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Implementation of membrane bioreactor fouling models based on linear and bilinear autoregressive model structures

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ABSTRACT

The focus of this research is to create pragmatic and novel membrane bioreactor (MBR) models which can be applied for plant design, control and optimisation. Consequently, this research compares the traditional mechanistic models based on existing well known MBR filtration and biochemical processes with alternatives forms based on autoregressive input–output model formulations that in turn are based on system identification methods. Both model types are calibrated and validated using the same plant layouts and datasets derived for this purpose. This collated plant information included data obtained from carrying out standard flux-stepping experiments on a membrane filtration unit, and long term filtration experiments on a pilot MBR plant. In order to overcome the inherent deficiencies in any traditional approach, a novel alternative approach was tried in order to predict membrane filtration and fouling process for a MBR in a quick and easy manner. The rationale behind this novel approach is that it is simple to apply and that it does not require an intimate knowledge of the exact processes occurring in the MBR, so it could be applied by any non-specialist who was new to wastewater treatment modelling. This alternative approach uses linear and bilinear autoregressive model structures. Initial results from both the traditional and novel approaches indicate reasonable model predictive capabilities.

Keywords: Membrane; Fouling; Modelling; Autoregressive

1. Introduction

The aim of this study was to create practical membrane bioreactor (MBR) computer models that can then be applied for plant design, control and optimisation. It was intended that the outcomes of this research would lead both to the improvement of existing models and the creation of new, innovative models. The eventual application of both model types would be to optimise a real treatment plant and thereby eventually develop a long-term energy saving control strategy [1].

1.1. Disadvantages of using phenomenological membrane fouling models for plant design, operation and control

Most current researchers model the membrane fouling process using a phenomenological mechanistic

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approach that obeys the fundamental laws of physics. This is the traditional approach used to model MBR systems that treat wastewater. However, it has been found that it does suffer from the following disadvantages:

- Membrane fouling is in reality highly complex and currently poorly understood as a process. Hence any mechanistic fouling model, either simple or complex, cannot hope adequately to address all aspects involved in the fouling procedure [2].
- Usually a mechanistic fouling model needs to be made bespoke for each individual filtration system, so that it accurately depicts the specific hydrodynamics of the process and the membrane operational regime [2].
- These models are normally highly dimensional and contain several parameters requiring determination by real-life plant datasets (e.g. flux stepping trials, extended specialist laboratory experiments, etc.).
- Parameter estimation and optimisation require expert knowledge and proves to be complex as most models of this type are over-parameterised with too many degrees of freedom.
- For many applications insufficient quality data is usually available to allow a full model calibration and validation, and thus any verified model is not accurate for every situation.
- The general application of such complex models means their take up for process control and the development of future operational strategies will always prove limited [3].

In a bid to overcome the distinct disadvantages of a traditional mechanistic approach, it has been suggested that a non-traditional approach can be used to describe the membrane fouling process for a MBR system. The non-traditional approach which was used in this study is based on time series system identification methods [4,5]. At its simplest, it uses the plant data set itself to determine that best fit model from a range of standard numerical model structures (e.g. autoregressive, state-space, sub-space, etc.), that are described in greater detail in the next section.

1.2. "Model conceptualisation procedure" required to embed the alternative modelling approaches in reality

Under this study two different model types, namely, a phenomenological model structure and an autoregressive time series model structure, were tested to ascertain which gave the best results. These autogressive model types, which are based on standard mathematical formulations such as ordinary differential equations or difference equations of various orders, can be used as a quick method for model prediction as no prior process knowledge is required for model calibration and validation [6,7]. The procedure automatically selects the best order model-based on the number of lags in output data that give the optimal prediction. Little skill is needed by the simulator to obtain the best-fit, and a significant amount of time is saved when compared to the complex needs by verifying a typical mechanistic model. Additionally, many of the complex tests, both laboratory-based and in situ, that are required to validate numerous model parameters are not required, or the need to carry out extensive literature reviews of parameter values used by previous reputable researchers.

However, it is recommended if these model types are used as real practical alternatives to phenomenological approaches, extreme care should be taken in selecting appropriate variables when forming the autoregressive model structure. This is where a "Model Conceptualisation Procedure" developed by prior researchers, such as Paul [8] will prove invaluable as it underpins the basic knowledge needed by a lay person when developing models of this type. This procedure means that various structures have already been developed and tested based on expert biochemical and hydrodynamic process knowledge, and the user only has to implement them. Fig. 1 describes part of such a MBR "Model Conceptualisation Procedure" developed under this study [8].

