

IDAES Unit Model – NAWI ProteusLib Nanofiltration

1) Model specifications and general **notes**:

- i. Model dimensionality: 0D model
- ii. Model dynamics: Steady-state only
- iii. Valid phases: Single liquid phase only
- iv. Notes: Modified from RO unit model

2) List all required unit model **sets**:

- v. Set description: Time
- vi. Set symbol: $t \in T$
- vii. Pyomo notation: t
- viii. Pyomo set declaration: `flowsheet().config.time`

- i. Set description: Components
- ii. Set symbol: $j \in J$
- iii. Pyomo notation: j
- iv. Pyomo set declaration: `config.property_package.component_list`

3) List all required unit model **parameters**:

- i. Parameter description: Water permeability coefficient
- ii. Parameter symbol: A_t
- iii. Pyomo notation: A
- iv. Parameter indices: Time (t)
- v. Parameter initial value: $3.77\text{e-}11$
- vi. Parameter bounds: $[1\text{e-}18, 1\text{e-}6]$
- vii. Parameter unit: $\text{m}/(\text{Pa}\cdot\text{s})$
- viii. Parameter data source: [Nair et al. (2018), ESNA membranes for Water]
- ix. Note: $10.52 \text{ L}/(\text{m}^2\cdot\text{h}\cdot\text{bar}) = 10.52/(1,000 \times 100,000 \times 3,600) \text{ m}/(\text{Pa}\cdot\text{s})$

- i. Parameter description: Salt permeability coefficient
- ii. Parameter symbol: B_t
- iii. Pyomo notation: B
- iv. Parameter indices: Time (t)
- v. Parameter initial value: $4.724\text{e-}5$
- vi. Parameter bounds: $[1\text{e-}11, 1\text{e-}5]$
- vii. Parameter unit: m/s
- viii. Parameter data source: [Nair et al. (2018), ESNA membranes for Na⁺/Cl⁻]
- ix. Note: Assume permeability coefficients for Na⁺/Cl⁻ are additive for NaCl

i. Parameter description:	Pure water density
ii. Parameter symbol:	ρ^{H2O}
iii. Pyomo notation:	dens_H2O
iv. Parameter indices:	---
v. Parameter initial value:	1,000
vi. Parameter bounds:	[1, 1e6]
vii. Parameter unit:	kg/m ³
viii. Parameter data source:	Common knowledge
i. Parameter description:	Reflection coefficient
ii. Parameter symbol:	σ
iii. Pyomo notation:	sigma
iv. Parameter indices:	---
v. Parameter initial value:	0.28
vi. Parameter bounds:	---
vii. Parameter unit:	--- (dimensionless)
viii. Parameter data source:	Nair et al. (2018), ESNA membranes for Na ⁺ /Cl ⁻
x. Note:	Assume reflection coefficients for Na ⁺ /Cl ⁻ are <u>additive for NaCl</u>

4) List all required unit model decision **variables**:

i. Variable description:	Flux at feed inlet
ii. Variable symbol:	$J_{t,j}^{in}$
iii. Pyomo notation:	flux_mass_comp_in
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	1e-3
vi. Variable bounds:	[1e-8, 1e6]
vii. Variable unit:	kg / (m ² x s)
i. Variable description:	Flux at feed outlet
ii. Variable symbol:	$J_{t,j}^{out}$
iii. Pyomo notation:	flux_mass_comp_out
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	1e-3
vi. Variable bounds:	[1e-8, 1e6]
vii. Variable unit:	kg / (m ² x s)
i. Variable description:	Membrane area
ii. Variable symbol:	x^A
iii. Pyomo notation:	area

iv. Variable indices:	---
v. Variable initial value:	1
vi. Variable bounds:	[1e-8, 1e6]
vii. Variable unit:	m ²
i. Variable description:	Average concentration at feed inlet
ii. Variable symbol:	\bar{c}_t^{in}
iii. Pyomo notation:	avg_concentration_in
iv. Variable indices:	Time (t)
v. Variable initial value:	1e-3
vi. Variable bounds:	[1e-8, 1e6]
vii. Variable unit:	kg/m ³
i. Variable description:	Average concentration at feed outlet
ii. Variable symbol:	\bar{c}_t^{out}
iii. Pyomo notation:	avg_concentration_out
iv. Variable indices:	Time (t)
v. Variable initial value:	1e-3
vi. Variable bounds:	[1e-8, 1e6]
vii. Variable unit:	kg/m ³
i. Variable description:	Average component mass flux
ii. Variable symbol:	$J_{t,j}^{Avg}$
iii. Pyomo notation:	flux_mass_comp_avg
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	kg/(m ² x s)

