Dynamic modeling of diafiltration system for a biorefinery application

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Abstract

Application of membrane technologies in biorefinery processes has been studied for some time. The heterogenous nature of biorefinery steams, however, results in unideal performance of membrane systems and considerable fouling of membranes, which is decreasing the efficiency of separation. As a part of BioSPRINT project, this study focuses on application of separating monomeric sugars from the hemicelluloses fraction of lignocellulosic biomass, where pressure-driven nanofiltration with several diafiltration stages has been proposed for the separation task. Diafiltration is required to overcome the decreased separation efficiency when the retentate concentrations and viscosity increases. A lumped parameter dynamical model of the diafiltration plant is applied. The key model parameters are identified from experimental data from a laboratory membrane unit to reflect the considered biorefinery process. The model is then simulated to study the sensitivity of the uncertain model parameters (related to membrane fouling, solute concentrations, viscosity, and mass transfer coefficients) to the diafiltration plant performance (product purity, operation time). The model is implemented in the MATLAB®/Simulink environment. The simulation results are expected to identify potential sources of scale-up challenges in biorefinery-related membrane applications. The developed dynamic model also allows to investigate different operational strategies of diafiltration plants in the future.

1. Introduction

In order to mitigate the global challenges related to the environmental impact and climate change, the bio-based economy drives to substitute fossil-based fuels and chemicals with their more sustainable, bio-based counterparts (European Commission and Directorate-General for Research and Innovation, 2017). Chemical industries are energy-intensive and mostly relied on fossil-based petrochemical feedstocks; the use of biomass as a feedstock for intermediate chemicals production can be seen as a major shift toward more sustainable production (Fiorentino *et al.*, 2019). From the potential raw materials, lignocellulosic biomass has a great potential having a good availability and being a non-food biomass.

In the BioSPRINT project,[1] the hemicellulosic fraction of lignocellulosic biomass is valorized into furan-based polymers. The hemicelluloses are heterogenous polysaccharides comprising a range of sugar monomers, such as xylose, glucose, arabinose, mannose *etc*. However, in biomass side streams from different biorefineries (*e.g.*, pulping, steam explosion or fermentation), the hemicelluloses are in a water-solute mixture also containing impurities such as short-chain acids, degradation products, phenolic compounds, and soluble inorganic species. In catalytic conversion, these can have considerable interactions with the catalyst. Thus, efficient purification of hemicellulosic sugars is needed prior to the catalytic conversion steps to produce bio-based chemicals.

Membrane technologies have been proposed for different kinds of biorefinery applications (Abels *et al.*, 2013). Applicability studies of nanofiltration (NF), reverse osmosis (RO) and ultrafiltration (UF) membranes for lignocellulosic hydrolysates includes examples such as fractionating hemicelluloses from pulp mill process waters (Krawczyk, 2013), concentration and purification of lignin from pulping liquors (Jönsson *et al.*, 2008), and development of purification cascades for the Organosolv process (Nitzsche *et al.*, 2022). Some of the results have also been transferred to the pre-industrial scale (Nguyen *et al.*, 2016). Diafiltration is a membrane purification technology, where the retentate (stream that the membrane rejects) is diluted to overcome the decreased separation efficiency when the retentate viscosity increases, and thus enables further removal of the impurities to the permeate (stream

[1] https://www.biosprint-project.eu/

that passes the membrane) (Doran, 2013; Nguyen *et al.*, 2016).

Process modeling typically plays an important role in process design and scale-up. In the case of membrane systems, the scale-up is governed by permeate flux values, which affect the separation efficiency, purity of product stream and required membrane surface area (sizing). The membrane fouling, which is accumulation of material to membrane surfaces and pores thus decreasing the permeate flux, is another important factor in process design. Theoretical analysis cannot offer tools to predict all of the aspects (Doran, 2013). For instance, (Nguyen *et al.*, 2016) stated that the pilot-scale membranes may have 30—45% lower water permeability than observed in laboratory membrane units. Thus, the mathematical modeling of diafiltration processes has focused, for example, on studying intermittent diluent addition scenarios in different levels of details (Wang *et al.*, 2008; Tan and Franzreb, 2022), prediction of fouling dynamics (López-Murillo *et al.*, 2021), or integrated process and control design (Hunter, 2000; Yee *et al.*, 2012; Saltık *et al.*, 2017).

