Electronic Supplementary Material (ESI) for Green Chemistry.

Supplementary Information for: Recovery of Low Molecular Weight Compounds from Alkaline Pretreatment Liquor via Membrane Separations†

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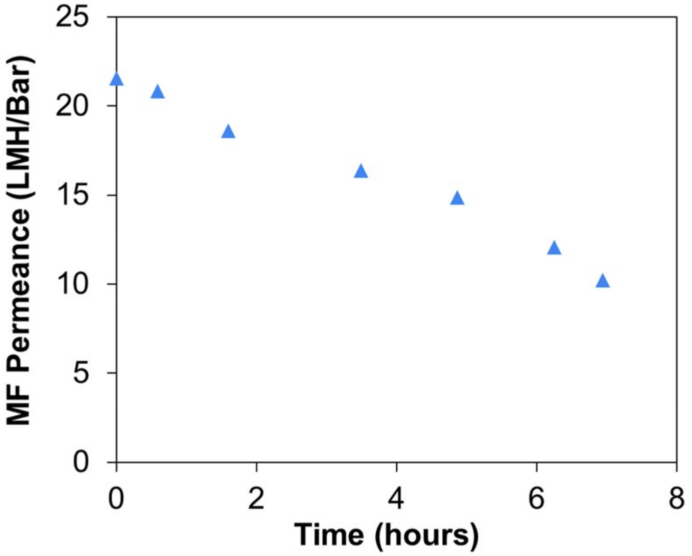


Figure S1. MF permeance. The permeance from an Alfa Laval tangential flow system using the MFP5 microfiltration membrane. APL filtration is shown over 7 hours at which time an 80% volume reduction was reached (initial volume of 20L APL).

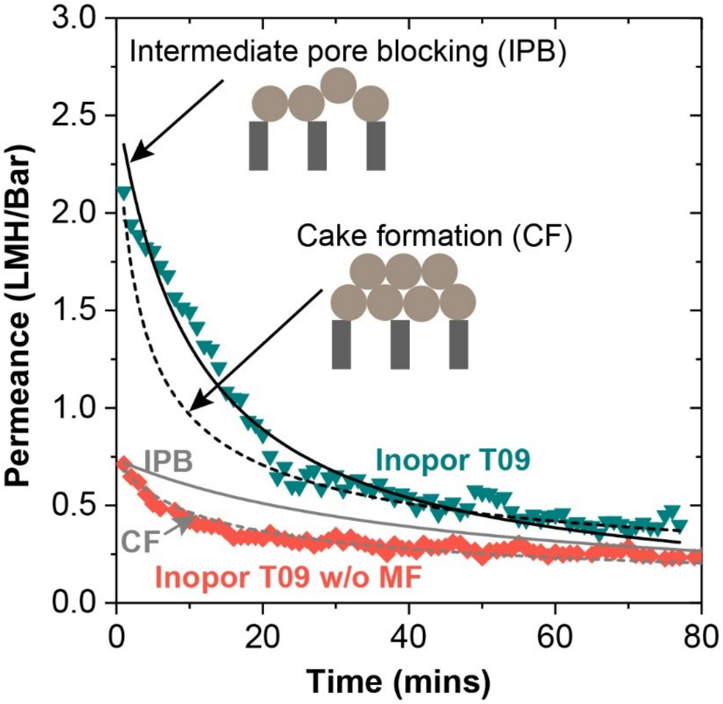


Figure S2. Flux decline. When MF is used for APL pretreatment, the NF permeance decline over time fits to the intermediate pore blocking model more closely than the cake filtration fouling model. However, without the use of MF, the NF permeance decline fits the cake filtration model more closely (see Table S1).

The cake formation model

$$J = J_o(1 + k_c t)^{-0.5}$$

J is the flux, J_o is the initial flux, k_c is the cake filtration constant ($s \cdot m^{-2}$) and t is time (s).

The intermediate pore blocking model:

$$\frac{1}{J^2} = \frac{1}{J_o^2} + kt$$

J is the flux, J_o is the initial flux, k is the intermediate pore blocking constant (m^2) and t is time (s).

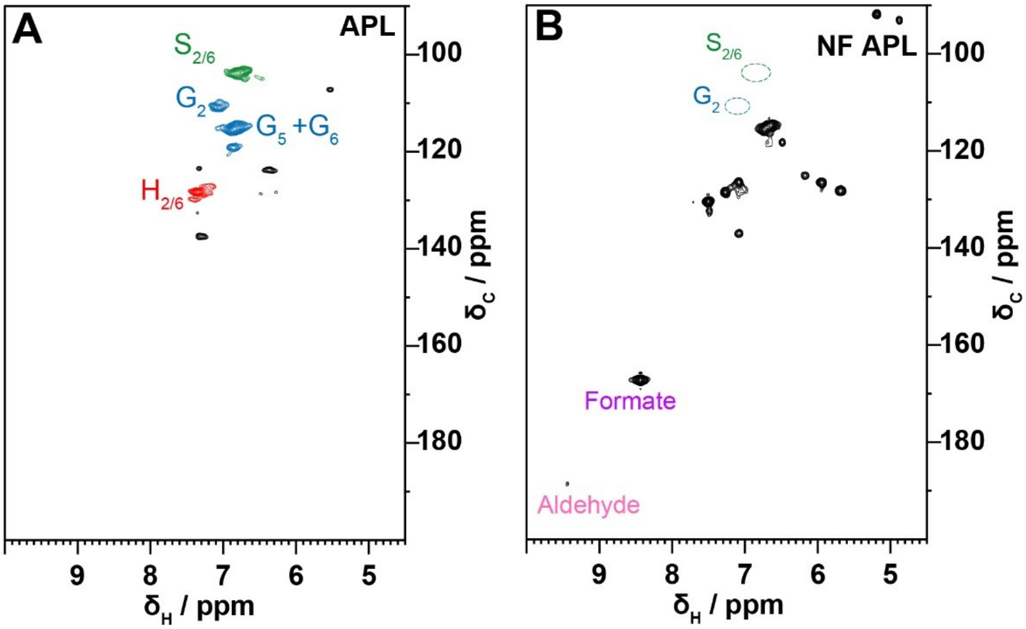


Figure S3. 2D HSQC NMR. 2D HSQC NMR of the (A) APL starting material aromatic region; (B) NF permeate APL aromatic region.