A model of a process is typically represented by an ordinary differential equation as shown in Eq. (1) where the following vectors are: $x(t)$ the state of the system, $m(t)$ the manipulated (control) variables, $z(t)$ the input variables from external environment, $u(t)$ the input variables connections from other subsystems and $y(t)$ the output variables for a subsystem.

$$\dot{x}(t) = f(x(t), m(t), z(t), u(t), y(t)) \quad (1)$$

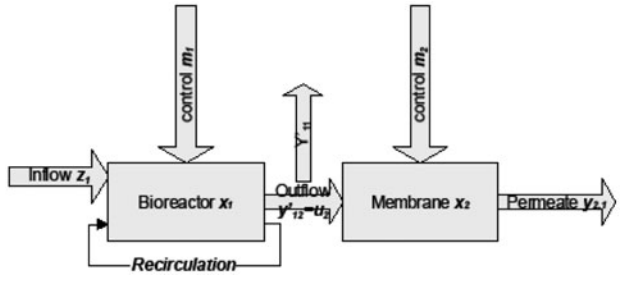

Fig. 1. Part of a "model conceptualisation procedure" used to develop rational relationships between input and output variables for an approximate decomposed MBR model.

$$\text{Input variables} \qquad \text{State and output variables}$$

$$y'_{12} = u_2 = \begin{bmatrix} S_{PS} \\ S_{PP} \\ C_b \\ X_{EPS} \\ \mu(T) \end{bmatrix} \text{ and } m_2 = \begin{bmatrix} \omega_{pump} \\ v_{throttle} \\ f_{bwash} \end{bmatrix}; \quad x_2 = \begin{bmatrix} I_{foul} \\ R_{foul} \\ B_{cake} \end{bmatrix} \text{ and } y'_{21} = \begin{bmatrix} TMP \\ q_{perm} \end{bmatrix}$$

So for a general membrane undergoing filtration as shown in Fig. 1, the following generalised vector representation can be used for a typical side stream MBR scenario as shown above.

2. Methodology

This research work uses phenomenological models based on both traditional MBR filtration and biochemical processes to measure the effectiveness of alternative time series input–output (IO) models based upon system identification time series analysis methods. Both model types are calibrated and validated using the same plant layouts and data sets derived for this purpose.

2.1. Duclos–Orsello phenomenological model

A phenomenological dead-end filtration model [9], was used in this study that depicts the three main fouling mechanisms occurring on membranes, namely, cake build-up, complete pore blocking and pore constriction, as originally described in Hermia [10] under constant trans-membrane pressure (TMP) operation. In this model, Duclos–Orsello et al. [9], splits the total flow, Q_t, through the membrane into flow through the unblocked membrane surface area and flow through the blocked membrane surface area as shown in Eq. (2). Hence the first algebraic term relates to the unblocked flow whilst the second integral term relates to blocked flow.

$$Q_t = \frac{Q_0}{(1+\beta Q_0 C_b t)^2} \cdot e^{\left(-\frac{\alpha C_b J_0 t}{1+\beta Q_0 C_b t}\right)} + Q_0 \int_0^t \frac{(\alpha C_b J_0/(1+\beta Q_0 C_b t_p)^2) e^{(-(\alpha C_b J_0 t_p/(1+\beta Q_0 C_b t_p)))}}{\sqrt{[(R_{p0}/R_m)+(1+\beta Q_0 C_b t_p)^2]^2 + 2(f' R' \Delta p C_b/\mu R_m^2)(t-t_p))}} dt_p \tag{2}$$

This initial model was extensively modified and added to by Paul et al. [11], so that it could be used to model a variety of real-life MBR configurations. Modifications and add-ons to this basic model included: alteration so that it could be used for varying flux and varying TMP operations; inclusion of a backwash mode; it described pore constriction (i.e. irreversible fouling) in relation to the concentration of soluble microbial products (SMP) in the liquor with SMP being the key agent thought to determine membrane fouling [12,13]; and, it could be used in a cross-flow scenario by the addition of scouring terms in the model formulation. Using data collected from a pilot membrane filtration unit, this modified deterministic model was calibrated and validated in Matlab©.