This study takes the first steps related to the integrated process and control design of a diafiltration plant processing hemicelluloses from lignocellulosic biomass. A dynamical mass-balance based model of the diafiltration plant is implemented, the key model parameters are identified from laboratory membrane experiments and the scaled-up purification step of the biorefinery process is simulated. The simulations in this study focus on assessing the uncertainty of laboratory data derived model parameters on a selected design criterion.

The process model is presented in Section 2 together with a short description of acquisition of the experimental data. Section 3 focuses on the parameter estimation of the model and the development of a scaled-up simulator. The sensitivity of the selected model parameters is studied in Section 4, followed by the summary in Section 5.

2. Material and methods

2.1. Simulation model

A lumped parameter dynamical model of the diafiltration plant originated from (Hunter, 2000) is applied. The model comprises retentate mass balances of component *j* (see Eq. 1) over membrane stage *i* given in volumetric flows *Q* and concentrations *C* as weight fractions. Subscripts *F*, *DF*, *P* and *R* stand for feed, diafiltration, permeate and retentate, respectively. Fig. 1 illustrates the stage *i* with inputs, outputs and state variables given in Eq. 2 and Eq. 3.

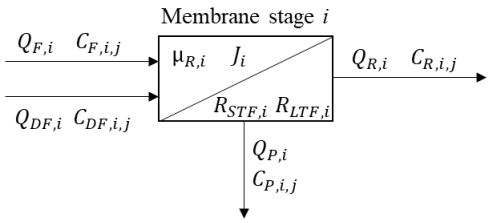

Figure 1: Model boundaries and variables for a single membrane stage.

The equation set for the case, where the feed flow is treated as a degree of freedom, is as follows:

$$\begin{aligned}\rho_{R,i}V_i\frac{dC_{R,i,j}}{dt} = {} & \rho_{F,i}Q_{F,i}C_{F,i,j} \\ & + \rho_{DF,i}Q_{DF,i}C_{DF,i,j} \\ & - \rho_{P,i}Q_{P,i}\left(1-R_j\right)C_{R,i,j} \\ & - \left(\rho_{F,i}Q_{F,i}+\rho_{DF,i}Q_{DF,i}\right. \\ & \left. - \rho_{P,i}Q_{P,i}\right)C_{R,i,j}\end{aligned} \quad (1)$$

$$\frac{dR_{STF,i}}{dt} = 10^{-13}\frac{k_1 J_i C_{R,i,foul}\mu_{R,i}}{\rho_{R,i}} - k_2 R_{STF,i} \quad (2)$$

$$\frac{dR_{LTF,i}}{dt} = k_3 R_{STF,i} \quad (3)$$

$$J_i = \frac{\Delta P_{TMP} - \Delta\pi_i}{\mu_{P,i}R_{tot,i}} \quad (4)$$

$$R_{tot,i} = R_{P,i} + 10^{13}\left(R_{STF,i} + R_{LTF,i}\right) \quad (5)$$

$$R_{P,i} = max\left\{\begin{array}{c}\dfrac{\Delta P_{TMP} - \Delta\pi_i}{\mu_{P,i}K_{m,i}ln\left(\frac{C_{gel,i}}{C_{R,i,foul}}\right)} - R_m \\ \\ 0\end{array}\right\} \quad (6)$$

Where $\rho_{R,i}$ is the retentate stream density in stage *i*, V_i is the stage volume, $\rho_{F,i}$, $\rho_{DF,i}$, $\rho_{P,i}$ are the stream densities and R_j is the retention coefficient for component *j*. In Eq. 2, the short-term fouling ($R_{STF,i}$) is given as a function of permeate flux J_i, concentration of fouling components ($C_{R,i,foul}$), dynamic viscosity of the retentate stream ($\mu_{R,i}$) and density ($\rho_{R,i}$). The two parameters k_1 and k_2 determine the rate of change. The long-term fouling (Eq. 3) is dependent on the short-term fouling via the parameter k_3.