5) List all utilized unit model (IDAES-internal) decision **variables**:

i. Variable description:	Mass transfer to permeate
ii. Variable symbol:	$M_{t,j}^P$
iii. Pyomo notation:	properties_permeate[t].mass_transfer_comp[j]
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	kg/s
viii. Note:	IDAES-internal variable
i. Variable description:	Feed pressure
ii. Variable symbol:	P_t^F
iii. Pyomo notation:	feed_side.properties_in[t].pressure
iv. Variable indices:	Time (t)

v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	Pa
viii. Note:	IDAES-internal variable

i. Variable description:	Permeate pressure
ii. Variable symbol:	P_t^P
iii. Pyomo notation:	properties_permeate[t].pressure
iv. Variable indices:	Time (t)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	Pa
viii. Note:	IDAES-internal variable

i. Variable description:	Brine pressure
ii. Variable symbol:	P_t^B
iii. Pyomo notation:	feed_side.properties_out[t].pressure
iv. Variable indices:	Time (t)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	Pa
viii. Note:	IDAES-internal variable

i. Variable description:	Feed osmotic pressure
ii. Variable symbol:	π_t^F
iii. Pyomo notation:	feed_side.properties_in[t].pressure_osm
iv. Variable indices:	Time (t)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	Pa
viii. Note:	IDAES-internal variable

i. Variable description:	Permeate osmotic pressure
ii. Variable symbol:	π_t^P
iii. Pyomo notation:	properties_permeate[t].pressure_osm
iv. Variable indices:	Time (t)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	Pa
viii. Note:	IDAES-internal variable

i. Variable description:	Brine osmotic pressure
ii. Variable symbol:	π_t^B
iii. Pyomo notation:	feed_side.properties_out[t].pressure_osm

iv. Variable indices:	Time (t)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	Pa
viii. Note:	IDAES-internal variable
i. Variable description:	Feed concentration
ii. Variable symbol:	$C_{t,j}^F$
iii. Pyomo notation:	feed_side.properties_in[t].conc_mass_comp[j]
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	kg/m ³
viii. Note:	IDAES-internal variable
i. Variable description:	Permeate concentration
ii. Variable symbol:	$C_{t,j}^P$
iii. Pyomo notation:	properties_permeate[t].conc_mass_comp[j]
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	kg/m ³
viii. Note:	IDAES-internal variable
i. Variable description:	Brine concentration
ii. Variable symbol:	$C_{t,j}^B$
iii. Pyomo notation:	feed_side.properties_out[t].conc_mass_comp[j]
iv. Variable indices:	Time (t), Component (j)
v. Variable initial value:	---
vi. Variable bounds:	---
vii. Variable unit:	kg/m ³
viii. Note:	IDAES-internal variable

6) List all required unit model **performance equations**:

i. Constraint description:	Average flux
ii. Constraint validity:	$\forall t \in T, j \in J$
iii. Symbolic constraint:	$J_{t,j}^{Avg} = 0.5 \cdot (J_{t,j}^{in} + J_{t,j}^{out})$
iv. Pyomo constraint:	flux_mass_comp_avg[t,j] = 0.5 * (flux_mass_comp_in[t,j] + flux_mass_comp_out[t,j])
v. Constraint source:	[adopted from RO unit model]
i. Constraint description:	Permeate mass flow
ii. Constraint validity:	$\forall t \in T, j \in J$

