{ax}/V_{tot} = 0.50$ the
338 anoxic mass fraction in our plant is in fact very low and equals $M_{ax}/M_{tot} = 0.124$.
339 Hence, it seems, that although membrane technology allows us to reduce aerobic
340 volume, the benefits with regards to N and, similarly, biological phosphorus (P) re-
341 moval are less obvious, at least in pre-denitrification systems with such configuration
342 of tanks and recirculation streams as used in our benchmark model.

343 Effluent soluble concentrations produced from IBMF-MBR and BSM-MBR are

Table 8: Comparison of steady-state effluent soluble concentrations between IBMF-MBR and BSM-MBR.

Output	Unit	BSM-MBR		IBMF-MBR	
		Open-loop	Closed-loop ^{*)}	Open-loop	Closed-loop ^{*)}
S_I	gO ₂ m ⁻³	30.00	30.00	9.00	9.00
S_S	gO ₂ m ⁻³	0.68	0.69	1.90	1.94
S_{UAP}	gO ₂ m ⁻³	–	–	5.99	5.91
S_{BAP}	gO ₂ m ⁻³	–	–	14.96	14.73
S_O	gO ₂ m ⁻³	7.69	5.19	7.08	4.49
S_{NO}	gN m ⁻³	12.03	11.71	12.43	11.67
S_{NH}	gN m ⁻³	0.076	0.080	0.23	0.24
S_{ND}	gN m ⁻³	0.59	0.59	0.88	0.89
S_{ALK}	molHCO ₃ ⁻ m ⁻³	3.89	3.92	3.87	3.93

^{*)} DO, NO₃⁻-N, and SAD_m control

344 compared in Table 8. The results show that the outputs of both models are very
 345 similar with minor differences in S_S , S_{NO} and S_{NH} . Particulate components are
 346 omitted in the table as they all have zero concentrations.

347 5.2. Dynamic results

348 Dynamic simulations were performed with BSM-MBR and IBMF-MBR models
 349 in dry-, rain- and storm-weather under four levels of process control: (a) open-loop,
 350 (b) closed-loop with DO control, (c) closed-loop with DO and NO₃⁻-N control and
 351 (d) closed-loop with DO, NO₃⁻-N and SAD_m control. Alike in BSM1 and BSM-MBR
 352 benchmarks the results constitute the last 7 days of outputs.

353 The flow-proportionally averaged effluent concentrations from open-loop and closed
 354 loop simulations under all three weather scenarios are listed, respectively in Tables 9
 355 and 10. Alike in steady-state simulations, closed loop dynamic simulation refers to
 356 the simulation scenario with DO, SAD_m and NO₃⁻-N control. The results show that
 357 IBMF-MBR predicts, on average, ~ 1 mgN L⁻¹ higher effluent total nitrogen (TN)

358 than the ASM1-based BSM-MBR due to slightly higher produced effluent NO_3^- -N
359 and ammoniacal nitrogen (NH_4^+ -N) concentrations. Effluent total Kjeldahl nitro-
360 gen (TKN) produced by IBMF-MBR is again about 1.5 mgN L^{-1} higher than those
361 in the BSM-MBR benchmark model as a result of higher NH_4^+ -N and soluble or-
362 ganic N concentrations. The rest of the effluent state and composite variables in
363 both models have similar values except soluble inert organics (S_I) which are lower
364 in IBMF-MBR due to lower influent S_I concentrations which had been reduced in
365 order to accommodate three new biopolymer state variables in the influent (input)
366 files.

367 The selected effluent concentrations from the last 7 days of dynamic simulation
368 under different weather conditions and process control variants are presented in Fig-
369 ures 3-6. Figure 3 indicates that, in response to the changes in the influent flow
370 rate, MLSS concentrations in the individual reactors fluctuate significantly as the
371 biomass is shifted downstream under high flows and then returned upstream with
372 RAS flow after the influent flow rate has subsided. This behaviour is observed during
373 the periods when the flow of wastewater is large enough for the flux of suspended
374 solids along the bioreactor to exceed the sludge return rate. As a result, during these
375 periods, the sludge is shifted downstream to the membrane tank. Unfortunately,
376 these increased sludge loading events in the membrane tank usually coincide with
377 high permeate fluxes, ultimately leading to a simultaneous increase in the rates of
378 reversible fouling and irreversible fouling, the latter, as shown in Janus and Ulanicki
379 (2015b), increasing exponentially with the permeate flux.

380 Figure 4 indicates that DO concentration in both aerobic tanks fluctuates sig-
381 nificantly in an open-loop process control scenario. Once automatic DO control is
382 switched on, DO concentration in the second aerobic tank is kept at an almost steady
383 level of $1.5 \text{ mgO}_2 \text{ L}^{-1}$ whilst S_O in the first aerobic tank varies between $1.4 \text{ mgO}_2 \text{ L}^{-1}$

Table 9: Flow proportionally averaged effluent concentrations from dynamic open-loop simulations with BSM-MBR and IBMF-MBR in dry-, rain- and storm-weather.

Variable	Unit	BSM-MBR			IBMF-MBR		
		Dry	Rain	Storm	Dry	Rain	Storm
Effluent state variables							
S_I	$\text{gO}_2 \text{ m}^{-3}$	30.00	22.86	26.30	9.00	6.86	7.89
S_S	$\text{gO}_2 \text{ m}^{-3}$	0.73	0.75	0.76	1.96	1.97	2.02
X_I	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_S	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_H	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_A	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_{EPS}	$\text{gO}_2 \text{ m}^{-3}$	–	–	–	0.00	0.00	0.00
S_{UAP}	$\text{gO}_2 \text{ m}^{-3}$	–	–	–	6.20	6.05	6.30
S_{BAP}	$\text{gO}_2 \text{ m}^{-3}$	–	–	–	15.26	13.68	14.63
X_P	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
S_O	$\text{gO}_2 \text{ m}^{-3}$	6.97	6.32	6.27	5.96	5.35	5.23
S_{NO}	gN m^{-3}	12.21	10.76	11.26	12.74	11.14	11.63
S_{NH}	gN m^{-3}	0.15	0.15	0.17	0.45	0.44	0.54
S_{ND}	gN m^{-3}	0.61	0.62	0.64	0.89	0.89	0.90
X_{ND}	gN m^{-3}	0.00	0.00	0.00	0.00	0.00	0.00
S_{ALK}	$\text{molHCO}_3^- \text{ m}^{-3}$	3.88	4.52	4.23	3.87	4.52	4.23
Effluent composite variables							
TSS	g m^{-3}	0.00	0.00	0.00	0.00	0.00	0.00
TKN	gN m^{-3}	0.76	0.78	0.81	2.25	2.15	2.31
TN	gN m^{-3}	12.98	11.54	12.07	14.99	13.29	13.94
COD	$\text{gO}_2 \text{ m}^{-3}$	30.73	23.61	27.06	32.43	28.55	30.84
BOD ₅	$\text{gO}_2 \text{ m}^{-3}$	0.18	0.19	0.19	0.49	0.49	0.50