The total permeate flux (J_i) in Eq. 4 is dependent on the trans-membrane pressure (ΔP_{TMP}), the osmotic pressure ($\Delta\pi_i$), the permeate stream viscosity ($\mu_{P,i}$), and the total membrane resistance ($R_{tot,i}$, Eq. 5), which is a sum of the above fouling terms together with the concentration polarization resistance (R_P, Eq. 6). R_P is given as a function of ΔP_{TMP}, $\mu_{P,i}$, mass-transfer coefficient ($K_{m,i}$), threshold for fouling components concentration

($C_{gel,i}$), and constant membrane resistance (R_m). However, in this study a negligible osmotic pressure is assumed due to the low feed flow and working in narrow volumetric reduction ratio.

Finally, by multiplying the permeate flux with the membrane cross-sectional area (A_i), the permeate flow is attained. In addition, the model implementation involves a perfectly mixed buffer tank for the purified stream (Eq. 7) and first-order dynamics for the diafiltration addition based on the permeate flux of the previous stage (Eq. 8). In the simulations, the inlet mass flow ($\dot{m}_{B,j,in}$) to the buffer tank is the final retentate stream and no outflow from the buffer tank is assumed. Thus, Eq. 7 simplifies into an integral.

$$\frac{d\dot{m}_{B,j}}{dt} = \dot{m}_{B,j,in} - \dot{m}_{B,j,out} \quad (7)$$

$$G(s) = \frac{Q_{DF,i+1}}{Q_{P,i}} = \frac{1}{0.95s + 1} \quad (8)$$

Other assumptions related to the diafiltration simulation model are as follows:

- No hydraulic losses along the flow direction.
- Stream consists of monomeric sugars, impurity components (small-chain acids and degradation products), phenolic compounds (lignin) and inorganics mixed to water.
- Only sugar and phenolic concentrations contribute to fouling ($C_{R,i,foul}$).
- The water content of the feed and permeate streams are high, thus the density and dynamic viscosity are equal to water at 25°C.
- The changes in the dynamic viscosity of retentate streams ($\mu_{R,i}$) are assumed to follow the relation for aqueous solution of glucose given in (Converti *et al.*, 1999).
- Retention coefficients R_j do not change in the studied range of flows, concentrations, and operation conditions.
- The model parameters k_1, k_2, k_3, K_m, R_m and C_{gel} are similar for all stages *i*.

The stage model was implemented as a Matlab® function and extended to the diafiltration plant model in Simulink where several stage models can be connected to each other and solved simultaneously. In order to improve the numerical performance of the simulator, the exponential factors were used in Eq. 2 and Eq. 5. This allowed to balance the amplitudes of the derivatives during the numerical integration, where in total 52 ordinary differential equations were solved simultaneously. The initial states were zero, corresponding a start-up of a membrane system initially filled with water only. The 'ode45' variable-step solver was used in these simulations.

2.2 Experimental data

The laboratory-scale batch membrane filtration unit CELFA P-28 (CM-Celfa Membrantechnik AG, Switzerland) was used in the experiments with a commercially available thin film composite NF membrane. The experimental conditions correspond to the cross-flow velocity of 0.63 m/s and trans-membrane pressure of 19 kPa. The permeate flux values were recorded during the batch trial with a duration of 120 minutes, when the system was tested with a lignocellulosic hydrolysate comprising different sugar monomers, short-chain acids and degradation products, soluble phenols, and inorganic compounds. The unit was also run with pure water before and after the experiments to evaluate the flux degradation and calculating the model parameter R_m analytically. The average values of the permeate flux in four consecutive experiments were used in the parameter estimation in Section 3. The experiments were conducted in a concentration mode, but due to the low flux values, and the unavailability of reliable and frequent concentration measurements, it was assumed that the feed concentrations in the experiments are constant.