2.2. Using system identification time series analysis methods to create input–output models as possible non-traditional alternatives

System identification is an iterative process in which models with different structures are identified from data, and the individual model performance is compared. The normal start point is determined by estimating the parameters of very simple model structures. If the performance still proves poor, then the model structure is gradually increased in complexity. Ultimately the simplest of all model structures tested is eventually selected, in which the best describes the dynamics of the system under scrutiny. In this iterative process, which can be automated, the system identification procedure commences by initially using linear continuous IO model structures. This followed by using more complex non-linear structures the simplest of which is the bilinear one [14]. The best-fit structure is then chosen as the optimal model formulation.

Table 1
Operational data for pilot membrane filtration unit

ITT Sanitaire membrane filtration unit (without bioreactor)	
Membrane type and area	Horizontal "Kolon" fibres; PVDF 0.1 μm pore size; 20 m^2
Feed flow; permeate flow; backwash	1–2.4 m^3/h; 0.6–1 m^3/h; 1.2–1.8 m^3/h
Backwash interval & duration	Every 4 min with 30 s ON
TMP	300–500 mbar
Aeration rate	13 Nm^3/h from coarse bubble tube diffuser
Cleaning regime	Hypochlorite dosed 4 times daily into permeate tank
Feed flow biological data	COD concentration 50 mgO_2/l; TSS concentration 25 mg/l
Indicative feed flow SMP data	Measured glucose concentration 5 mg/l; measured protein concentration 100 mg/l

In this study, a linear continuous IO state-space model structure is tested using Matlab© and the supplied time series data. The state-space model structure is a good choice for quick estimation because it requires only two parameters, namely the model order and one or more input delays. These model formulations are usually solved using iterative optimisation techniques and algorithms like the least squares method. However, this requires a lot of computing power and they are prone to inherent inaccuracies. A much more attractive model formulation is the sub-space one which does not need to be solved using iterative optimisation techniques and algorithms, but by only using algebraic calculations [15]. This means the sub-space model formulation is a very powerful version of the state-space one that uses only a single-shot solving procedure with improved accuracy. Hence this sub-space method was also tested under this study for comparative purposes on two different data sets. Finally, a more complex but less robust temperature dependent bilinear model structure was tested on one of these data sets.

Picture 1. ITT Sanitaire pilot MBR plant.

2.3. Pilot membrane filtration unit

Both the phenomenological and the state- and sub-space fouling model types have been tested on the data obtained from flux stepping tests performed on an ITT Sanitaire Ltd pilot membrane filtration unit. This unit treated tertiary effluent from Cardiff's sequence batch reactor wastewater treatment plant, and its basic operational information is described in Table 1 above.

2.4. Pilot MBR plant

In a separate but related study, the sub-space fouling model type is tested with a bilinear fouling model type using long term filtration data taken from an ITT Sanitaire Ltd pilot MBR depicted in Picture 1. This pilot treated brewery effluent generated from a Coors (UK) plant, and its basic operational information is described in Table 2 above. The dimensions of the filtration portion of the pilot MBR plant were identical

Table 2
Pilot MBR plant operational data

ITT Sanitaire MBR plant (with bioreactor)	
Membrane type and area	Vertical "Puron" fibres; PES 0.04 μm pore size; 20 m^2
Permeate flow; backwash flow	0.6 m^3/h; 1.1 m^3/h
Permeate recirculation flow	0.27 m^3/h
Backwash interval & duration	Every 6 min with 45 s ON
TMP	300–500 mbar
Bioreactor DO operating range	2–4 mg/l
Full air scour flow	27 Nm^3/h for 15 s every 60 s
Low air scour flow	~2 Nm^3/h for 45 s every 60 s
Bioreactor data (membrane feed)	MLSS concentration ~7,500 mg/l
Bioreactor tank data	Volume 1 m^3; operating level of weir 1.9–2.0 m

to filtration unit used earlier for the flux-stepping tests. This validation was done on standard mixed liquor from a MBR plant, in order to test the autoregressive models validity during filtration of liquids with high biological solids content. The other advantage of this dataset was that it was accumulated over several months and consisted of regular measurements taken on-line. Consequently, for a single month there were hundreds of thousands of data points that could be potentially used in any model simulation. Further, the mixed liquor temperature was regularly measured on-line so could be used as an input variable to see whether a bilinear model gave a more representative fit for the data.

3. Results and discussion

3.1. Model simulation for flux stepping—results for Duclos–Orsello traditional approach

After various assumptions and simplifications of the plant data, the eight best flux steps were used to test the modified phenomenological model. Fig. 2, shows the result obtained when using the calculated optimal parameter sets for the best eight flux steps for this pilot unit, with the pore blockage parameter, α, calculated as 3,469 and the pore constriction parameter, β, as 0.14. The model fit is extremely good, with the genetic algorithm (GA) mean fit being 1.0377 for a population generation of 5,000 when using the Matlab© standard GA routine.