384 and $2.1 \text{ mgO}_2 \text{ L}^{-1}$. Introduction of an automatic DO control scheme prevents over-
385 aeration of the bulk liquid in low organic and N loading periods, decreases the effluent
386 NH_4^+ -N concentration, albeit at already very low level, but also leads to an increase
387 in effluent TN concentrations, as can be seen when we cross examine Table 11 and
388 Table 12. This behaviour can be explained as follows. The system has a high aerobic
389 sludge retention time (SRT), hence nitrification rates are ultimately high whilst ni-
390 trogen removal is limited by denitrification. Under open-loop operation, fluctuation
391 of DO concentration in both aerobic tanks leads to a temporary cyclic development

Table 10: Flow proportionally averaged effluent concentrations from dynamic closed-loop simulations (DO, NO_3^- -N and SAD_m control) with BSM-MBR and IBMF-MBR in dry-, rain- and storm-weather.

Variable	Unit	BSM-MBR			IBMF-MBR		
		Dry	Rain	Storm	Dry	Rain	Storm
Effluent state variables							
S_I	$\text{gO}_2 \text{ m}^{-3}$	30.00	22.86	26.30	9.00	6.86	7.89
S_S	$\text{gO}_2 \text{ m}^{-3}$	0.70	0.72	0.73	2.01	2.03	2.07
X_I	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_S	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_H	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_A	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.00	0.00	0.00
X_{EPS}	$\text{gO}_2 \text{ m}^{-3}$	–	–	–	0.00	0.00	0.00
S_{UAP}	$\text{gO}_2 \text{ m}^{-3}$	–	–	–	6.07	5.95	6.09
S_{BAP}	$\text{gO}_2 \text{ m}^{-3}$	–	–	–	14.93	13.48	14.14
X_P	$\text{gO}_2 \text{ m}^{-3}$	0.00	0.00	0.00	0.0	0.00	0.00
S_O	$\text{gO}_2 \text{ m}^{-3}$	5.33	5.65	5.20	3.90	4.29	3.75
S_{NO}	gN m^{-3}	12.19	10.35	11.15	11.89	10.27	10.86
S_{NH}	gN m^{-3}	0.10	0.10	0.10	0.39	0.37	0.40
S_{ND}	gN m^{-3}	0.60	0.61	0.62	0.91	0.91	0.92
X_{ND}	gN m^{-3}	0.00	0.00	0.00	0.00	0.00	0.00
S_{ALK}	$\text{molHCO}_3^- \text{ m}^{-3}$	3.88	4.24	4.23	3.93	4.58	4.28
Effluent composite variables							
TSS	g m^{-3}	0.00	0.00	0.00	0.00	0.00	0.00
TKN	gN m^{-3}	0.70	0.71	0.72	2.19	2.09	2.17
TN	gN m^{-3}	12.89	11.06	11.87	14.08	12.36	13.03
COD	$\text{gO}_2 \text{ m}^{-3}$	30.70	23.58	27.03	32.00	28.32	30.20
BOD_5	$\text{gO}_2 \text{ m}^{-3}$	0.18	0.18	0.18	0.50	0.51	0.52

392 of anoxic conditions inside both aerobic tanks thus increasing denitrification capac-
393 ity in the system. Once DO control is switched on, both aerobic tanks become fully
394 aerobic at all times reducing the overall anoxic mass fraction in the system and hence
395 its denitrification potential. The simulations thus show that although DO control
396 offers benefits, usually in the form of energy savings, it may cause some detrimental
397 effects in the plant such as unwanted reduction of denitrification potential, as in case
398 of our system.

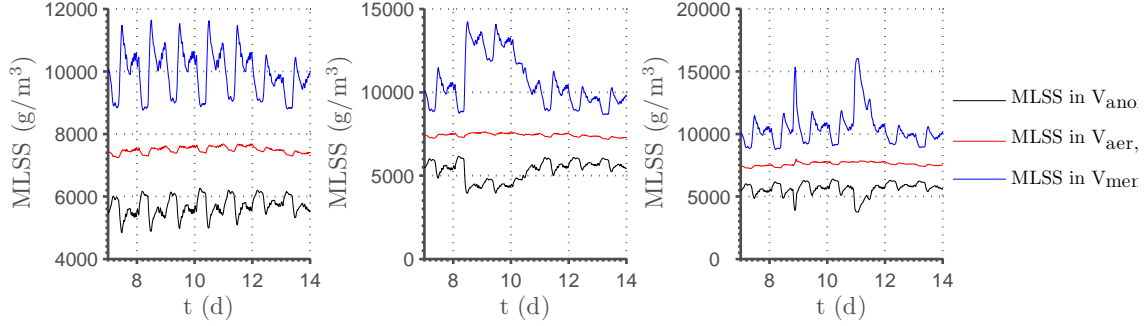


Figure 3: MLSS concentrations in open-loop simulation during (from left to right) dry-, rain- and storm-weather conditions.

399 DO concentration in the membrane tank fluctuates significantly between nearly
 400 $0 \text{ mgO}_2 \text{ L}^{-1}$ to almost its saturation concentration of $\sim 9 \text{ mgO}_2 \text{ L}^{-1}$. At such high
 401 oxygen concentrations, significant amounts of oxygen are being carried over into the
 402 anoxic zones with RAS stream, what in turn impairs denitrification. Once SAD_m
 403 control is switched on DO concentration in the membrane tank is reduced, what in
 404 turn decreases the ingress of the mass of oxygen into anoxic tanks, ultimately leading
 405 to reduction in effluent TN concentrations and the amount of time at violation for
 406 TN. The level of improvement in TN removal with introduction of SAD_m control
 407 can be judged from Table 13. Impact of SAD_m control on N removal is one of the
 408 examples how operation of the membrane might have an impact on the performance
 409 of an entire plant.

410 As already mentioned, effluent $\text{NH}_4^+\text{-N}$ concentration is very low at all times dur-
 411 ing all weather conditions and under all operating scenarios due to high nitrification
 412 capacity of the system. As can be seen in Figure 5 at no point in time effluent $\text{NH}_4^+\text{-N}$
 413 exceeds the effluent $\text{NH}_4^+\text{-N}$ constraint $S_{\text{NH,max}} = 4 \text{ mgN L}^{-1}$ whilst S_{NH} is below
 414 1 mgN L^{-1} at around $\sim 90\%$ of the time.

