Supplementary Material

### Material Balances for Inlet Streams

Equation 1 states that feed streams entering the network can be distributed to the PDISDB, directly to the waste or lean streams, or directly to the regenerators via the NFSDB.

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| $$F\_{i}= \sum\_{np=1}^{NP}f\_{i,np} + \sum\_{nt=1}^{NT}f\_{i,nt} + \sum\_{j=1}^{J}f\_{i,j}+f\_{i}^{WW} +\sum\_{q=1}^{Q}f\_{i,q}$$ | $∀i \in I $(S1) |

The flowrate of the freshwater stream is the sum of freshwater going to the lean streams, as shown in Equation 2. Because freshwater is assumed to be pure, none of it can be sent to the regenerator network or effluent stream. It is also prohibited to send freshwater to the waste stream.

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| $$F^{FW}= \sum\_{j=1}^{J}f\_{j}^{FW}$$ |  (S2) |

### Material Balances for Outlet Streams

Lean streams can receive water from the freshwater stream, feed streams, the regenerator permeate or retentate streams and the pressurisation/depressurization streams as shown in Equation 3. Since it is desirable to minimize the freshwater consumed, wastewater generated and the load imposed on the regenerator network, the wastewater sink is only used as a final resort and cannot receive water from the freshwater source or permeate streams. Only the original feed streams and the regenerator retentate streams can be sent to the wastewater stream as demonstrated in Equation 4. The concentration in sinks and the wastewater stream is dependent on the concentrations and flowrates of incoming streams, as shown in Equations 5 and 6, respectively.

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| $$f\_{j}= f\_{j}^{FW}+\sum\_{i=1}^{I}f\_{i,j}+ \sum\_{q=1}^{Q}f\_{q,j}^{P}+\sum\_{q=1}^{Q}f\_{q,j}^{R}+\sum\_{nt=1}^{NT}f\_{nt,j}^{NT}+ \sum\_{np=1}^{NP}f\_{np,j}^{NP}$$ | $∀j \in J $**(****S3)** |
| $$f^{WW}=\sum\_{i=1}^{I}f\_{i}^{WW} +\sum\_{q=1}^{Q}f\_{q}^{R,WW}+\sum\_{nt=1}^{NT}f\_{nt}^{WW}+ \sum\_{np=1}^{NP}f\_{np}^{WW}$$ | **(****S4)** |
| $$f\_{j}c\_{j,m}= \sum\_{i=1}^{I}f\_{i,j}C\_{i,m}+ \sum\_{q=1}^{Q}f\_{q,j}^{P}c\_{q,m}^{P}\sum\_{q=1}^{Q}f\_{q,j}^{R}c\_{q,m}^{R}+ \sum\_{nt=1}^{NT}f\_{nt,j}^{NT}c\_{nt,m}^{NT}+\sum\_{np=1}^{NP}f\_{nt,j}^{NP}c\_{np,m}^{NP}$$ | $∀j\in J$***;***$ $$∀m \in M $**(****S5)** |
| $$f^{WW}c\_{m}^{WW}= \sum\_{i=1}^{I}f\_{i}^{WW}C\_{i,m}+ \sum\_{q=1}^{Q}f\_{q}^{R,WW}c\_{q,m}^{R}+ \sum\_{nt=1}^{NT}f\_{nt}^{WW}c\_{nt,m}^{NT} + \sum\_{np=1}^{NP}f\_{np}^{WW}c\_{np,m}^{NP}$$ | $∀m \in M $**(****S6)** |

Each sink has a maximum concentration limit, which is determined using the purity required for end use in that sink. In the case of the wastewater sink, the limit is dictated by environmental restrictions. Constraints 7 and 8 ensure that these limits are observed.

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| $$C\_{j,m}^{U}\geq c\_{j,m}$$ | $∀j \in J$***;***$ ∀m \in M$ **(****S7)** |
| $$C\_{m}^{WW}^{U}\geq C\_{m}^{WW}$$ | $∀m \in M$ **(****S8)** |

### Material Balances for Pumps and Turbines

The total flow through the PDISDB and PDMB via node *np* or *nt* is the sum of flowrates entering that node from the feed and regenerators, as shown in Equations 9 and 11. The corresponding concentration balances are shown in Equations 10 and 12.