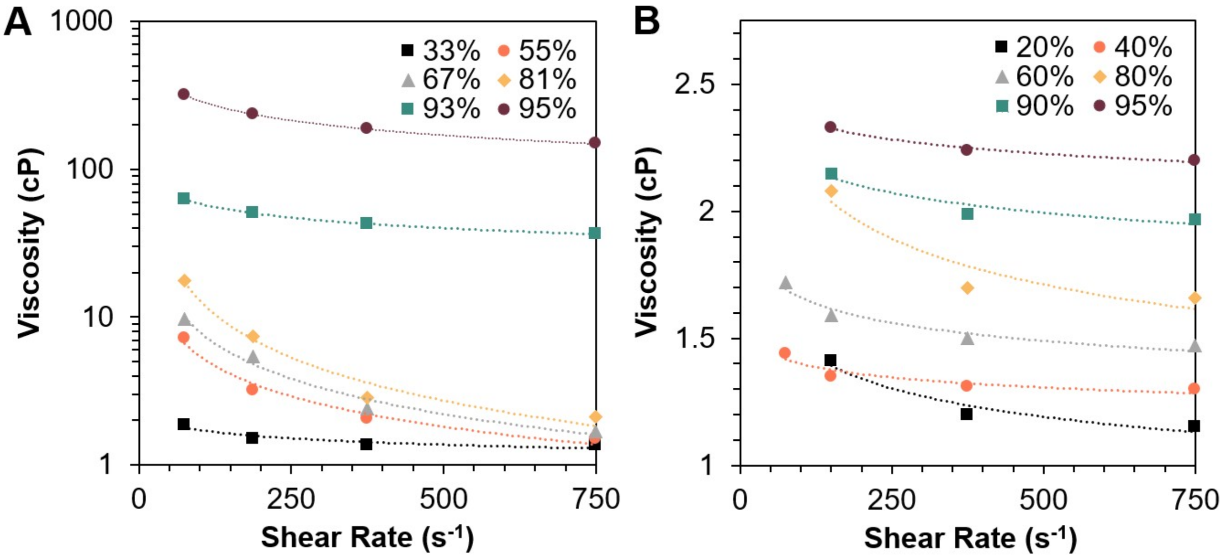


Figure S4. Experimental viscosity. The viscosity (cP) of the APL retentate stream for (A) microfiltration and (B) nanofiltration as a function of the shear rate (s^{-1}) at six different volume recoveries between 20% and 95%. The APL retentate is classified as a Non-Newtonian, shear thinning fluid where viscosity decreases with increasing shear rate according to a power law model.

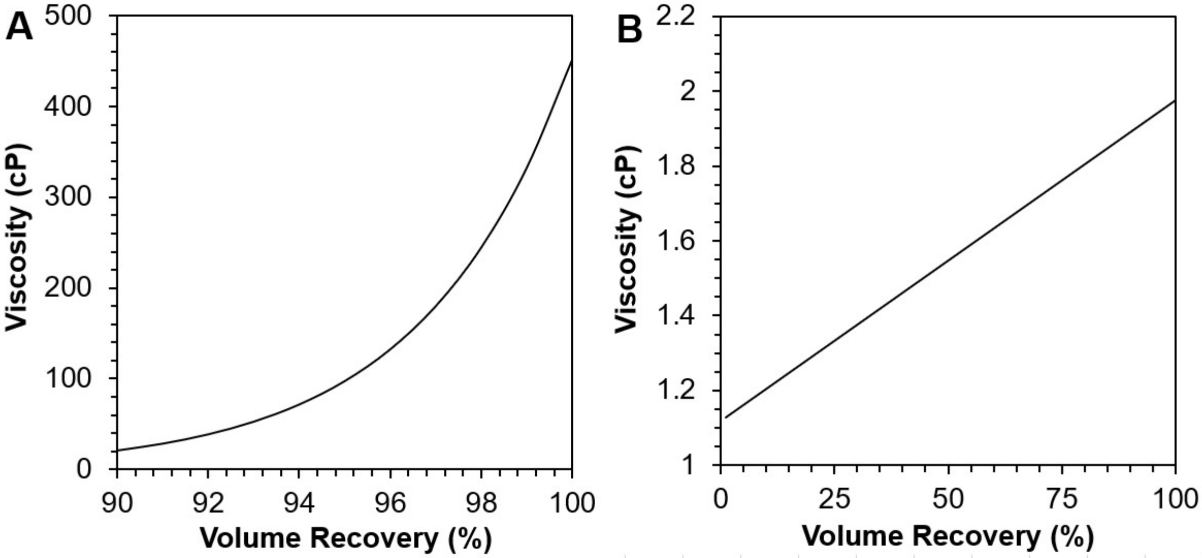


Figure S5. Model viscosity. The modeled viscosity (cP) of the APL retentate stream for (A) microfiltration and (B) nanofiltration as a function of the volume recovery. The viscosities are calculated using a power law model (Equation S23) with parameters estimated from experimental data (Figure S6) at shear rates of 1000 s^{-1} and 2700 s^{-1} for MF and NF, respectively.