415 On the other hand, effluent total nitrogen (TN) concentration exceeds the effluent

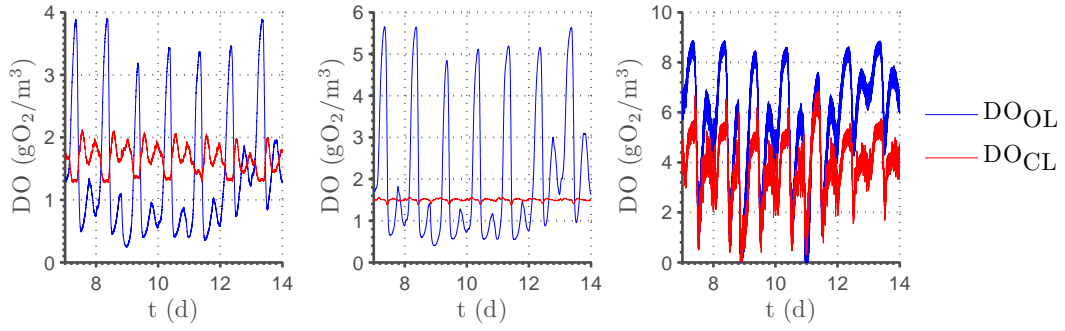


Figure 4: DO concentrations during in the (from left to right) first aerobic tank, second aerobic tank, and membrane tank in dry-weather conditions.

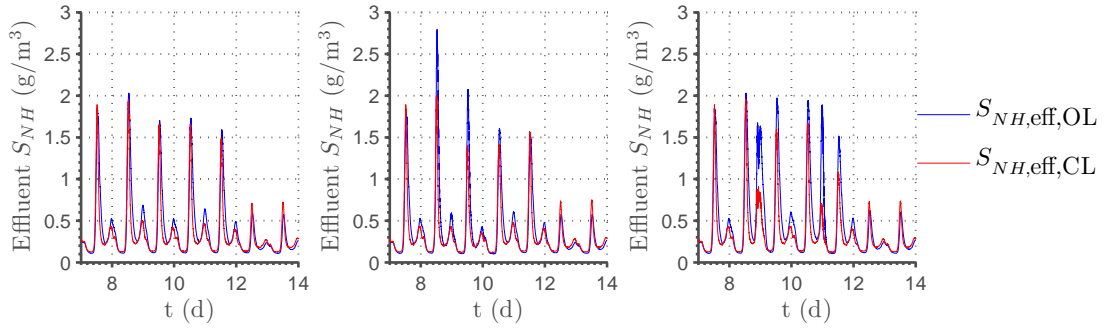


Figure 5: Effluent NH_4^+ -N concentrations during (from left to right) dry-, rain- and storm-weather conditions.

416 TN constraint of 18 mgN L^{-1} at some point of time in each weather scenario and
 417 under each process control variant, as demonstrated in Figure 6. It is clear that
 418 although the plant achieves a complete and stable nitrification, N removal efficiency
 419 is rather low in comparison to nitrification due to slow denitrification rates as a result
 420 of high SRT and ingress of DO mass from the membrane tank to the first anoxic
 421 tank.

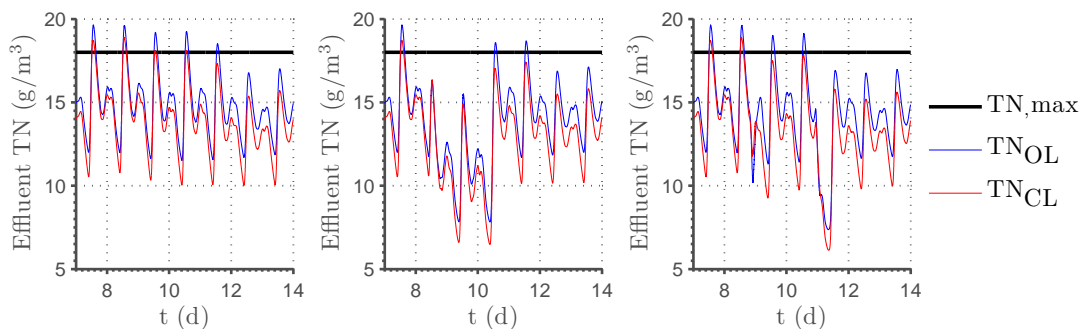


Figure 6: Effluent TN concentrations during (from left to right) dry-, rain- and storm-weather conditions - Reprinted from Janus and Ulanicki (2014).

422 5.3. Effluent quality measures and cost performance

423 Performance of the BSM-MBR benchmark simulation model and IBMF-MBR
 424 in each weather scenario and under each level of process control is summarised in
 425 Tables 11, 12, 13 and 14 which correspond, as mentioned earlier on, to the following
 426 process control scenarios: open-loop, closed-loop with DO control, closed-loop with
 427 DO and SAD_m control, and closed-loop with DO, SAD_m and NO_3^- -N control.

428 IBMF-MBR produces higher effluent TN concentrations than BSM-MBR, as in-
 429 dicated by the 95-th percentile of the total nitrogen concentration (TN_{95}), number
 430 of TN consent limit violations, and % of time under violation. While BSM-MBR
 431 produces no TN violations under the open-loop scenario and under the closed-loop

432 scenario with DO, SAD_m and NO_3^- -N control, IBMF-MBR exceeds the TN constraint
433 under all weather conditions and under all levels of process control despite having a
434 higher anoxic volume fraction. Effluent TN_{95} concentration produced by BSM-MBR
435 is on average about 2 mgN L^{-1} lower than in IBMF-MBR. As already mentioned
436 in Section 2, higher effluent TN concentrations in IBMF-MBR are a direct result of
437 lower denitrification rates in the CES-ASM1 biological model compared to ASM1.
438 In turn, lower denitrification rates are a consequence of an addition of biopolymer
439 kinetics into the biological model which alter the death-regeneration loop in ASM1
440 causing less of readily biodegradable substrates to be produced during bacterial ly-
441 sis. Although not validated numerically, lower denitrification rates in CES-ASM1 are
442 theoretically and practically justified as ASM1 was found to overestimate denitrifi-
443 cation rates in high SRT systems where the death-regeneration model perpetually
444 produces readily biodegradable organic substrates in the bioreactor.