3. Parameter estimation and scale-up

The three fouling parameters k_1, k_2, k_3 and the mass-transfer coefficient K_m were estimated based on the flux behavior in a lab-scale unit. The model identification assumed a spiral-wound membrane leaf with similar cross-flow velocity as in the laboratory experiments. According to (Roy *et al.*, 2015), the leaf area of 1 m^2 and the channel height of 0.7 mm was chosen for a single leaf. These results in a feed flowrate of 1.58 m^3/h (0.00044 m^3/s).

The optimization of the parameters was conducted with the Nelder-Mead Simplex Method using Matlab® function 'fminsearch'. Fig. 2 shows the observed and modelled permeate flux given as a volumetric flow per unit area.

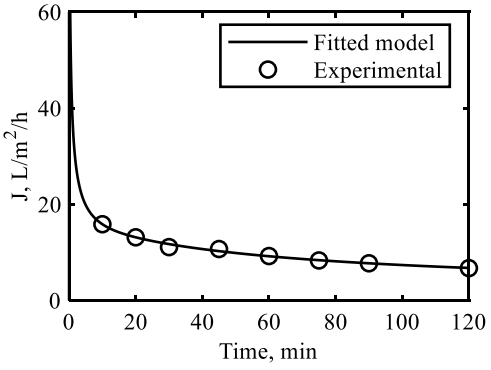

Figure 2: Permeate flux.

The estimated parameters are given in Tab. 1. Other model parameters are listed in Tab. 2. The lumped retention coefficients for sugars, impurities and inorganics are selected based on the experimental results and the retention coefficient of phenols is assumed to follow the sugar retention for simplicity.

Finally, the system was scaled-up for the feed flow value of 20,000 m^3/h. The total membrane area was selected to be near the minimal feed flow rate of 60 L/h for each leaf to minimize the effect of osmotic pressure in NF (Roy *et al.*, 2015). Seven diafiltration stages with identical membrane areas and cross-membrane pressures were assumed to the scaled-up plant configuration.

Table 1: Estimated model parameters.

K_m*10^{-5} [m/s]	k_1*10^{24} [s/m^4]	k_2*10^{-3} [1/s]	k_3*10^{-4} [1/s]
7.54	1.74	1.81	5.36

Table 2: Other model parameters.

Parameter	Value	Unit	Note
A	330	m^2	
ΔP_{TMP}	19	kPa	
ρ_P	997.05	g/L	Equal to water in 25°C
ρ_R	997.05	g/L	Equal to water in 25°C
C_{gel}	0.15	-	Estimated from (Doran, 2013)
μ_P	889.1	mPas	Equal to water in 25°C
R_m	3*10^{13}	1/m	
R_{sugars}	0.93	-	
$R_{impurities}$	0.22	-	Retention coefficients
$R_{phenols}$	0.93	-	
$R_{inorganics}$	0.67	-	
$Q_{F,1}$	0.0056	m^3/s	Plant feed flow
C_{sugars}	80	g/L	
$C_{impurities}$	20	g/L	Feed concentrations
$C_{phenols}$	7.04	g/L	
$C_{inorganics}$	0.97	g/L	

4. Sensitivity analysis

Even the continuous membrane systems are actually operated in a batchwise-continuous manner, as the static operation cannot be achieved due to the progressive membrane fouling, requiring periodic production breaks for cleaning (Hunter, 2000). Thus, it is assumed that in the simulated biorefinery case, two operational boundaries hold; (1) The sugar purity in the buffer tank need always to be over 80% to be viable in downstream conversion steps, and (2) the maximum running time of diafiltration plant is 8 hours before service (cleaning).

By simulating the system with the feed concentrations shown in Tab. 2, these thresholds are barely met. Fig. 3 shows the buffer purity as a function time, closing to value of 80% after 8 hours (480 minutes). The model was then simulated to study the sensitivity of uncertain model parameters (related to membrane fouling, solute concentrations, viscosity, and mass transfer coefficients) to the diafiltration plant performance by recording the operation time, where the purity threshold was violated.