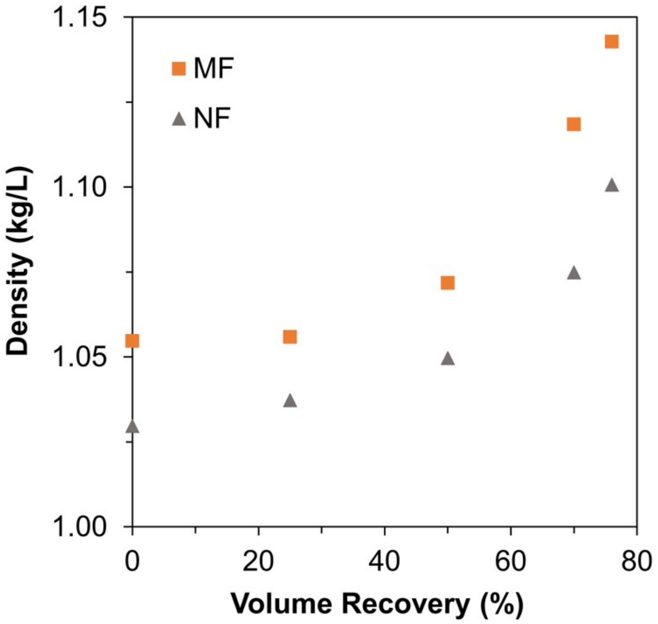


Figure S6. Density. The density (kg/L) of the APL retentate stream for microfiltration and nanofiltration as a function of the volume recovery.

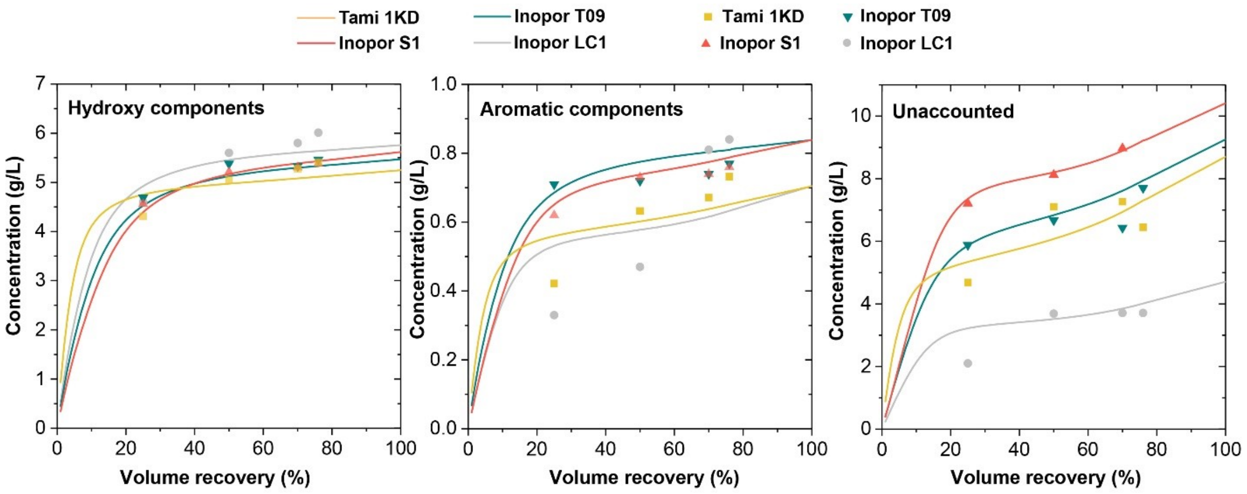
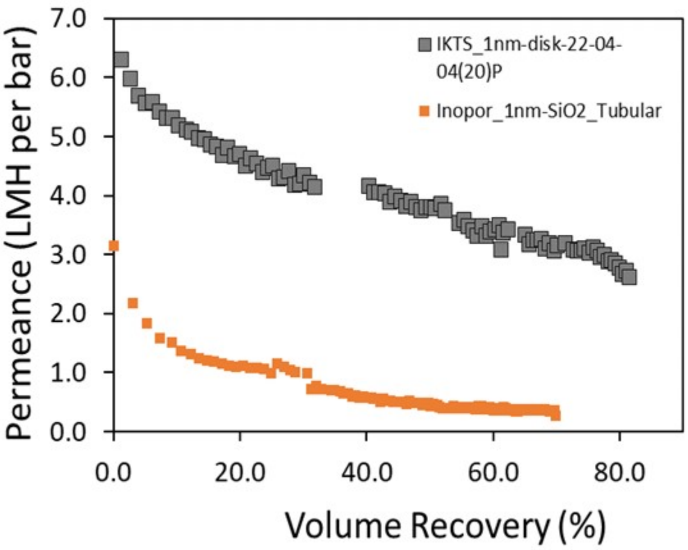


Figure S7. Mixing cup output. The concentration (g/L) of hydroxy (non-aromatic), aromatic and unaccounted lignin in NF APL permeate measured from the batch tangential flow filtration experiments (markers) compared to the concentrations predicted using the batch TFF model (solid lines). The concentration data is presented as a function of the volume recovery of the system for the four nanofiltration membranes screened.



Sample treatment	Membrane ID	Membrane Material	Nominal cut-off	HMW rejection (%)	M_w	PDI	LMH/bar (Average)
MF/NF	Inopor S1 (Tubular)	SiO_2	600 Da	93.4	630	1.6	0.96
MF/NF	IKTS 1.0 nm (Disk)	Coated TiO_2	600 Da	93.0	620	1.9	5.0

Figure S8. RCD performance. APL permeance of the IKTS 1-nm disk membrane and the Inopor 1-nm tubular membrane. The membrane ID, material, nominal cut-off, HMW rejection, and permeate molecular weight (Mw), PDI, and permeance are listed below the graph.