445 IBMF-MBR also generates less waste activated sludge (WAS) leading to $\sim 20\%$
446 lower observed sludge yield (Y_{obs}) and therefore, higher aerobic and total SRT. Whilst
447 energy demand for fine bubble aeration is slightly higher in IBMF-MBR, energy de-
448 mand for air scouring is less due to lower installed membrane area. In consequence,
449 similar overall energy requirements for aeration are predicted in both models. Mix-
450 ing energy requirement is $\sim 24\%$ higher in IBMF-MBR due to larger total anoxic
451 tank volume, whilst energy consumption for pumping is significantly lower due to
452 lower energy requirements for permeate pumping, which were found to be grossly
453 overestimated in BSM-MBR. The calculated transmembrane pressures (TMPs)
454 in IBMF-MBR are ~ 8 times lower from the values predicted in the BSM-MBR
455 model despite rather average, for ultrafiltration (UF) modules, permeabilities of 80–
456 100 Lmh bar^{-1} , due to very conservative permeate fluxes of 8–20 Lmh in dry-weather
457 and up to 32 Lmh and 38 Lmh in rain and storm weather, respectively.

458 5.4. Biopolymer production and membrane fouling

459 Bulk liquid SMP concentrations in the membrane tank under all three weather
 460 scenarios are plotted in Figure 7 which indicates that S_{UAP} and S_{BAP} vary rather
 461 moderately in time in response to diurnal changes in influent load during dry weather
 462 and as a result of dilution effects during rain and storm weather. Since CES-ASM1,
 463 similarly to other published biopolymer ASM models, does not describe the mecha-
 464 nisms of biopolymer production in response to stress conditions such as extreme DO
 465 concentrations, salinity, pH, changes in the type of organic substrates, toxic effects,
 466 shear stress, etc. these system dynamics have not been captured in IBMF-MBR.
 467 Hence, the simulations only show how dynamic changes in influent flow and compo-
 468 sition alter normal Monod-based substrate limiting SMP dynamics and these effects
 469 seem to be rather insignificant to have an observable effect on membrane fouling. It
 470 is likely that a full-scale WWTP might experience additional SMP dynamics under
 471 time varying conditions in response to environmental stress and thus, variations in
 472 bulk liquid SMP concentrations might actually be larger, but this is the topic for
 473 further research.

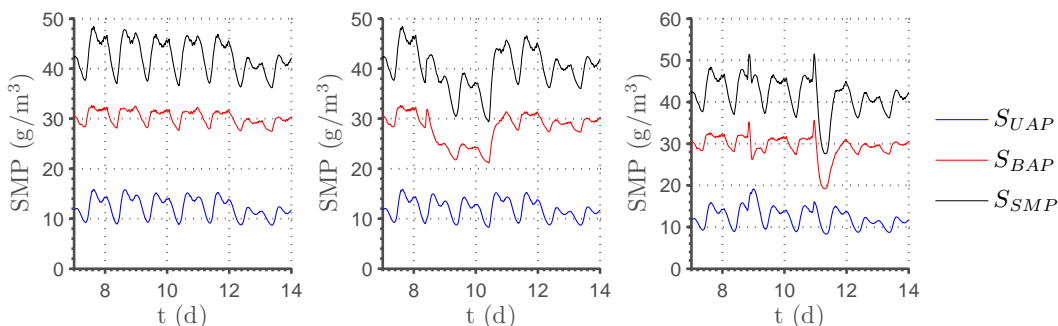


Figure 7: SMP concentrations in the membrane bioreactor during (from left to right) dry-, rain- and storm-weather conditions.

474 Figure 8 shows how irreversible fouling resistance (R_i) and SMP/MLSS ratio

475 in the membrane tank change in time in all three weather scenarios. If we look
 476 at sub-figure (a) we can see that whilst under dry-weather conditions R_i increases
 477 slowly and steadily at the rate of about $1.10 \times 10^{-2} \text{ m kg}^{-1} \text{ h}^{-1}$, under elevated
 478 flow conditions in wet periods the rate of R_i increase is up to four times larger and
 479 around $4.58 \times 10^{-2} \text{ m kg}^{-1} \text{ h}^{-1}$ in rain weather, and up to $\sim 0.21 \text{ m kg}^{-1} \text{ h}^{-1}$ in
 480 storm weather. If we then look at sub-figure (b) presenting the SMP/MLSS ratio
 481 in the membrane tank, we can see that the rate of irreversible fouling coincides
 482 with a decrease in the SMP/MLSS ratio. The results thus indicate that the rate of
 483 irreversible fouling depends much more on flux than on SMP concentrations which,
 484 in our case, decrease in wet-periods due to dilution with rain and storm water.

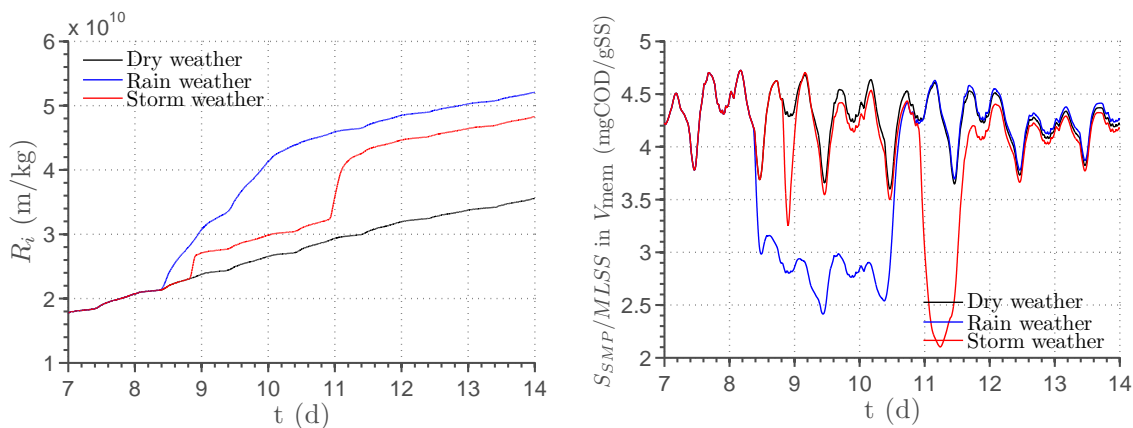


Figure 8: (a) Resistance due to irreversible fouling R_i and (b) SMP fraction in MLSS vs. time during open-loop simulation in dry-, wet-, and storm-weather conditions - Reprinted from Janus and Ulanicki (2014).