3.2. Model simulation for flux stepping—results for non-traditional approach using IO models

After various assumptions and simplifications of the plant data, the eight best flux steps were used to test the proposed multi-input single output (MISO) model structure. As the plant layout for this unit is very simple with no bioreactor to complicate matters, the selected MISO model structure should give a very high degree of accuracy. In this case, the permeate flux, the measured SMP levels, and the measured bulk mixed liquor concentration into the membrane were used as variables in the input model vector with the TMP being the single variable in the output model vector. First, an IO model-based on a standard iterative state-space formulation, was tested using the parameter estimation method (PEM) in the Matlab© graphical user interface (GUI) system identification toolbox. This was followed by using a quicker single-shot algebraic sub-space method as a comparison, which was developed by Chen and Maciejowski [15] to run as a specialist Matlab© sub-space analysis toolbox that overcomes the deficiencies of the PEM GUI procedure. Results are described below.

3.2.1. Best-fit for eight flux steps of MISO normal state-space model

Fig. 3 shows the result obtained when using the calculated optimal parameter sets for the best eight flux steps for this pilot unit. The model fit is extremely poor.

The fully calculated state-space model vectors and matrices for this specific simulation are as follows:

The generalised state-space model is shown in Eqs. (3) and (4) with $e(t)$ being system disturbance or noise; T_S the sampling interval; and A, B, C, D and K as determined parameter sets.

$$x(t + T_S) = A \cdot x(t) + B \cdot u(t) + K \cdot e(t) \quad (3)$$

$$y(t) = C \cdot x(t) + D \cdot u(t) + e(t) \quad (4)$$

where

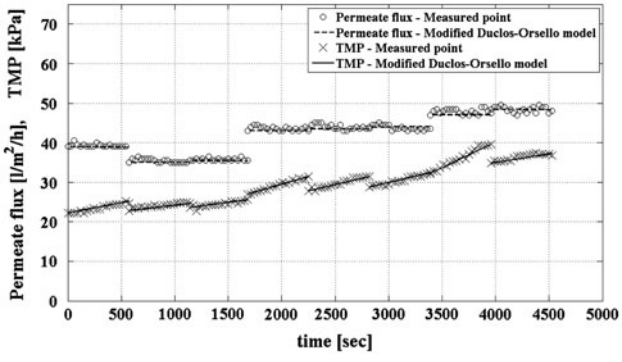

Fig. 2. Modified phenomenological model - best model fit for eight flux steps.

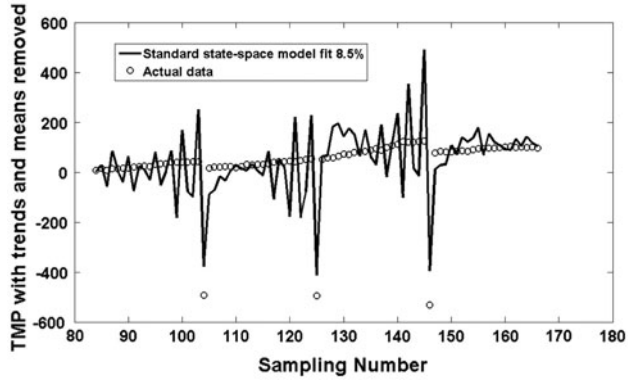

Fig. 3. Best model fit for eight flux steps (four for validation) for standard state-space formulation.

$$A = \begin{bmatrix} 0.83394 & -0.29167 & 0.2897 & 0.062391 \\ 0.34065 & -0.27338 & -0.85698 & -0.077276 \\ -0.45991 & -0.71571 & -0.051448 & 0.70936 \\ 0.65204 & -1.1375 & -0.99252 & -0.7441 \end{bmatrix}$$

$$B = \begin{bmatrix} -0.012929 & -0.072907 & 0.27366 \\ -0.02189 & -0.64752 & 0.040819 \\ -0.36466 & 0.53015 & 4.6264 \end{bmatrix}$$

$$C = [130.32 \quad 46.421 \quad -30.711 \quad -30.999]$$

$$D = [0 \quad 0 \quad 0] \qquad K = \begin{bmatrix} 0.0027854 \\ -0.0019581 \\ -0.041576 \\ 0.071596 \end{bmatrix}$$

3.2.2. Best-fit for eight flux steps for MISO sub-space model

Fig. 4 shows the result obtained when using the calculated optimal parameter sets for the best eight flux steps for this pilot unit. The model fit is very good. For the sake of brevity the fully calculated sub-space model vectors, matrices and parameter sets are not given here.