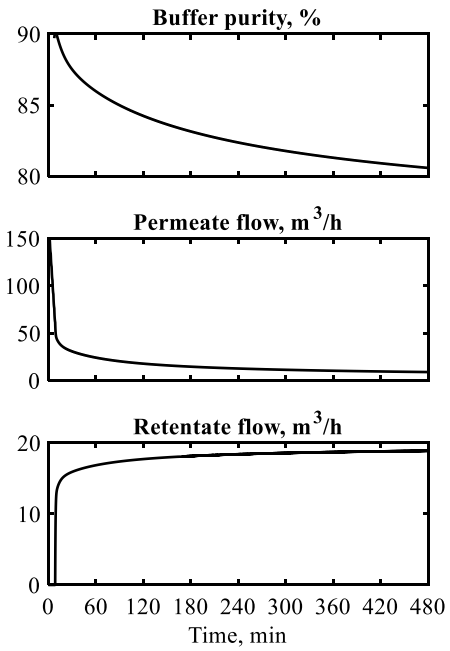

Figure 2: Base case simulation of a diafiltration plant. From top to bottom, sugar purity in buffer tank, total permeate flow, and product flow to the buffer tank, respectively.

In total, 33 simulations were performed by varying model parameters one-at-a-time in different extent. Tab. 3 presents qualitatively the direction of change (in product purity) and quantitatively the operational time, where the above-mentioned purity threshold was not met in the simulation. It can be seen that most of the parameters have only a small effect on this criterion; Even changes ±50% in K_m, R_m or C_{gel} show no effect on the selected criterion. Less surprisingly, the three fouling parameters (k_1, k_2, k_3) show more sensitivity to the selected criterion. ρ_R was only simulated with slightly higher values (up to +5%) as it can be expected that the stream density cannot exceed substantially higher values due to low permeate fluxes and diafiltration water addition. μ_R shows a moderate effect only after an increment of over 30% in its value. This kind of an increment in a stream dynamic viscosity is not expected unless the stream contains longer hydrocarbons (such as oligomeric sugars, alcohols), which is not the case with the studied stream.

Table 3: Direction of change in product purity and the time of threshold violation (in minutes). The target operation time for the diafiltration plant was 480 minutes.

Parameter	-50%	-25%	-15%	+5%	+15%	+25%	+30%	+50%
ρ_R				↑				
μ_R				↓	↓	↓	**466**	
R_m	↓		↓			↑		↑
K_m	↓	↓						
C_{gel}	↓	↓	↓		↑	↑		
k_1			↑			↓	**466**	**401**
k_2	**299**	**454**	↓			↑		
k_3		↑				↓	**471**	
$C_{phenols}$	↑	↑	↑		↓	**463**		**336**

The solute feed concentration changes were simulated by adjusting the ratio of impurities and phenolic compounds, and this way keeping the initial stream purity at constant value. As the retention coefficient of phenols is equal to that of sugars, the higher amount of phenols in the feed stream make the purification less efficient. This can also be seen in the results presented in Table 3, where the increment of phenol concentration quite easily results in a violation of the purity threshold. Thus, in the case of inhomogeneous diafiltration feedstock composition, the dimensioning should be made for the worst-case scenario, *i.e.*, for the high phenolic concentration. Otherwise, too optimistic performance of the membrane system is expected, having a considerable effect on the operational and cleaning cycles.

K_m, R_m or C_{gel} are all related to the fixed membrane resistance and the concentration polarization fouling in the applied model (Eq. 6). It has been reported that the concentration polarization is the major fouling mechanism in these kinds of real hydrolysate streams, contributing 71—82% to the total resistance (Nitzsche *et al.*, 2021). Hence, the negligible sensitivity in these simulation results indicate that the applied model cannot adequately represent the concentration polarization behavior and the fouling is dominated by the short-term and long-term fouling instead (Eq. 2 and Eq. 3).

According to the simulation results (Tab. 3), the fouling parameters related to the short-term and long-term fouling (k_1, k_2, k_3) require quite significant changes before the purity threshold is compromised. By looking at Eq. 2, it can be observed that the parameter k_1 should be the most dominant as it initializes the dynamic fouling effects. Indeed, around 30% larger value for k_1 results in a shortened operation time. The effect of parameter k_2 is opposite; it is a negative gain term for the short-term fouling (see Eq. 2) and thus a smaller value accelerates the fouling, whereas a larger value mitigates the fouling dynamics. Finally, parameter k_3 basically describes the shift from short-term fouling to long-term fouling and it takes of around +30% change in the parameter value to deteriorate the diafiltration process outside of the performance criteria.