485 As explained in Janus and Ulanicki (2015b), specific cake resistance (α_c) is calcu-
 486 lated with the equation of Ahmed et al. (2007) which has been additionally modified
 487 to include a proportionality coefficient m that has been assigned an arbitrary value of
 488 10 in order to raise the calculated α_c values to a level leading to sufficiently high ‘ob-
 489 servable’ fouling levels in the simulation model. As shown in Figure 9, the changes in

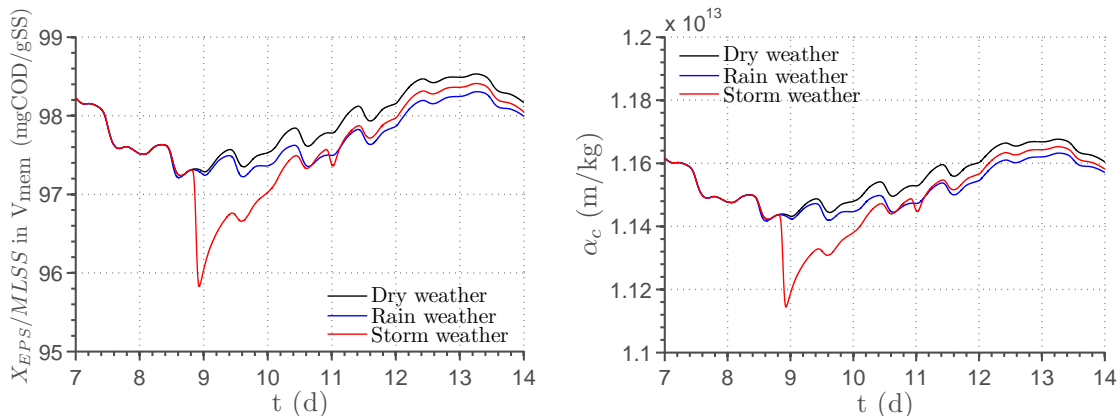


Figure 9: (a) EPS fraction in MLSS and (b) specific cake resistance α_c vs. time during the open-loop simulation in dry-, wet-, and storm-weather conditions - Reprinted from Janus and Ulanicki (2014).

490 α_c are proportional to the EPS content in the activated sludge due to a linear nature
 491 of Ahmed et al.'s equation. However, as X_{EPS} does not change much over the course
 492 of the simulations, α_c remains at a relatively constant value of $\sim 1.12 - 1.16 \text{ m kg}^{-1}$.
 493 Although, as shown in Janus and Ulanicki (2015a), under steady state conditions
 494 the operating parameters such as DO or SRT have a noticeable effect on the EPS
 495 content in activated sludge and hence α_c , the EPS dynamics with respect to DO and
 496 temperature are slow. Hence, as pointed out above, the temporal variability of EPS
 497 content in the activated sludge is therefore small. Since the EPS production kinetics
 498 in our model are based on the standard Monod equation, similarly to SMP kinet-
 499 ics, the model excludes the effects of possible additional dynamics such as release
 500 of EPS in response to shock loading, toxicity, salinity etc. which might additionally
 501 affect the bulk liquid EPS concentrations and thus, α_c . Nevertheless, production
 502 of biopolymers under highly dynamic conditions is a topic for further research and
 503 therefore shall not be considered in this publication.

504 Figure 10 shows the calculated TMPs for a selected simulation time period under

505 two control scenarios: (a) open-loop and (b) closed-loop with the SAD_m controller
506 adjusting the amount of airflow in proportion to the permeate flux (Maere et al.,
507 2011). Coarse bubble aeration reduces trans-membrane pressure (TMP) by creat-
508 ing shear on the cake surface which leads to cake detachment. As the rate of cake
509 detachment is also proportional to cake thickness, a steady-state cake thickness ulti-
510 mately develops for a given flux and air scouring rate. Upon reaching that thickness
511 TMP will reach a plateau resulting in concave down pressure gradients, as shown
512 in Figure 10. The figure demonstrates how air scouring affects TMP in the model.
513 In our case the amount of air scouring in the open-loop scenario is excessive and
514 thus energy is wasted on aeration without leading to further reduction in TMP.
515 Once SAD_m control is applied, energy demand for coarse bubble aeration reduces
516 by about a third whilst reversible fouling under low flux rates increases only slightly
517 but is still insignificantly small compared to the overall membrane resistance, hence
518 indicating a significant potential for energy savings. The above case study shows
519 how the simulation model can be used for energy optimisation in MBR plants by
520 testing different control scenarios, such as this simple feedback air scouring control,
521 and demonstrates how addition of membrane fouling into BSM-MBR benchmark
522 model, on top of biopolymer kinetics, expands its capabilities.

523 *5.5. Energy consumption*

524 Unit energy consumption values per m^3 of treated wastewater calculated from
525 IBMF-MBR and BSM-MBR, and measured on three full-scale MBR plants are com-
526 pared in Table 15, which extends the table originally published in Maere et al. (2011).

527 The energy demand predicted by IBMF-MBR in the open-loop configuration is
528 similar to the energy consumption estimated by BSM-MBR, apart from the ear-
529 lier mentioned energy for permeate pumping, which is the lowest among all effluent

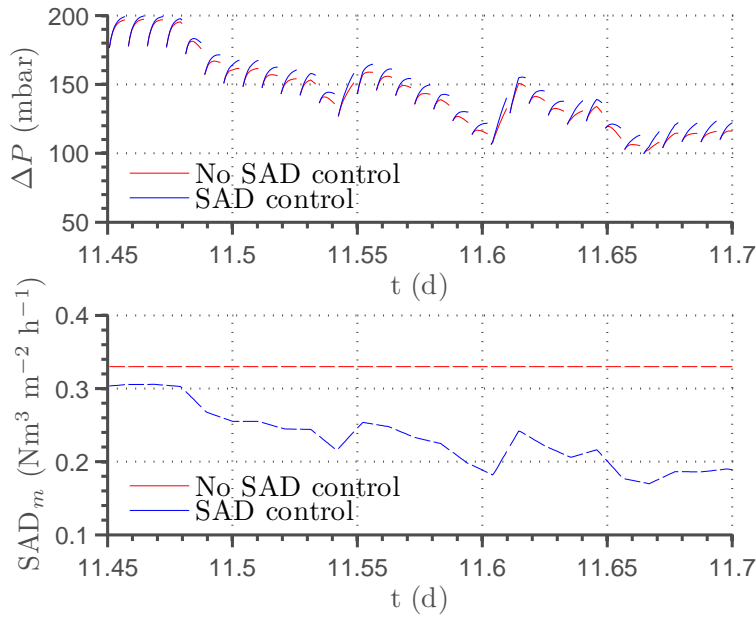


Figure 10: TMP gradients in filtration cycles for a selected time period in a simulation scenario with and without SAD_m control.