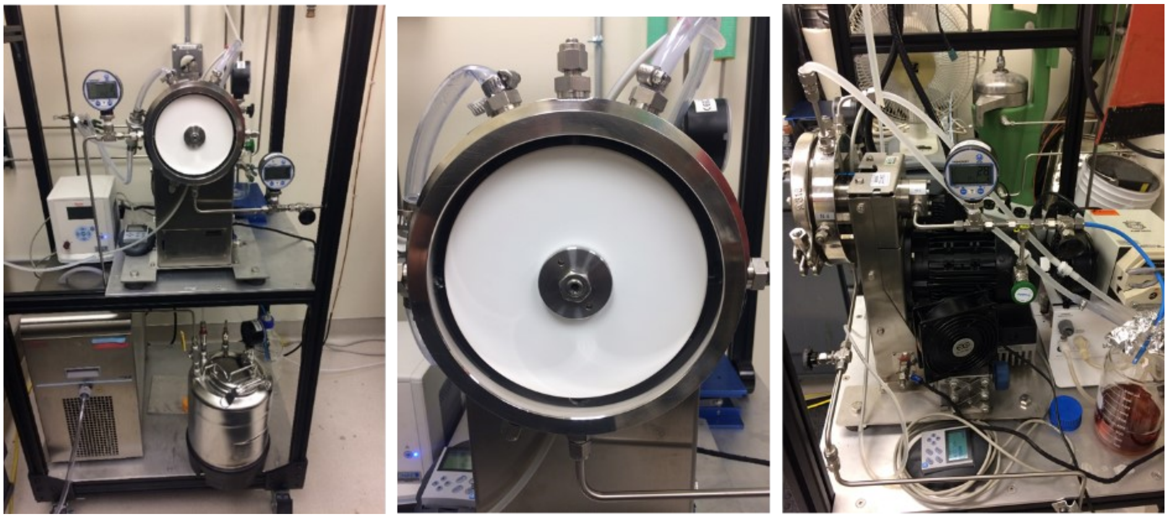


Figure S9. RCD module. Photos of the RCD (rotating ceramic disk) system (Andritz, DCF 152/S). This is the smallest unit available from Andritz and features a single ceramic disk that is interchangeable.

Table S1. Flux decline parameters. The permeance of NF membranes was fit to the cake formation and intermediate pore blocking models. The chi-squared value (X^2) gives an indication of goodness of fit with a low X^2 corresponding to a higher confidence in the fit.

APL sample treatment	Membrane ID	Nominal cut-off	Water permeance (LMH/bar)	Cake formation constant	Intermediate pore blocking constant	Cake formation X^2	Intermediate pore blocking X^2
MF/NF	Tami 1KD	1 kDa	3.4	0.036	0.0023	2.11	0.64
MF/NF	Inopor S1	600 Da	10.1	0.024	0.0022	12.28	4.55
MF/NF	Inopor T09	450 Da	11.6	0.03	0.0027	8.06	1.52
MF/NF	Inopor LC1	200 Da	8.9	0.03	0.0027	10.82	2.15
NF	Inopor T09	450 Da	11.6	0.09	0.0022	0.18	3.25

	wt.% Ash	**wt.% Lignin**	**wt.% Glucan**	**wt. % Xylan**	**wt.% Galactan**	**wt.% Arabinan**	**wt.% Acetyl**	**wt. % total**
APL	29.77	28.75	3.26	10.02	1.95	4.10	5.07	82.91
Inopor T09 Retentate	19.36	36.45	3.65	13.13	2.50	5.32	0.36	80.78
Inopor T09 Permeate	52.54	4.36	2.44	0.62	0.52	0.42	13.17	74.06

Table S2. Compositional analysis.

Table S3. Tracked compounds. Concentration of tracked compounds in APL and permeate samples at 70 vol.% recovery.

	Component	**MW (Da)**	**APL (g/L)**	**MF APL (g/L)**	**Tami 1KD (g/L)**	**Inopor S1 (g/L)**	**Inopor T09 (g/L)**	**Inopor LC1 (g/L)**
	Total carbon	n/a	24.9	12.5	5.1	5.6	5.5	4.4
Non-aromatic species								
1	Acetic acid	60.1	3.59	3.59	3.39	3.43	3.59	3.59
2	Lactic acid	90.1	0.52	0.52	0.45	0.47	0.45	0.52
3	Glycolic Acid	76.1	0.22	0.22	0.17	0.19	0.19	0.22
4	Malic Acid	134.1	0.60	0.60	0.51	0.54	0.54	0.55
5	Formic Acid	46.0	0.61	0.61	0.54	0.56	0.58	0.61
6	Oxalic Acid	90.0	0.21	0.21	0.21	0.22	0.21	0.23
7	Propionic Acid	74.1	0.04	0.04	0.00	0.00	0.00	0.10
8	Glycerol	92.1	0.20	0.20	0.20	0.20	0.20	0.20
9	Glyceric acid	106.1	0.21	0.21	0.21	0.21	0.21	0.21
10	Malonic Acid	104.1	0.16	0.16	0.00	0.00	0.00	0.16
11	Succinic Acid	118.1	0.04	0.04	0.00	0.00	0.00	0.04
12	Fumaric Acid	116.1	0.05	0.05	0.00	0.00	0.00	0.12
Aromatic species								
13	p-coumaric acid	164.0	0.73	0.73	0.48	0.56	0.64	0.67
14	Ferulic acid	194.2	0.09	0.09	0.07	0.08	0.08	0.08
15	4-Hydroxybenzaldehyde	122.1	0.04	0.04	0.04	0.04	0.04	0.04
16	4-Hydroxybenzoic Acid	138.1	0.01	0.01	0.01	0.01	0.01	0.01
17	Vanillic Acid	168.1	0.01	0.01	0.01	0.01	0.01	0.00
18	Syringic Acid	198.2	0.01	0.01	0.01	0.01	0.01	0.00
19	Vanillin	152.2	0.02	0.02	0.02	0.02	0.02	0.02
20	Acetovanillone	166.2	0.01	0.01	0.01	0.01	0.01	0.00
21	Syringaldehyde	182.2	0.00	0.00	0.01	0.01	0.01	0.00
22	Acetosyringone	196.2	0.05	0.05	0.01	0.01	0.02	0.07