3.2.3. Discussion of model simulation results with pilot membrane filtration unit data

The standard state-space formulation gave a workable fit, albeit not a very good one of 8.5% as shown in Fig. 3. However, the shape and direction of the fit is correct even though the simulated data is prone to gradually attenuating fluctuations around a mean point. This poor fit could be attributed to the regular backwash events that cause a sudden large negative drop in the TMP that the simulated model in this case is unable to cope with.

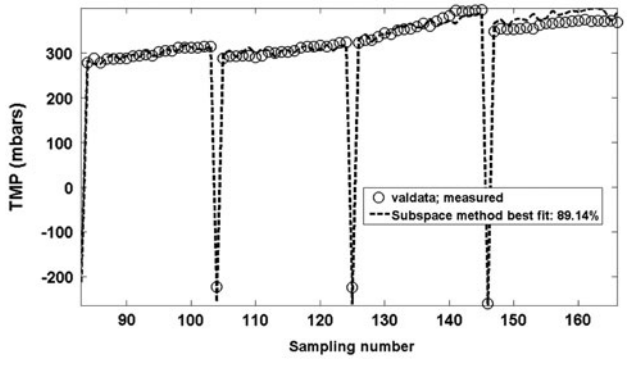

Fig. 4. Best model fit for eight flux steps (four for validation) for sub-space method.

When this MISO model structure is run as a sub-space formulation, the best-fit is for a sixth order model with an algorithm block size of four. This fit is carried out by using the last four flux stepping cycles as the validation data set. The result as shown in Fig. 4 depicts an excellent fit amounting to 89.14%. The shape of the fit is extremely good and is in the right direction (i.e. TMP increases with time), and thus validating the use of additional input biochemical data (e.g. SMP and mixed liquor concentration levels) to improve the overall model fit.

3.3. Model simulation for long term filtration—results for sub-space linear and temperature dependent bilinear models

In this case the permeate flux, the measured bulk mixed liquor concentration into the membrane, and the liquid temperature were used as variables in the input model vector with the TMP being the single variable in the output model vector. Data taken for the full month of January was used and consisted of nearly 24,000 data points.

3.3.1. Best-fit for long term filtration for MISO sub-space and bilinear models

Fig. 5 is a combined plot of the actual TMP values plotted against both the sub-space method and the bilinear model version. Again for the sake of brevity, neither model's fully calculated vectors, matrices and parameter sets are given here. As can be seen the bilinear model which includes for temperature dependence gives greater predictive accuracy at 43% best-fit, although it proved more difficult to set up and less robust than the sub-space method which only gave a 26% best-fit.

The following summarised points can be made regarding IO model structures used in this section:

- If the IO model structure is not selected judiciously then the resulting model will prove of little predictive value. Therefore very careful thought has to be applied to develop appropriate and sensible IO model structures that best reflect reality.
- Different plant layout seem to favour different IO model formulations, so some achieve a better fit using state space formulations, whilst others are better reflected using autoregressive iterative formulations. However, the sub-space method always performed adequately and so should always be tried first.

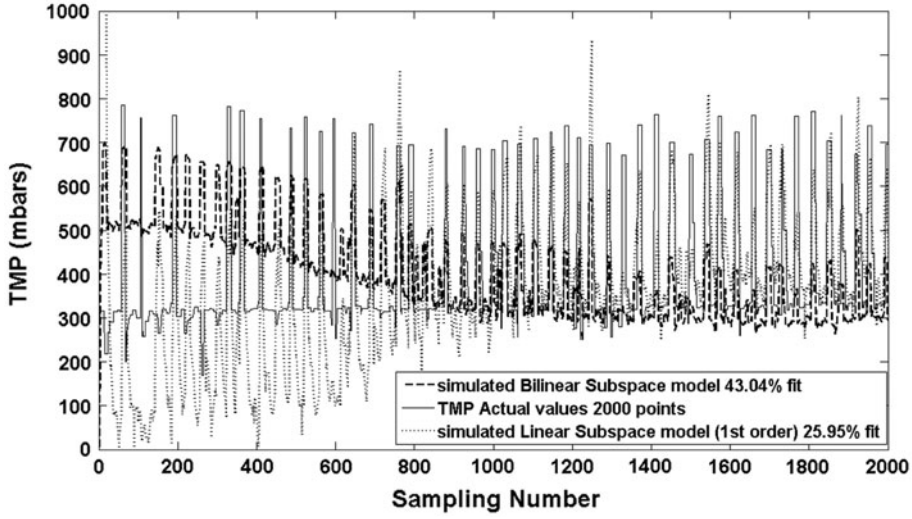

Fig. 5. Actual TMP vs. simulated subspace and bilinear model calculated values.