530 pumping energy values listed in Table 15. The reasons for this are two-fold. First,
 531 the energy costs in BSM-MBR are calculated using previously assumed unit energy
 532 consumption factors per m^3 of pumped liquid, whilst in IBMF-MBR the permeate
 533 pumping costs are directly calculated from the pumping energy equation (see Equa-
 534 tion 1) in which the pumping head is given or, in the case of permeate pumping,
 535 calculated from the TMP values predicted by the fouling model. Since the permeate
 536 fluxes under dry-weather conditions are at the lower end of sustainable long-term
 537 fluxes used with this type of membranes, very low pressure losses across the mem-
 538 brane calculated by the fouling model are justifiable whilst, at the same time, the unit
 539 permeate pumping cost assumed in BSM-MBR seems to be overestimated. Second,
 540 the effects of irreversible fouling on the overall operational costs cannot be evalu-
 541 ated in such a short time scale as 14 days due to very slow dynamics of irreversible

542 fouling under sustainable fluxes. The only plausible way to include the effects of
543 irreversible fouling over a longer time period in our short-term simulation would be
544 either to specify an initial condition for the membrane resistance which represented
545 a typical ‘average’ membrane resistance over its entire life-span or to extrapolate the
546 contribution of irreversible fouling into a longer period of time using the calculated
547 irreversible fouling rates. It is also tempting to extend the simulation horizon to a
548 period of a few months in order to quantify the overall permeate pumping costs, but
549 such a long-term simulation would necessitate an appropriately designed simulation
550 scenario which would take into account the variability in the influent flow, influent
551 load, and temperature, and which would require a careful selection of a sequence of
552 dry- and wet-weather conditions.

Table 11: Comparison of dynamic open-loop effluent quality and operating cost performance criteria between BSM-MBR and IBMF-MBR models.

Criterion	Unit	BSM-MBR			IBMF-MBR		
		Dry	Rain	Storm	Dry	Rain	Storm
I.Q.	kgPU d ⁻¹	52115.2	52115.2	54074.5	52052.1	52050.2	54029.5
E.Q.	kgPU d ⁻¹	3216.9	3423.6	3423.6	4177.5	4935.9	4544.6
$S_{NH,95}$	gN m ⁻³	0.475	0.473	0.491	1.42	1.40	1.59
TN ₉₅	gN m ⁻³	16.49	15.42	16.32	18.64	17.73	18.55
TSS ₉₅	g m ⁻³	0	0	0	0	0	0
COD ₉₅	gO ₂ m ⁻³	30.90	30.80	30.86	34.78	34.31	35.16
BOD _{5,95}	gO ₂ m ⁻³	0.225	0.232	0.237	0.605	0.610	0.638
$S_{NH,violations}$ (4 gN m ⁻³)	– % of time	0	0	0	0	0	0
TN _{violations} (18 gN m ⁻³)	– % of time	0	0	0	5	3	4
BOD _{5,violations} (10 gO ₂ m ⁻³)	– % of time	0	0	0	8.16	4.31	6.87
COD _{violations} (100 gO ₂ m ⁻³)	– % of time	0	0	0	0	0	0
TSS _{violations} (30 g m ⁻³)	– % of time	0	0	0	0	0	0
SP _{tot}	kgTSS d ⁻¹	1971.2	1982.9	2198.5	1590.1	1587.6	1772.0
SP _{disp}	kgTSS d ⁻¹	1971.2	1982.9	2198.5	1590.1	1587.6	1772.0
AE _{bioreactor}	kWh d ⁻¹	3878.6	3878.6	3878.6	4075.6	4075.6	4075.6
AE _{membrane}	kWh d ⁻¹	9680.7	9680.7	9680.7	9018.1	9018.1	9018.1
AE _{total}	kWh d ⁻¹	13559.3	13559.3	13559.3	13093.7	13093.7	13093.7
PE _{total}	kWh d ⁻¹	2209.2	2639.6	2403.2	1023.6	1128.3	1078.2
PE _{sludge}	kWh d ⁻¹	840.1	840.1	840.1	835.2	835.2	835.2
PE _{permeate}	kWh d ⁻¹	1369.2	1800.0	1563.2	188.33	293.03	243.00
PE _{q_w}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	8.00	8.00	8.00
PE _{q_{int}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_r}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_{eff}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	145.94	250.53	200.55
PE _{q_{back}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	42.39	42.50	42.25
ME	kWh d ⁻¹	576	576	576	714.38	714.38	714.38
OCI	–	26200.4	26690.0	27531.2	22763.9	22856.1	23728.2
Total SRT	d	27.51	25.90	26.83	33.38	31.24	32.47
Aerobic SRT	d	18.85	18.17	18.56	20.41	19.67	20.09
Y _{obs}	–	0.700	0.743	0.732	0.565	0.603	0.591
FI _i	m ⁻¹ L ⁻¹				4616.9	6380.8	6715.5
FI _r	m ⁻¹ L ⁻¹				30334.2	33228.0	32855.5

Table 12: Comparison of dynamic closed-loop effluent quality and operating cost performance criteria between BSM-MBR and IBMF-MBR models with DO control.

Criterion	Unit	BSM-MBR			IBMF-MBR		
		Dry	Rain	Storm	Dry	Rain	Storm
I.Q.	kgPU d ⁻¹	52115.4	52115.4	54074.5	52052.1	52050.2	54029.5
E.Q.	kgPU d ⁻¹	3222.5	3714.4	3456.8	4145.9	4894.3	4504.4
$S_{NH,95}$	gN m ⁻³	0.169	0.175	0.176	0.784	0.783	0.747
TN ₉₅	gN m ⁻³	17.43	16.18	17.23	19.62	18.52	19.54
TSS ₉₅	g m ⁻³	0	0	0	0	0	0
COD ₉₅	gO ₂ m ⁻³	30.82	30.75	30.78	34.13	33.60	34.49
BOD _{5,95}	gO ₂ m ⁻³	0.205	0.210	0.215	0.584	0.591	0.612
$S_{NH,violations}$ (4 gN m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
TN _{violations} (18 gN m ⁻³)	– % of time	4 2.38	1 0.743	4 2.53	5 11.06	3 6.11	5 10.00
BOD _{5,violations} (10 gO ₂ m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
COD _{violations} (100 gO ₂ m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
TSS _{violations} (30 g m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
SP _{tot}	kgTSS d ⁻¹	1978.2	1990.6	2182.1	1588.4	1584.7	1764.3
SP _{disp}	kgTSS d ⁻¹	1978.2	1990.6	2182.1	1588.4	1584.7	1764.3
AE _{bioreactor}	kWh d ⁻¹	3834.3	3791.5	3945.3	4070.6	3981.4	4169.5
AE _{membrane}	kWh d ⁻¹	9680.7	9680.7	9680.7	9018.1	9018.1	9018.1
AE _{total}	kWh d ⁻¹	13515.0	13472.2	13626.0	13088.7	12999.5	13187.6
PE _{total}	kWh d ⁻¹	2209.2	2639.6	2403.2	1023.5	1128.2	1078.2
PE _{sludge}	kWh d ⁻¹	840.1	840.1	840.1	835.22	835.22	835.22
PE _{permeate}	kWh d ⁻¹	1369.2	1799.5	1563.2	188.32	293.01	242.98
PE _{q_w}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	8.00	8.00	8.00
PE _{q_{int}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_r}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_{eff}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	145.93	250.52	200.54
PE _{q_{back}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	42.39	42.49	42.44
ME	kWh d ⁻¹	576	576	576	714.38	714.38	714.38
OCI	–	26191.3	26640.8	27505.8	23954.9	22765.5	25123.1
Total SRT	d	27.51	25.89	26.83	33.38	31.24	32.48
Aerobic SRT	d	18.85	18.17	18.56	20.41	19.67	20.10
Y _{obs}	–	0.702	0.744	0.732	0.565	0.603	0.591
FI _i	m ⁻¹ L ⁻¹				4532.0	6311.2	6473.7
FI _r	m ⁻¹ L ⁻¹				30363.6	33256.0	32897.2

