IDAES Unit Model – NAWI ProteusLib **Nanofiltration**

1. Model specifications and general ***notes***:
2. Model dimensionality: 0D model
3. Model dynamics: Steady-state only
4. Valid phases: Single liquid phase only
5. Notes: Modified from RO unit model
6. List all required unit model ***sets***:
7. Set description: Time
8. Set symbol:
9. Pyomo notation: t
10. Pyomo set declaration: flowsheet().config.time
11. Set description: Components
12. Set symbol:
13. Pyomo notation: j
14. Pyomo set declaration: config.property\_package.component\_list
15. List all required unit model ***parameters***:
16. Parameter description: Water permeability coefficient
17. Parameter symbol:
18. Pyomo notation: A
19. Parameter indices: Time (t)
20. Parameter initial value: 3.77e-11
21. Parameter bounds: [1e-18, 1e-6]
22. Parameter unit: m/(Pa-s)
23. Parameter data source: [Nair et al. (2018), ESNA membranes for Water]
24. Note: 10.52 L/(m2-h-bar) =

10.52/(1,000x100,000x3,600) m/(Pa-s)

1. Parameter description: Salt permeability coefficient
2. Parameter symbol:
3. Pyomo notation: B
4. Parameter indices: Time (t)
5. Parameter initial value: 4.724e-5
6. Parameter bounds: [1e-11, 1e-5]
7. Parameter unit: m/s
8. Parameter data source: [Nair et al. (2018), ESNA membranes for Na+/Cl-]
9. Note: Assume permeability coefficients for Na+/Cl- are

additive for NaCl

1. Parameter description: Pure water density
2. Parameter symbol:
3. Pyomo notation: dens\_H2O
4. Parameter indices: ---
5. Parameter initial value: 1,000
6. Parameter bounds: [1, 1e6]
7. Parameter unit: kg/m3
8. Parameter data source: Common knowledge
9. Parameter description: Reflection coefficient
10. Parameter symbol:
11. Pyomo notation: sigma
12. Parameter indices: ---
13. Parameter initial value: 0.28
14. Parameter bounds: ---
15. Parameter unit: --- (dimensionless)
16. Parameter data source: Nair et al. (2018), ESNA membranes for Na+/Cl-
17. Note: Assume reflection coefficients for Na+/Cl- are