- It was found that when the backwash data was entirely removed from the dataset, the fits for all methods considerably improved. It is recommended it is always discarded from a dataset before use if at all possible, since it will negatively skew the fit especially, the shape and direction of the fit.
- As expected, the bilinear sub-space model gives a better fit than its linear version, although its formulation is more complex in nature, and the algorithm used is very sensitive and thus, apt to fail or not be able to provide a solution.
- It is abundantly evident from these simulation results that IO model structures can give useful predictive results when compared to traditional phenomenological mechanistic approaches for wastewater treatment.

4. Conclusions

Overall it is clear that the phenomenological model performed very well even though it took a considerable time to be developed into a useful format, and the model had to be calibrated using complex genetic algorithm procedures. Conversely, the sub-space method gave consistent results for the IO models used, and was very easy to set up and calibrate. The bilinear formulation even managed to improve upon this but was much more difficult to setup and calibrate and even more fragile to run.

It initially looks like this novel approach has many advantages over traditional mechanistic models while giving comparable results for some IO structures. Early simulation results described in this study prove this, especially for subspace methods. However these methods can prove very fragile and prone to crashing. Additionally a comprehensive "Model Conceptualisation Procedure" is required to tie it into reality which needs expert know-how to set up. They also require very large data sets to produce accurate formulations, and these linear models are only useful around a very narrow operating range or operating point. Non-linear model versions, such as the bilinear structure tested in this study, can improve upon predictive accuracy but are even more fragile than their linear counterparts.

In summary, it may prove advantageous to use these methods for model prediction under most circumstances apart from the following instances:

- Not for design of new plant (particularly for processes with long time constants), and the biological operation of plant (i.e. off-line measurements).
- No good as research tools to investigate membrane fouling. Cannot predict one-off fouling events, only generalised scenarios.

The situation in which they may particularly prove themselves superior to traditional model structures is for model predictive control (possibly in real time) for processes with very short time constants (i.e. rapidly changing flux/TMP data). However, they would need constant automated updating of historical data sets using on-line sensors. In conclusion, further research is required using longer historical data sets to definitively ascertain whether this non-traditional modelling approach can be further developed and improved upon.

Nomenclature

B_{cake} — general unspecified term relating to cake build up
C_b — bulk concentration (mg/l)
f — fractional amount of total foulant contributing to deposit growth
f_{bwash} — general unspecified term relating to backwash frequency, intensity, duration (and relaxation steps)
I_{foul} — general unspecified term relating to irreversible fouling (i.e. pore constriction) and its amelioration (e.g. chemical clean, etc.)
J_0 — initial flux rate of clean membrane (m/s)
q_{perm} — permeate flow rate (m^3/s)
Q_t — total volumetric flow rate (m^3/s)
Q_0 — initial volumetric flow rate (m^3/s)
R_{foul} — general unspecified term relating to reversible fouling (i.e. pore blocking) and its amelioration dependant on configuration (e.g. air scour, cross flow velocity, backwash, forward permeate run, relaxation, etc.)
R_m — resistance of the clean membrane (m^{-1})
R_{p0} — original resistance of the deposit (m^{-1})
R — specific protein layer resistance (m/kg)
S_{PS} — soluble polysaccharide concentration (mg/l)
S_{PP} — soluble protein concentration (mg/l)
t — filtration time (s)
t_p — filtration time after initial membrane blocking occurs(s)
TMP — trans-membrane pressure (Pa)
X_{EPS} — particulate (bound) extracellular polymeric substances (mg/l)
Δ_p — constant total membrane pressure (Pa)

Greek letters

α — pore blockage parameter (m^2/kg)
β — pore constriction parameter (kg)
$\mu(T)$ — temperature dependant viscosity (cP)
ω_{pump} — general unspecified term relating to recirculation pump speed, duration, etc.
$V_{throttle}$ — general unspecified term relating to throttle valve settings for external membrane unit

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