Table 13: Comparison of dynamic closed-loop effluent quality and operating cost performance criteria between BSM-MBR and IBMF-MBR models with DO and SAD_m control.

Criterion	Unit	BSM-MBR			IBMF-MBR		
		Dry	Rain	Storm	Dry	Rain	Storm
I.Q.	kgPU d ⁻¹	52115.4	52115.4	54074.6	52052.1	52050.2	54029.5
E.Q.	kgPU d ⁻¹	3197.2	3696.0	3432.0	4112.4	4871.0	4470.9
$S_{NH,95}$	gN m ⁻³	0.174	0.179	0.178	0.882	0.842	0.815
TN ₉₅	gN m ⁻³	17.32	16.08	17.12	19.31	18.26	19.22
TSS ₉₅	g m ⁻³	0	0	0	0	0	0
COD ₉₅	gO ₂ m ⁻³	30.82	30.75	30.79	34.28	33.76	34.62
BOD _{5,95}	gO ₂ m ⁻³	0.205	0.211	0.216	0.586	0.592	0.614
$S_{NH,violations}$ (4 gN m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
TN _{violations} (18 gN m ⁻³)	– % of time	3 1.63	1 0.594	3 1.63	5 10.16	3 5.56	5 8.81
BOD _{5,violations} (10 gO ₂ m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
COD _{violations} (100 gO ₂ m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
TSS _{violations} (30 g m ⁻³)	– % of time	0 0	0 0	0 0	0 0	0 0	0 0
SP _{tot}	kgTSS d ⁻¹	1977.1	1991.0	2181.2	1587.7	1584.7	1763.4
SP _{disp}	kgTSS d ⁻¹	1977.1	1991.0	2181.2	1587.7	1584.7	1763.4
AE _{bioreactor}	kWh d ⁻¹	3911.8	3848.2	4007.9	4152.4	4039.7	4246.2
AE _{membrane}	kWh d ⁻¹	5597.0	6647.8	5970.9	5469.5	6409.9	5809.3
AE _{total}	kWh d ⁻¹	9508.9	10486.0	9988.8	9621.9	10449.6	10055.7
PE _{total}	kWh d ⁻¹	2209.2	2639.6	2403.2	1025.5	1129.7	1080.0
PE _{sludge}	kWh d ⁻¹	840.07	840.07	840.07	835.22	835.22	835.22
PE _{permeate}	kWh d ⁻¹	1396.2	1799.5	1563.2	190.29	294.43	244.8
PE _{q_w}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	8.00	8.00	8.00
PE _{q_{int}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_r}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_{eff}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	147.90	251.93	202.36
PE _{q_{back}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	42.39	42.49	42.44
ME	kWh d ⁻¹	576	576	576	714.38	714.38	714.38
OCI	–	22179.6	23666.5	23864.1	19301.0	20217.2	20667.1
Total SRT	d	27.51	25.89	26.83	33.38	31.24	32.48
Aerobic SRT	d	18.85	18.17	18.56	20.41	19.67	20.10
Y _{obs}	–	0.701	0.744	0.732	0.565	0.603	0.591
FI _i	m ⁻¹ L ⁻¹				4566.2	6330.0	6515.0
FI _r	m ⁻¹ L ⁻¹				72730.4	55404.1	65751.0

Table 14: Comparison of dynamic closed-loop effluent quality and operating cost performance criteria between BSM-MBR and IBMF-MBR models with DO, SAD_m and NO_3^- -N control.

Criterion	Unit	BSM-MBR			IBMF-MBR		
		Dry	Rain	Storm	Dry	Rain	Storm
I.Q.	kgPU d ⁻¹	52115.4	52115.4	54074.5	52052.1	52050.2	54029.5
E.Q.	kgPU d ⁻¹	3174.8	3569.5	3345.7	3980.8	4679.1	4280.6
$S_{NH,95}$	gN m ⁻³	0.191	0.207	0.201	1.16	1.07	1.05
TN ₉₅	gN m ⁻³	16.72	15.22	16.48	17.82	16.64	17.45
TSS ₉₅	g m ⁻³	0	0	0	0	0	0
COD ₉₅	gO ₂ m ⁻³	30.80	30.75	30.79	34.10	33.61	34.50
BOD _{5,95}	gO ₂ m ⁻³	0.200	0.206	0.211	0.609	0.624	0.641
$S_{NH,violations}$ (4 gN m ⁻³)	– % of time	0	0	0	0	0	0
TN _{violations} (18 gN m ⁻³)	– % of time	0	0	0	4	1	2
BOD _{5,violations} (10 gO ₂ m ⁻³)	– % of time	0	0	0	0	0	0
COD _{violations} (100 gO ₂ m ⁻³)	– % of time	0	0	0	0	0	0
TSS _{violations} (30 g m ⁻³)	– % of time	0	0	0	0	0	0
SP _{tot}	kgTSS d ⁻¹	1978.2	1992.2	2180.5	1584.5	1577.0	1757.1
SP _{disp}	kgTSS d ⁻¹	1978.2	1992.2	2180.5	1584.5	1577.0	1757.1
AE _{bioreactor}	kWh d ⁻¹	3897.8	3806.9	3974.1	4096.4	3951.3	4159.2
AE _{membrane}	kWh d ⁻¹	5596.9	6647.6	5970.4	5469.4	6410.0	5809.2
AE _{total}	kWh d ⁻¹	9494.7	10454.5	9944.5	9565.8	10361.3	9968.4
PE _{total}	kWh d ⁻¹	2198.4	2682.0	2428.2	1092.3	1238.8	1188.0
PE _{sludge}	kWh d ⁻¹	829.18	882.42	864.98	902.14	945.00	943.63
PE _{permeate}	kWh d ⁻¹	1369.2	1799.5	1563.2	190.16	293.80	244.35
PE _{q_w}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	8.00	8.00	8.00
PE _{q_{int}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	480.53	523.39	522.02
PE _{q_r}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	413.61	413.61	413.61
PE _{q_{eff}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	147.77	251.31	201.91
PE _{q_{back}}	kWh d ⁻¹	Not recorded	Not recorded	Not recorded	42.39	42.49	42.44
ME	kWh d ⁻¹	576	576	576	714.38	714.38	714.38
OCI	–	22160.0	23673.3	23851.3	20479.6	20199.6	20656.3
Total SRT	d	27.44	26.04	26.91	33.80	31.90	33.11
Aerobic SRT	d	18.85	18.17	18.56	20.41	19.67	20.10
Y_{obs}	–	0.706	0.743	0.732	0.566	0.599	0.587
FI_i	m ⁻¹ L ⁻¹				4530.2	6282.8	6446.7
FI_r	m ⁻¹ L ⁻¹				71639.6	54281.4	64244.2