iii. Symbolic constraint:	$M_{t,j}^P = x^A \cdot J_{t,j}^{Avg}$
iv. Pyomo constraint:	mass_transfer_comp[t, j] = area * flux_mass_comp_avg[t, j] =
v. Constraint source:	[adopted from RO unit model]
i. Constraint description:	Inlet water flux
ii. Constraint validity:	$\forall t \in T, j \in \{H2O\}$
iii. Symbolic constraint:	$J_{t,j}^{in} = A_t \cdot \rho^{H2O} \cdot (P_t^F - P_t^P) - \sigma \cdot (\pi_t^F - \pi_t^P)$
iv. Pyomo constraint:	flux_mass_comp_in[t, j] = A[t] * dens_H2O * (feed_side.properties_in[t].pressure - properties_permeate[t].pressure) - sigma * (feed_side.properties_in[t].pressure_osm - properties_permeate[t].pressure_osm)
v. Constraint source:	Wang et al. (2014)
i. Constraint description:	Inlet salt flux
ii. Constraint validity:	$\forall t \in T, j \in \{NaCl\}$
iii. Symbolic constraint:	$J_{t,j}^{in} = B_t \cdot (C_{t,j}^F - C_{t,j}^P) + (1 - \sigma) \cdot J_{t,j}^{in} \cdot \frac{1}{\rho_{H2O}} \cdot \bar{c}_t^{in}$
iv. Pyomo constraint:	flux_mass_comp_in[t, j] = B[t] * (feed_side.properties_in[t].conc_mass_comp[j] - properties_permeate[t].conc_mass_comp[j]) + (1 - sigma) * flux_mass+comp_in[t, j] * 1/dens_H2O * avg_concentration_in
v. Constraint source:	Wang et al. (2014)
i. Constraint description:	Outlet water flux
ii. Constraint validity:	$\forall t \in T, j \in \{H2O\}$
iii. Symbolic constraint:	$J_{t,j}^{out} = A_t \cdot \rho^{H2O} \cdot (P_t^B - P_t^P) - \sigma \cdot (\pi_t^B - \pi_t^P)$
iv. Pyomo constraint:	flux_mass_comp_out[t, j] = A[t] * dens_H2O * (feed_side.properties_out[t].pressure - properties_permeate[t].pressure) - sigma * (feed_side.properties_out[t].pressure_osm - properties_permeate[t].pressure_osm)
v. Constraint source:	Wang et al. (2014)
i. Constraint description:	Outlet salt flux
ii. Constraint validity:	$\forall t \in T, j \in \{NaCl\}$
iii. Symbolic constraint:	$J_{t,j}^{in} = B_t \cdot (C_{t,j}^F - C_{t,j}^P) + (1 - \sigma) \cdot J_{t,j}^{out} \cdot \frac{1}{\rho_{H2O}} \cdot \bar{c}_t^{out}$
iv. Pyomo constraint:	flux_mass_comp_out[t, j] = B[t] * (feed_side.properties_out[t].conc_mass_comp[j] - properties_permeate[t].conc_mass_comp[j]) + (1 - sigma) * flux_mass+comp_out[t, j] * 1/dens_H2O * avg_concentration_out
v. Constraint source:	Wang et al. (2014)

i. Constraint description:	Average inlet concentration
ii. Constraint validity:	$\forall t \in T, j \in \{NaCl\}$
iii. Symbolic constraint:	$\bar{c}_t^{in} = (C_{t,j}^F \cdot C_{t,j}^P \cdot (C_{t,j}^F + C_{t,j}^P)/2)^{1/3}$
iv. Pyomo constraint	$b.avg_concentration_in[t] ==$ $(feed_side.properties_in[t].conc_mass_comp[j]$ $* properties.permeate[t].conc_mass_comp[j] *$ $(feed_side.properties_in[t].conc_mass_comp[j]$ $+ properties.permeate[t].conc_mass_comp[j])/2)^{**}$ $(1/3)$
v. Constraint source:	Bruggen (2013)
vi. Note:	<p>The original average concentration expression</p> $\bar{c}_t^{in} = (C_{t,j}^F - C_{t,j}^P)/\ln(C_{t,j}^F/C_{t,j}^P)$ <p>is approximated for numerical robustness</p>
i. Constraint description:	Average outlet concentration
ii. Constraint validity:	$\forall t \in T, j \in \{NaCl\}$
iii. Symbolic constraint:	$\bar{c}_t^{out} = (C_{t,j}^B \cdot C_{t,j}^P \cdot (C_{t,j}^B + C_{t,j}^P)/2)^{1/3}$
iv. Pyomo constraint:	$b.avg_concentration_out[t] ==$ $(feed_side.properties_out[t].conc_mass_comp[j] *$ $properties.permeate[t].conc_mass_comp[j] *$ $(feed_side.properties_out[t].conc_mass_comp[j]$ $+ properties.permeate[t].conc_mass_comp[j])/2)^{**}$ $(1/3)$
v. Constraint source:	Bruggen (2013)
vi. Note:	<p>The original average concentration expression</p> $\bar{c}_t^{out} = (C_{t,j}^B - C_{t,j}^P)/\ln(C_{t,j}^B/C_{t,j}^P)$ <p>is approximated for numerical robustness</p>

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