Table S4. Rejection Coefficient (%)

Component	MF	Tami 1KD	Inopor S1	Inopor T09	Inopor LC1
Non-aromatic	0	12	9	9	9
Aromatic	0	27	25	11	48
Unaccounted	57	70	63	70	82
Total Carbon	50	60	54	59	68

$$R = 1 - \frac{C_p}{C_f}$$

R is the rejection coefficient, C_p is the concentration of the component in the permeate $(g \cdot L^{-1})$, and C_f is the concentration of the component in the feed $(g \cdot L^{-1})$.

Table S5. Parameter assumptions for batch TFF model

Component Group	Diffusivity x 10^{10} (m^2/s)	Van't Hoff Coefficient
Non-aromatic	9.9	1
Aromatic	8.4	0.63
Unaccounted	4.3	0.03

Diffusivity values are based on those for acetic acid, p-aminobenzoic acid and raffinose for tracked compounds and unaccounted lignin, respectively.[1, 2]

The osmotic factor and Van't Hoff coefficient of the hydroxy group is based on glycolic acid data,[3] and the Van't Hoff coefficients are scaled with MW. The MW of p-coumaric acid is used for the aromatic group, and the mean MW from HMW GPC data (Figure 2) is used for the unaccounted group.

Table S6. Constant parameter inputs for batch TFF model

Parameter	Value	Unit
Number of cells per module	10	n/a
Module length	0.357	m
Module inner diameter	0.70	cm
Transmembrane pressure	1.33	MPa
Osmotic Factor	32.4	MPa

Table S7. Flow rates. Stream flow rates in two-stage process

Stream #	Stream name	Flow rate (L/h)
1	Feed	10,000
2	Recycle + Feed	13,115
3	MF Inlet	19,866
4	MF Permeate	12,459
5	MF Retentate	7,407
6	Purge	656
7	MF Recirculation	6,751
8	NF Inlet	53,535
9	NF Permeate	9,344
10	NF Retentate	44,190
11	NF Recirculation	41,076
12	Recycle	3,115

Table S8. Required membrane area

	Tami 1KD	Inopor S1	Inopor T09	Inopor LC1
MF area (m^2)	716	716	716	716
NF area (m^2)	1038	703	806	820

Table S9. Capital expenses.

Capital expense	Tami 1KD	Inopor S1	Inopor T09	Inopor LC1
MF modules ($)	1,768	1,768	1,768	1,768
NF modules ($)	116,904	80,316	90,701	92,293
Pumps ($)	29,334	29,334	29,334	29,334
Auxiliary equipment ($)	37,627	37,627	37,627	37,627
Total Capital expenses ($)	185,633	149,045	159,431	161,022
Taxes ($/$m^3$)	0.038	0.038	0.038	0.038
Total Capital expenses ($/$m^3$)	0.12	0.11	0.11	0.11

Table S10. TEA assumptions

Parameter	Value	Unit
Plant lifetime	30	years
Plant operating time	7884	hours/year
Membrane module cost	25	% of membrane material cost
Energy price	0.068	$/kWh
Internal rate of return (IRR)	10	%
MF membrane material cost	10	$/$m^2$
MF membrane material lifetime	2	years
NF membrane material cost	450	$/$m^2$
NF membrane material lifetime	15	years

Table S11. Membrane properties.

Membrane name	Membrane ID	Membrane Material	Porosity	HMW rejection (%)	Nominal cut-off	LMH/bar (Average)
Alfa Laval MFP5	MF	Polypropylene support/ Fluoro polymer active layer		2.7	0.5 µm	17.4
Tami MSKTT01001KD	Tami 1KD	TiO_2	n/a	94.0	1 kDa	0.66
Inopor AA0250-A3S1G	Inopor S1	SiO_2	30-40%	93.4	600 Da	0.96
Inopor AA0250-A3T09G	Inopor T09	TiO_2	30-40%	97.6	450 Da	0.85
Inopor AA0250-A3LC1G	Inopor LC1	TiO_2	30-40%	98.6	200 Da	0.84

n/a: not available

Process Model Operating Guide

The process model code made available on Github consists of two main parts – the batch TFF model and the energy consumption model. The batch TFF model contains two Python files: 'Module.py' and 'TFF_Functions.py' and two Jupyter Notebook files: 'Selectivity Optimization.ipynb' and 'Batch TFF Main.ipynb'. The Module file contains the parameters specific to the membrane module such as its geometry and free water permeance. The TFF Functions file contains functions used to simulate a TFF module, including viscosity and flux decline fits and retentate and permeate concentration solvers. Each NF membrane being modeled will have a unique Module file, while the TFF_Functions file does not need to be updated. The Selectivity Optimization file is used to determine the membrane selectivity of each component and does so using a least squares optimization function. Once the selectivity values are determined using the Selectivity Optimization file, they can be inputted into the Batch TFF Main file which calculates the stream concentrations as a function of volume recovery for our batch TFF experimental process.