Table 15: Comparison of energy costs between IBMF-MBR, BSM-MBR and three full-scale municipal MBR WWTPs - modified from Maere et al. (2011) - Reprinted from Janus and Ulanicki (2014).

Energy cost (kWh m ⁻³)	Schilde ¹⁾	Varsseveld ²⁾	Nordkanal ³⁾	BSM-MBR	IBMF-MBR	
					Open-loop ^{*)}	Closed-loop ^{*)}
ME	0.05	0.04	0.11	0.03	0.039	0.039
PE _{sludge}	0.10	0.11	0.01	0.05	0.046	0.049
PE _{effluent}	0.07	0.12	0.02	0.07	0.008	0.008
AE _{bioreactor}	0.07	0.24	0.11	0.21	0.22	0.22
AE _{membrane}	0.23	0.34	0.45	0.53	0.49	0.30
Total	0.52	0.85	0.71	0.90	0.81	0.62

^{*)} dry-weather conditions with average permeate flow rate $q_{perm,ave} = 18286.3 \text{ m}^3 \text{ d}^{-1}$

¹⁾ Fenu et al. (2010)

²⁾ Wever et al. (2009)

³⁾ Brepols et al. (2010)

553 6. Conclusion

554 In summary, IBMF-MBR was found to be in a good agreement with the ASM1-
555 based BSM-MBR benchmark model whilst additionally providing information on
556 biopolymer production and membrane fouling. Although the simulations showed a
557 few discrepancies between both models with regards to some biological constituents
558 and process parameters, these differences were not significant. IBMF-MBR was
559 found to predict lower denitrification rates compared to BSM-MBR. Although it is
560 impossible at this stage to say if the denitrification rates predicted by IBMF-MBR
561 are closer to the typical values observed on physical systems than those predicted
562 by BSM-MBR, ASM1 was already reported in literature to over-predict denitrifica-
563 tion in high SRT systems due to infinite recirculation of biodegradable substrates in
564 the implemented death-regeneration model. IBMF-MBR also predicts lower sludge
565 yields and thus higher SRTs to BSM-MBR due to an altered flow of organic sub-
566 strates in the biological model caused by the introduction of biopolymer kinetics.
567 Qualitatively, this change is again in a good direction as MBR systems have been
568 reported numerously to produce lower sludge yields to those predicted by standard
569 mathematical models due to large SRTs (Lubello et al., 2009).

570 The simulations also revealed that irreversible fouling, albeit traditionally pre-
571 dominantly attributed to bulk liquid SMP concentrations, is much more sensitive
572 to flux than SMP. Additionally, under high flow rates across the plant, solids shift
573 downstream from the bioreactor to the membrane tank causing high solids loading
574 on the membrane and thus producing higher reversible fouling simultaneously co-
575 inciding with high irreversible fouling. These findings suggest that flow control in
576 MBRs is of an utmost importance. In order to compare the degree of fouling asso-
577 ciated with different operating strategies in a MBR benchmark model, two fouling

578 indices, respectively for irreversible and reversible fouling, have been introduced and
579 calculated for each control strategy investigated in this paper. These fouling indices
580 can also be used to calculate fouling cost indices in order to quantify the financial
581 operational costs associated with fouling mitigation.

582 The simulated bulk liquid SMP and EPS concentrations exhibit rather modest
583 variabilities under all dynamic weather conditions, mainly due to diurnal loading
584 pattern in dry weather and dilution effects in wet weather, while steady-state bulk-
585 liquid SMP and EPS concentrations were earlier found to change noticeably with
586 the operating conditions such as e.g. SRT (Janus and Ulanicki, 2015a). It is pos-
587 sible that the variability of SMP and EPS in physical full scale WWTPs would be
588 higher as the biopolymers were found to be produced predominantly under stress
589 conditions such as toxicity, osmotic shocks, large disturbances in influent flow and
590 loading rates or high shear intensities (Noguera et al., 1994; Barker and Stuckey,
591 1999; Wingender et al., 1999) while our CES-ASM1 biological model describes the
592 biopolymer kinetics only with a standard Monod equations. Therefore, the contribu-
593 tion of SMP and EPS to irreversible and reversible fouling under dynamic conditions
594 may be underestimated in the model as, first, some biopolymer production dynamics
595 might not have been identified during calibration and, second, the model itself may
596 not describe these dynamics. Lack of validation of standard biopolymer production
597 models in activated sludge systems operating under dynamic conditions is the main
598 bottleneck of the IBMF-MBR model as well as other integrated MBR models, along-
599 side the nature of the functional relationships between biopolymer concentrations
600 and fouling. These topics need to be researched in the future to allow development
601 of more realistic MBR models.

602 In summary, IBMF-MBR, despite of its shortcomings listed above, offers addi-
603 tional benefits compared to the BSM-MBR model as it additionally allows to quan-

604 tify the bulk liquid biopolymer concentrations, the rates of fouling and the energy
605 consumption for air-scouring and pumping. These features allow the modeller to
606 benchmark process control schemes while taking into account the effects of fouling
607 on process performance, which is not currently possible with the BSM-MBR bench-
608 mark model. They also allow the modeller to build fully functional MBR simulation
609 models which can be used for process design, process optimisation, controller design
610 and testing new plant configurations.

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