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| $$f\_{np}= \sum\_{i=1}^{I}f\_{i,np}+ \sum\_{q=1}^{Q}f\_{q,np}^{P}+\sum\_{q=1}^{Q}f\_{q,np}^{R}$$ | $∀np\in NP$ **(****S9)** |
| $$f\_{np}c\_{np,m}= \sum\_{i=1}^{I}f\_{i,np}C\_{i,m}+ \sum\_{q=1}^{Q}f\_{q,np}^{P}c\_{q,m}^{P}+\sum\_{q=1}^{Q}f\_{q,np}^{R}c\_{q,m}^{R}$$ | $∀np\in NP$***;***$ ∀m \in M$ **(****S10)** |
| $$f\_{nt}= \sum\_{i=1}^{I}f\_{i,nt}+ \sum\_{q=1}^{Q}f\_{q,nt}^{P}+\sum\_{q=1}^{Q}f\_{q,nt}^{R}$$ | $∀nt\in NT$ **(****S11)** |
| $$f\_{nt}c\_{nt,m}= \sum\_{i=1}^{I}f\_{i,nt}C\_{i,m}+ \sum\_{q=1}^{Q}f\_{q,nt}^{P}c\_{q,m}^{P}+\sum\_{q=1}^{Q}f\_{q,nt}^{R}c\_{q,m}^{R}$$ | $∀nt\in NT$***;***$ ∀m \in M$ **(****S12)** |

Flow going through these nodes after pressurisation or depressurization can be distributed to any of the regenerator stages or sent directly to the sinks and wastewater stream.

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| $$f\_{np}= \sum\_{q=1}^{Q}f\_{np,q}+ \sum\_{j=1}^{J}f\_{np,j}+f\_{np}^{WW}$$ | $∀np\in NP$**(S13)** |
| $$f\_{nt}= \sum\_{q=1}^{Q}f\_{nt,q}+ \sum\_{j=1}^{J}f\_{nt,j}+f\_{nt}^{WW}$$ | $∀nt\in NT$ **(S14)** |

### Material Balances for the Regenerator Network

The amount and concentration of feed to each stage $q\in Q$ of the regenerator network is dependent on the flow coming from the nodes to that stage, as shown in Equations 15 and 16

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| $$f\_{q}^{F}=\sum\_{np=1}^{NP}f\_{np,q}+\sum\_{nt=1}^{NT}f\_{nt,q}+\sum\_{i=1}^{I}f\_{i,q}$$ | $∀q \in Q$ **(****S15)** |
| $$f\_{q}^{F}c\_{q,m}^{F}= \sum\_{np=1}^{NP}f\_{np,q} c\_{np,m}+\sum\_{nt=1}^{NT}f\_{nt,q} c\_{nt,m}+\sum\_{i=1}^{I}f\_{i,q}C\_{i,m}$$ | $∀q \in Q; ∀m \in M$ **(****S16)** |

Equations 17 and 18 demonstrate that feed entering the regenerator is split into the permeate, a lean stream of low contaminant concentration, as well as the retentate, which contains a high contaminant concentration. The ratio of feed that reports in the permeate is known as the liquid recovery or liquid yield and is represented as $Y\_{q}$in Equation 19. The permeate concentration is dependent on the removal ratio ($RR\_{q}$), as shown in Equation 20. The removal ratio represents the amount of solute recovered in the retentate. In black box models, this value is a parameter, whereas detailed regenerator models use a variable recovery ratio.