The batch TFF model uses a single stage batch NF model to determine the selectivity values for the NF process, but the energy consumption model, consisting of one main Jupyter Notebook file 'Two-Stage TFF Energy Consumption.ipynb', is used to estimate the stream flowrates, compositions and recoveries, and TEA (energy consumption and membrane area) of the two-stage scaled-up MF/NF continuous filtration system. The process model code is customized specifically for our experimental apparatus, membrane type, operating conditions and feed stream, however the general approach can be applied to other tangential flow filtration systems and feedstocks. Equations S3-S19 provide a framework for estimating the membrane selectivity and permeate and retentate concentrations for a multicomponent NF TFF system, and the parameter inputs and assumptions can be easily modified depending on the feed material. In addition, the Module and Batch TFF Main files can be modified for different membranes and process flow structures. Finally, the energy consumption model provides a framework for a two-stage filtration system but could be adapted for a single-stage or cascade system with two or more membrane stages.

[*]Python codes used to generate Figure 5, Table 3, Table 4, and Table S7 are available on GitHub.com (NREL-SEPCON - https://github.com/NREL-SEPCON/Lignin-Filtration)

Batch TFF Model Equation List

Note: For all subsequent equations, subscript r indicates the retentate side, subscript p indicates the permeate side, subscript w indicates the membrane wall, and subscript m refers to the solute being considered (non-aromatic, aromatic, or unaccounted compounds).

Solvent and Solute Flux

This model uses equations for a reverse osmosis (RO) system that have been adapted to a multicomponent NF system.[4] First, the solvent flux is calculated; for this system, the solvent is water. In an RO system, the driving force for the solvent flux is the difference between the transmembrane pressure drop and the osmotic pressure difference across the membrane:

$$J_{solv} = K_{solv}\left[\left(P_r - P_p\right) - \sum_{m=1}^{R} \pi_{r,m}\left(x_{w,m}\right) - \pi_{p,m}\left(x_{p,m}\right)\right] \quad \text{(Equation S1)}$$

In Equation S1, J_{solv} is the mass flux of the solvent $\left(kg \cdot m^{-2} \cdot s^{-1}\right)$, K_{solv} is the permeance of the solvent $\left(kg \cdot Pa^{-1} \cdot m^{-2} \cdot s^{-1}\right)$, P is pressure (Pa), π_m is the osmotic pressure of the solute (Pa), and x_m is the mass fraction of the solute.

For RO and NF systems, concentration polarization must be considered. To account for concentration polarization, the concentration polarization modulus M is introduced:

$$M_m = \frac{x_{w,m}}{x_{r,m}} \quad \text{(Equation S2)}$$

In Equation S2, M_m is the concentration polarization modulus for the solute, $x_{w,m}$ is the mass fraction of the solute at the membrane wall, and $x_{r,m}$ is the mass fraction of the solute in the bulk retentate.

The osmotic pressure difference is calculated via the following:

$$\sum_{m=1}^{R} \left(\pi_{r,m}\left(x_{w,m}\right) - \pi_{p,m}\left(x_{p,m}\right)\right) = \sum_{m=1}^{R} \varphi * a_m\left(M_m x_{r,m} - x_{p,m}\right) \quad \text{(Equation S3)}$$

In Equation S3, π_m is the osmotic pressure of the solute (Pa), x_m is the mass fraction of the solute, φ is the osmotic pressure factor (Pa), a_m is the Van't Hoff coefficient, and M_m is the concentration polarization modulus.

Combining Equations S3 and S5, the following equation for solvent flux is derived:

$$J_{solv} = K_{solv}\left[\left(P_r - P_p\right) - \sum_{m=1}^{R} \varphi * a_m\left(M_m x_{r,m} - x_{p,m}\right)\right] \quad \text{(Equation S4)}$$

In Equation S4, J_{solv} is the mass flux of the solvent $\left(kg \cdot m^{-2} \cdot s^{-1}\right)$, K_{solv} is the permeance of the solvent $\left(kg \cdot Pa^{-1} \cdot m^{-2} \cdot s^{-1}\right)$, P is pressure (Pa), φ is the osmotic pressure factor (Pa), a_m is the Van't Hoff coefficient, M_m is the concentration polarization modulus and x_m is the mass fraction of the solute.

The driving force for the solute flux is the difference between the mass fraction of the solute at the membrane wall and in the permeate:

$$J_m = K_m\left(M_m x_{r,m} - x_{p,m}\right) \quad \text{(Equation S5)}$$

In Equation S5, J_m is the mass flux of solute $(kg \cdot m^{-2} \cdot s^{-1})$, K_m is the permeance of the solute $(kg \cdot m^{-2} \cdot s^{-1})$, M_m is the concentration polarization modulus for the solute, and x_m is the mass fraction of the solute.

The total flux is calculated as the sum of the individual component fluxes:

$$J_{tot} = \sum_{m=1}^{R} J_m + J_{solv} \qquad \text{(Equation S6)}$$

In Equation S6, J_{tot} is the total mass flux $(kg \cdot m^{-2} \cdot s^{-1})$, and J_m and J_{solv} are the mass fluxes of solute and solvent $(kg \cdot m^{-2} \cdot s^{-1})$, respectively.

Mass Fractions

The mass fraction of the solute can be calculated from a ratio of the flux values:

$$x_m = \frac{J_m}{J_{tot}} \qquad \text{(Equation S7)}$$

In Equation S7, x_m is the mass fraction of solute, J_m is the mass flux of solute $(kg \cdot m^{-2} \cdot s^{-1})$ and J_{tot} is the total mass flux $(kg \cdot m^{-2} \cdot s^{-1})$.