additive for NaCl

1. List all required unit model decision ***variables***:
2. Variable description: Flux at feed inlet
3. Variable symbol:
4. Pyomo notation: flux\_mass\_comp\_in
5. Variable indices: Time (t), Component (j)
6. Variable initial value: 1e-3
7. Variable bounds: [1e-8, 1e6]
8. Variable unit: kg / (m2 x s)
9. Variable description: Flux at feed outlet
10. Variable symbol:
11. Pyomo notation: flux\_mass\_comp\_out
12. Variable indices: Time (t), Component (j)
13. Variable initial value: 1e-3
14. Variable bounds: [1e-8, 1e6]
15. Variable unit: kg / (m2 x s)
16. Variable description: Membrane area
17. Variable symbol:
18. Pyomo notation: area
19. Variable indices: ---
20. Variable initial value: 1
21. Variable bounds: [1e-8, 1e6]
22. Variable unit: m2
23. Variable description: Average concentration at feed inlet
24. Variable symbol:
25. Pyomo notation: avg\_concentration\_in
26. Variable indices: Time (t)
27. Variable initial value: 1e-3
28. Variable bounds: [1e-8, 1e6]
29. Variable unit: kg/m3
30. Variable description: Average concentration at feed outlet
31. Variable symbol:
32. Pyomo notation: avg\_concentration\_out
33. Variable indices: Time (t)
34. Variable initial value: 1e-3
35. Variable bounds: [1e-8, 1e6]
36. Variable unit: kg/m3
37. Variable description: Average component mass flux
38. Variable symbol:
39. Pyomo notation: flux\_mass\_comp\_avg
40. Variable indices: Time (t), Component (j)
41. Variable initial value: ---
42. Variable bounds: ---
43. Variable unit: kg/(m2 x s)
44. List all utilized unit model (IDAES-internal) decision ***variables***:
45. Variable description: Mass transfer to permeate
46. Variable symbol:
47. Pyomo notation: properties\_permeate[t].mass\_transfer\_comp[j]
48. Variable indices: Time (t), Component (j)
49. Variable initial value: ---
50. Variable bounds: ---
51. Variable unit: kg/s
52. Note: IDAES-internal variable
53. Variable description: Feed pressure
54. Variable symbol:
55. Pyomo notation: feed\_side.properties\_in[t].pressure
56. Variable indices: Time (t)
57. Variable initial value: ---
58. Variable bounds: ---
59. Variable unit: Pa
60. Note: IDAES-internal variable
61. Variable description: Permeate pressure
62. Variable symbol:
63. Pyomo notation: properties\_permeate[t].pressure
64. Variable indices: Time (t)
65. Variable initial value: ---
66. Variable bounds: ---
67. Variable unit: Pa
68. Note: IDAES-internal variable
69. Variable description: Brine pressure
70. Variable symbol:
71. Pyomo notation: feed\_side.properties\_out[t].pressure
72. Variable indices: Time (t)
73. Variable initial value: ---
74. Variable bounds: ---
75. Variable unit: Pa
76. Note: IDAES-internal variable
77. Variable description: Feed osmotic pressure
78. Variable symbol:
79. Pyomo notation: feed\_side.properties\_in[t].pressure\_osm
80. Variable indices: Time (t)
81. Variable initial value: ---
82. Variable bounds: ---
83. Variable unit: Pa
84. Note: IDAES-internal variable
85. Variable description: Permeate osmotic pressure
86. Variable symbol:
87. Pyomo notation: properties\_permeate[t].pressure\_osm
88. Variable indices: Time (t)
89. Variable initial value: ---
90. Variable bounds: ---
91. Variable unit: Pa
92. Note: IDAES-internal variable
93. Variable description: Brine osmotic pressure
94. Variable symbol:
95. Pyomo notation: feed\_side.properties\_out[t].pressure\_osm
96. Variable indices: Time (t)
97. Variable initial value: ---
98. Variable bounds: ---
99. Variable unit: Pa
100. Note: IDAES-internal variable
101. Variable description: Feed concentration
102. Variable symbol:
103. Pyomo notation: feed\_side.properties\_in[t].conc\_mass\_comp[j]
104. Variable indices: Time (t), Component (j)
105. Variable initial value: ---
106. Variable bounds: ---
107. Variable unit: kg/m3
108. Note: IDAES-internal variable
109. Variable description: Permeate concentration
110. Variable symbol:
111. Pyomo notation: properties\_permeate[t].conc\_mass\_comp[j]
112. Variable indices: Time (t), Component (j)
113. Variable initial value: ---
114. Variable bounds: ---
115. Variable unit: kg/m3
116. Note: IDAES-internal variable
117. Variable description: Brine concentration
118. Variable symbol:
119. Pyomo notation: feed\_side.properties\_out[t].conc\_mass\_comp[j]
120. Variable indices: Time (t), Component (j)
121. Variable initial value: ---
122. Variable bounds: ---
123. Variable unit: kg/m3
124. Note: IDAES-internal variable
125. List all required unit model ***performance equations***:
126. Constraint description: Average flux
127. Constraint validity:
128. Symbolic constraint:
129. Pyomo constraint: flux\_mass\_comp\_avg[t,j] = 0.5 \*

(flus\_mass\_comp\_in[t,j] + flux\_mass\_comp\_out[t,j]

1. Constraint source: [adopted from RO unit model]
2. Constraint description: Permeate mass flow
3. Constraint validity:
4. Symbolic constraint:
5. Pyomo constraint: mass\_transfer\_comp[t, j] = area \*

flux\_mass\_comp\_avg[t,j] =

1. Constraint source: [adopted from RO unit model]
2. Constraint description: Inlet water flux
3. Constraint validity:
4. Symbolic constraint:
5. 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)

1. Constraint source: Wang et al. (2014)
2. Constraint description: Inlet salt flux
3. Constraint validity:
4. Symbolic constraint:
5. 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

1. Constraint source: Wang et al. (2014)
2. Constraint description: Outlet water flux
3. Constraint validity:
4. Symbolic constraint:
5. 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)

1. Constraint source: Wang et al. (2014)
2. Constraint description: Outlet salt flux
3. Constraint validity:
4. Symbolic constraint:
5. 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

1. Constraint source: Wang et al. (2014)
2. Constraint description: Average inlet concentration
3. Constraint validity:
4. Symbolic constraint:
5. 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)

1. Constraint source: Bruggen (2013)
2. Note: The original average concentration expression

is approximated for numerical robustness

1. Constraint description: Average outlet concentration
2. Constraint validity:
3. Symbolic constraint:
4. 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)

1. Constraint source: Bruggen (2013)
2. Note: The original average concentration expression

is approximated for numerical robustness