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| $f^{F}\_{q}= f^{P}\_{q}+f^{R}\_{q} $ | $∀q \in Q$ **(****S17)** |
| $f\_{q}^{F}c\_{q,m}^{F}= f\_{q}^{P}c\_{q,m}^{P}+f\_{q}^{R}c\_{q,m}^{R}$ | $∀q \in Q; ∀m \in M$ **(****S18)** |
| $Y\_{q}=\frac{f\_{q}^{P}}{f\_{q}^{F}}$ | $∀q \in Q$ **(****S19)** |
| $c\_{q,m}^{P}=(1-rr\_{q,m})c\_{q,m}^{F}$ | $∀q \in Q; ∀m \in M$ **(****S20)** |

Permeate and retentate streams leaving the regenerator stages can be sent to PDISDB for pressurisation/depressurization prior to being recycled to the regenerator stages or discharged to the sinks. They can also be sent directly to the sinks, and retentate can additionally be sent directly to the waste stream. This is stated in Equation 21 for permeate and Equation 22 for retentate.

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| $$f\_{q}^{P}= \sum\_{np=1}^{NP}f\_{q,np}^{P}+ \sum\_{nt=1}^{NT}f\_{q,nt}^{P}+ \sum\_{j=1}^{J}f\_{q,j}^{P} $$ | $∀q\in Q $**(****S21)** |
| $$f\_{q}^{R}= \sum\_{np=1}^{NP}f\_{q,np}^{R}+ \sum\_{nt=1}^{NT}f\_{q,nt}^{R}+ \sum\_{j=1}^{J}f\_{q,j}^{R} + f\_{q}^{R,WW}$$ | $∀q\in Q $**(****S22)** |

It must be ensured that the inlet feed to the regenerator is below the maximum allowable limit recommended by manufacturers. This is represented in constraint 23.

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| $C\_{q,m}^{U} \geq c\_{q,m}^{F}$ | $∀q\in Q; ∀m \in M$ **(****S23)** |

## Pressure Constraints

Pumps can only increase, while turbines can only decrease pressure. This is ensured by Equations 24 and 25.

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| $$p\_{np}^{out}-p\_{np}^{in}\geq 0$$ | $∀np\in NP$ **(S24)** |
| $$p\_{nt}^{in}-p\_{nt}^{out}\geq 0$$ | $∀nt\in NT$ **(S25)** |

Streams must mix at equal pressures as dictated by constraints 26 -37.

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| $$\left(p\_{np}^{in}-P\_{i}\right)f\_{i,np}=0$$ | $∀i\in I ; ∀np\in NP$**(S26)** |
| $$\left(p\_{nt}^{in}-P\_{i}\right)f\_{i,nt}=0$$ | $∀i\in I ; ∀nt\in NT$**(S27)** |
| $\left(p\_{np}^{in}-p^{P}\_{q}\right)f^{P}\_{q,np}=0$ | $∀q\in Q ; ∀np\in NP$ **(S28)** |
| $$\left(p\_{np}^{in}-p^{P}\_{q}\right)f^{R}\_{q,np}=0$$ | $∀q\in Q ; ∀np\in NP$ **(S29)** |
| $$\left(p\_{np}^{in}-p^{R}\_{q}\right)f^{R}\_{q,nt}=0$$ | $∀q\in Q ; ∀nt\in NT$ **(S30)** |
| $$\left(p\_{np}^{out}-p^{F}\_{q}\right)f\_{np,q}=0$$ | $∀q\in Q ; ∀np\in NP$ **(S31)** |
| $$\left(p\_{nt}^{out}-p^{F}\_{q}\right)f\_{nt,q}=0$$ | $∀q\in Q ; ∀nt\in NT$ **(S32)** |
| $$\left(p\_{np}^{out}-P\_{j}\right)f\_{np,j}=0$$ | $∀j\in J ; ∀np\in NP$ **(S33)** |
| $$\left(p\_{nt}^{out}-P\_{j}\right)f\_{nt,j}=0$$ | $∀j\in J ; ∀nt\in NT$ **(S34)** |
| $$\left(p\_{nt}^{out}-P^{WW}\right)f\_{nt}^{WW}=0$$ | $∀nt\in NT$ **(S35)** |
| $$\left(p\_{q}^{R}-P^{WW}\right)f\_{q}^{R,WW}=0$$ | $∀q\in Q $**(S36)** |
| $$\left(p\_{q}^{P}-P\_{j}\right)f\_{q,j}^{P}=0$$ | $∀q\in Q ;∀j\in J $**(S37)** |