Subsequently, the mass fraction of solvent can be calculated:

$$x_{solv} = 1 - \sum_{m=1}^{R} x_m = \frac{J_{solv}}{J_{tot}} \qquad \text{(Equation S8)}$$

In Equation S8, x_{solv} is the mass fraction of solvent, x_m is the mass fraction of solute. J_{solv} is the mass flux of solvent $(kg \cdot m^{-2} \cdot s^{-1})$ and J_{tot} is the total mass flux $(kg \cdot m^{-2} \cdot s^{-1})$.

Combining Equations S9 and S10 yields:

$$J_{tot} = \frac{J_m}{x_m} = \frac{J_{solv}}{x_{solv}} \qquad \text{(Equation S9)}$$

In Equation S9, J_{tot} is the total mass flux $(kg \cdot m^{-2} \cdot s^{-1})$, J_m and J_{solv} are the mass fluxes of solute and solvent $(kg \cdot m^{-2} \cdot s^{-1})$, respectively, and x_m and x_{solv} are mass fractions of the solute and solvent, respectively.

Substituting Equations S6 and S7 into Equation S11 yields:

$$\frac{K_m\,(M_m x_{r,m} - x_{p,m})}{x_{p,m}} = \frac{K_{solv}\left[(P_r - P_p) - \sum_{m=1}^{R} \varphi * a_m (M_m x_{r,m} - x_{p,m})\right]}{1 - \sum_{m=1}^{R} x_{p,m}} \qquad \text{(Equation S10)}$$

In Equation S10, K_m is the permeance of the solute $(kg \cdot m^{-2} \cdot s^{-1})$, M_m is the concentration polarization modulus for the solute, x_m is the mass fraction of the solute, K_{solv} is the permeance of the solvent $(kg \cdot Pa^{-1} \cdot m^{-2} \cdot s^{-1})$, P is pressure (Pa), φ is the osmotic pressure factor (Pa), a_m is the Van't Hoff coefficient, and M_m is the concentration polarization modulus.

The membrane selectivity of solute m can be defined as:

$$\alpha_m = \frac{K_{solv}}{K_m} \qquad \text{(Equation S11)}$$

In Equation S11, α_m is the membrane selectivity of solute (Pa^{-1}), K_{solv} is the permeance of the solvent $(kg \cdot Pa^{-1} \cdot m^{-2} \cdot s^{-1})$, and K_m is the permeance of the solute $(kg \cdot m^{-2} \cdot s^{-1})$.

Substituting Equation S11 into Equation S10 and rearranging yields:

$$1 - \sum_{m=1}^{R} x_{p,m} * (M_m x_{r,m} - x_{p,m}) = x_{p,m} * \alpha_m \left[(P_r - P_p) - \sum_{m=1}^{R} \varphi * a_m (M_m x_{r,m} - x_{p,m}) \right] \qquad \text{(Equation S12)}$$

In Equation S12, x_m is the mass fraction of the solute, M_m is the concentration polarization modulus, α_m is the membrane selectivity of solute (Pa^{-1}), P is pressure (Pa), φ is the osmotic pressure factor (Pa), and a_m is the Van't Hoff coefficient.

The retentate-side mass fractions can be calculated via a mass balance:

$$x_{r,m} = \frac{x_{in,m} - \theta * x_{p,m}}{1 - \theta} \qquad \text{(Equation S13)}$$

In Equation S13, $x_{r,m}$, $x_{in,m}$, and $x_{p,m}$ are the mass fraction of solute in the retentate, feed, and permeate, respectively, and θ is the volume recovery:

$$\theta = \frac{F_p}{F_{in}} \qquad \text{(Equation S14)}$$

In Equation S14, θ is the volume recovery and F_p and F_{in} are the permeate and feed flowrates $(L \cdot h^{-1})$, respectively.

Equations S12-S14 are written for each solute (non-aromatic, aromatic or unaccounted compounds) and solved simultaneously to calculate the permeate-side mass fractions. This is performed in Python using scipy.optimize.least_squares(), where a_m is varied and the output $x_{p,m}$ is compared to experimental data.

Concentration Polarization

Concentration polarization is calculated using an analytical solution derived for laminar flow in round tubes.[5] A dimensionless concentration polarization constant is calculated:

$$G = \frac{v_w^3 \, x \, R}{4 \, u_{in} \, D^2} \qquad \text{(Equation S15)}$$

In Equation S15, G is the concentration polarization constant, v_w is the solute velocity across the membrane $(m \cdot s^{-1})$, x is the axial distance along the membrane (m), R is the radius (m), u_{in} is the average axial velocity $(m \cdot s^{-1})$, and D is the solute diffusivity $(m^2 \cdot s^{-1})$.

The concentration polarization modulus is calculated as a function of the constant G. Two equations are presented, depending on whether the flow under study is in the entry region or sufficiently far into the tube. M_m is calculated using both equations, and the lower of the two values is used:

$$M_m = \frac{c_{w,m}}{c_{b,m}} = 1.536\ (G)^{1/3} + 1\ for\ G \leq 0.02 \qquad \text{(Equation S16)}$$

$$M_m = \frac{c_{w,m}}{c_{b,m}} = G + 6 - 5\ exp\left[-(G)^{1/2}\right] for\ G > 0.02 \qquad \text{(Equation S17)}$$

In Equations S16 and S17, M_m is the concentration polarization modulus for the solute, $c_{w,m}$ and $c_{b,m}$ are the concentrations of the solute at the wall and in the bulk retentate, respectively, and G is the concentration polarization constant.

Energy Demand Equation List

Area

For both the MF and NF stages, the required membrane area is calculated based off the experimentally measured flux values:

$$A = \frac{F_p}{J_M} \qquad \text{(Equation S18)}$$

In Equation S18, A is the required membrane area (m^2), F_p is the volumetric flow rate of the permeate stream $(L \cdot h^{-1})$, and J_M is the volumetric flux $(L \cdot h^{-1} \cdot m^{-2})$.