Fig. 3 presents the product purity as a function of time for the base case (thick dash-dotted line) and for the simulations with changes in parameters k_1, k_2, k_3 (thin gray lines). Obviously, three of the parameter combinations provide improved performance (as also qualitatively shown in Tab. 3), where the purity target is still clearly exceeded at time 480 minutes. For these cases, the total permeate flow at the end of simulation is slightly over 10 m^3/h, whereas for the base case, the total permeate flow was 8.93 m^3/h. Hence, even the modest changes in the flux values correspond to the increased availability of the membrane plant, decreased membrane area requirements, or increased throughput.

On the other hand, the worst simulated case (k_2 −50%) shows the total permeate flow of 6.3 m^3/h at the end of simulation. At the time of product purity violation (t = 299 minutes), the permeate flux in this case was around 8 m^3/h. It is known that the flux degradation of 30—45% can be expected during the scale-up of membranes (Nguyen *et al.*, 2016). In the simulated cases, the total permeate flow between the best and the worst cases was around −37%. Hence, the parameter ranges of the fouling parameters used may reflect the uncertainty related to the scale-up.

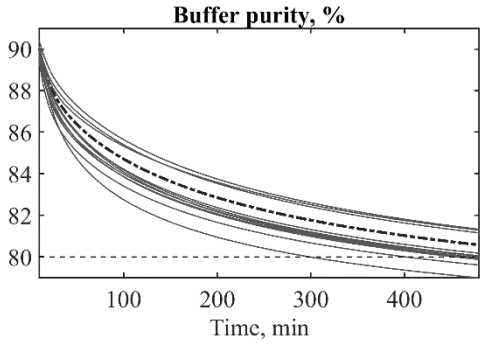

Figure 3: Envelope of diafiltration plant product purity in the simulated fouling scenarios.

5. Summary

This study presented the development of a dynamic simulation model describing a diafiltration system for hemicellulose purification in a biorefinery process. The key model parameters related to the membrane fouling were estimated based on experimental data from a laboratory membrane unit. The model was then scaled-up to reflect an industrial scale system.

Since the model is governed by high number of model parameters, this study focused on assessing the sensitivity of selected model parameters to operational aspect of the diafiltration plant. The simulation results showed that the expected range of uncertainty in many of the studied parameters had a sufficiently small effect on the process (dynamic) performance. This was unexpected especially for the parameters related to the concentration polarization behavior. However, the fouling parameters, together with the feed stream concentrations, showed an important effect on the product purity and operational time of the diafiltration plant.

The overall feasibility of such a diafiltration plant depends not only on the factors studied in these simulations. For example, recovery of valuable compounds can limit the process design; in the studied case, the monomeric sugars are not rejected completely (R_{sugars} = 0.93), therefore causing a loss of sugars to the permeate streams. The model should be accompanied with permeate mass balances to explore these in detail. These would also allow to implement calculation of trans-membrane pressure losses due to osmotic pressure (see *e.g.* (Nguyen *et al.*, 2016)) and this way probably enhance the modeling of the concentration polarization behavior.

Evaluation of economic performance of a diafiltration plant requires more detailed specifications on membrane module configurations and cleaning intervals. For instance, tubular modules instead of spiral-wound modules are more preferable if frequent cleaning is required, but they have lower packing density (Doran, 2013). In addition, energy costs need to be assessed. They are related to pumping costs of streams and diafiltration water and the need to maintain transmembrane pressure throughout the system.

The developed dynamic model allows to study different process configurations (number of stages, recycle flows, diafiltration strategies) and can be utilized in integrated process and control design in the future. It should be noted that the solver selection for this simulation model requires extra care for example in controllability studies, where new membrane modules or diafiltration feeds are started during the operation, thus creating discontinuities to the simulation.

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