The area of one module is then calculated based off the chosen module geometry:

$$A_{mod} = \pi \cdot N_c \cdot L \cdot D \qquad \text{(Equation S19)}$$

In Equation S19, A_{mod} is the area of one module (m^2), π is the mathematical constant, N_c is the number of channels in the module, L is the module length (m), and D is the channel inner diameter (m).

The number of modules required for the filtration stage is calculated:

$$N_{mod} = \frac{A}{A_{mod}} \qquad \text{(Equation S20)}$$

In Equation S20, N_{mod} is the number of modules required, A is the required area of the stage (m^2) and A_{mod} is the area of one module (m^2).

Retentate Viscosity

Non-Newtonian, shear thinning fluids obey a power law model:[6]

$$\mu = K\dot{\gamma}^{n-1} \qquad \text{(Equation S21)}$$

In Equation S21, μ is the apparent viscosity $(kg \cdot m^{-1} \cdot s^{-1})$, K is the power law coefficient $(kg \cdot m^{-1} \cdot s^{-(2-n)})$, $\dot{\gamma}$ is the shear rate (s^{-1}), and n is the power law exponent.

Parameters K and n are fit from experimental data as a function of volume reduction.

Retentate Density

Density is fit from experimental concentration data as a function of volume reduction.

Recirculation Loop Flowrates

The cross-flow velocity in each channel is set so that the shear rate at the membrane surface equals the desired shear rate (1000 s^{-1} for MF, 2700 s^{-1} for NF). From the Rabinowitsch-Mooney relationship,[6] the cross-flow velocity can be calculated:

$$v = \frac{\dot{\gamma}D}{8}\left(\frac{4n}{1+3n}\right) \qquad \text{(Equation S22)}$$

In Equation S22, v is the channel cross-flow velocity $(m \cdot s^{-1})$, $\dot{\gamma}$ is the desired shear rate at the membrane surface (s^{-1}), D is the channel inner diameter (m) and n is the power law parameter from Equation 21.

From the cross-flow velocity, the volumetric flowrate in a single channel can be calculated:

$$Q = \pi v\left(\frac{D}{2}\right)^2 \qquad \text{(Equation S23)}$$

In Equation S23, Q is the volumetric flow rate in a single channel $(m^3 \cdot s^{-1})$, π is the mathematical constant, v is the channel cross-flow velocity $(m \cdot s^{-1})$, and D is the channel inner diameter (m).

Subsequently, the total volumetric flowrate through the filtration stage can be calculated:

$$Q_{Tot} = N_c N_{mod} Q \qquad \text{(Equation S24)}$$

In Equation S24, Q_{Tot} is the total volumetric flowrate through the filtration stage and Q is the volumetric flow rate in a single channel $(m^3 \cdot s^{-1})$, N_c is the number of channels in a filtration module, and N_{mod} is the number of modules required for the filtration step.

Q_{Tot} defines the total volumetric flow rate required to achieve the desired shear rate at the membrane and is used to determine the microfiltration and nanofiltration recirculation rates.

Fanning Friction Factor

One factor that affects the pump power requirement is the pressure drop through the module during filtration. To calculate this pressure drop, we must first solve for the modified Reynolds number for non-Newtonian fluids defined by Metzner and Reed:[6]

$$K^{'} = K\left[\frac{1+3n}{4n}\right]^{n} \qquad \text{(Equation S25)}$$

$$Re_{MR} = \frac{D^{n^{'}}V^{2-n^{'}}\rho}{K'8^{n^{'}-1}} \qquad \text{(Equation S26)}$$

In Equations S25 and S26, K' is the modified power law coefficient and K is the power law coefficient from Equation S21 ($kg \cdot m^{-1} \cdot s^{-(2-n)}$), n is the power law exponent from Equation S21, Re_{MR} is the modified Reynolds number, D is the channel inner diameter (m), V is the channel cross-flow velocity $\left(m \cdot s^{-1}\right)$, ρ is the feed-side fluid density $\left(kg \cdot m^{-3}\right)$, and $n^{'} = n$.

Now, the fanning friction factor can be calculated:[7]

$$f^{-0.5} = 4log\left(Re_{MR}f^{0.5}\right) - 0.4 \qquad \text{(Equation S27)}$$

In Equation S27, f is the fanning friction factor and Re_{MR} is the modified Reynolds number calculated in Equation S28.

Pump Power Consumption

The pressure drop through the module is calculated:

$$\Delta P = \frac{2\rho f V^{2}L}{D} \qquad \text{(Equation S28)}$$

In Equation S28, ΔP is the pressure drop through the module (Pa), ρ is the feed-side fluid density $\left(kg \cdot m^{-3}\right)$, V is the channel cross-flow velocity $\left(m \cdot s^{-1}\right)$, L is the module length (m), and D is the channel inner diameter (m).

Finally, the pump power consumption can be determined:

$$P_{n} = \frac{Q_{Tot}\Delta P}{\xi} \qquad \text{(Equation S29)}$$

$$P = \frac{P_{n}}{Q_{perm}} \qquad \text{(Equation S30)}$$

In Equations S29 and S30, P_n is the net power requirement of the pump (W), Q_{Tot} is the total volumetric flowrate through the filtration stage $\left(m^{3} \cdot s^{-1}\right)$, ΔP is the pressure drop through the module (Pa), ξ is the pump efficiency, set to 0.6, P is the power requirement per volume permeate produced $\left(kWh \cdot m^{-3}\right)$, and Q_{perm} is the permeate flow rate $\left(m^{3} \cdot h^{-1}\right)$.

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