Simultaneous Water and Energy Optimization in Chemical Plants

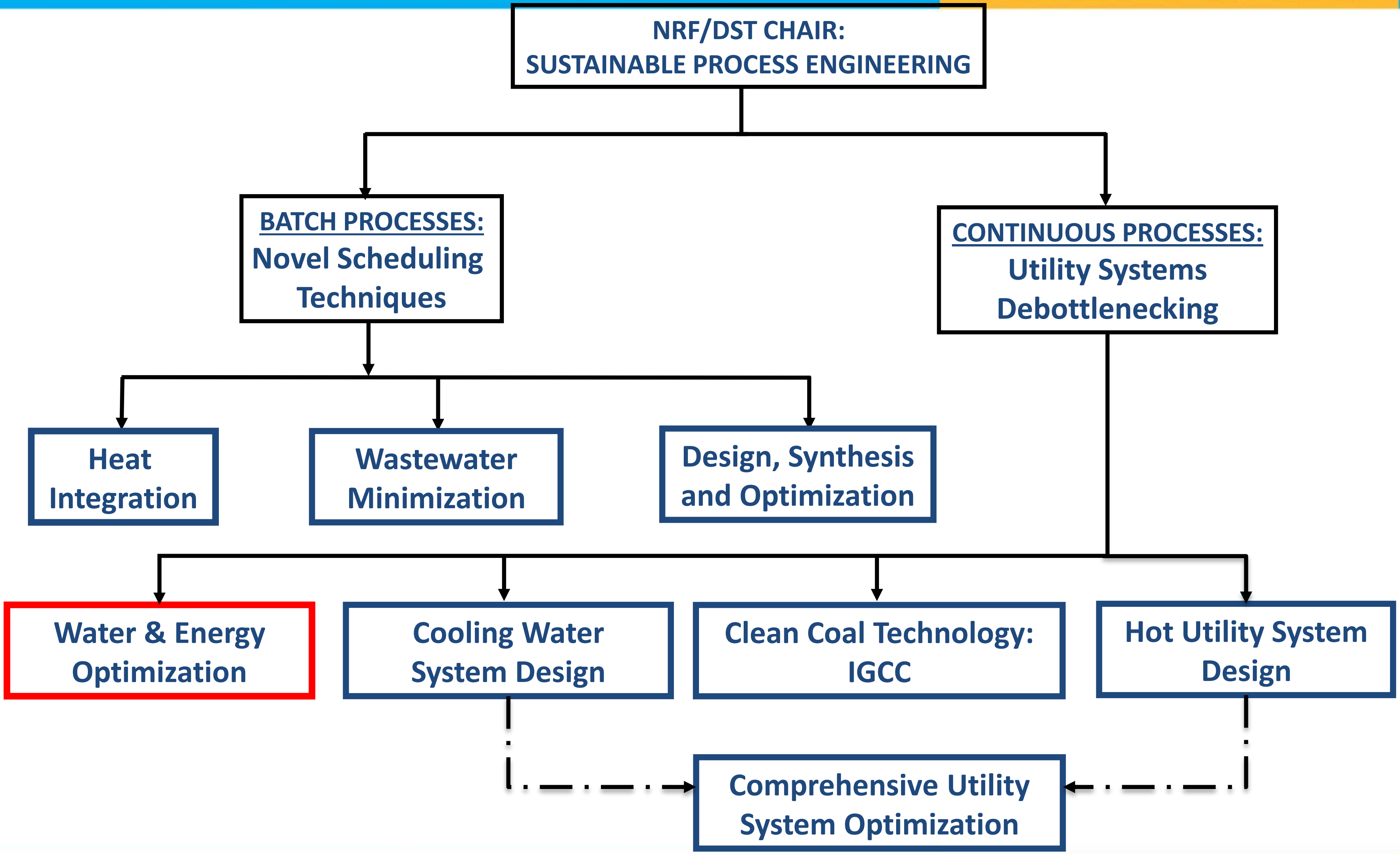
Thokozani Majozi

University of the Witwatersrand, Johannesburg

NRF/DST Chair: Sustainable Process Engineering

School of Chemical and Metallurgical Engineering

Group Structure



NRF/DST CHAIR:
SUSTAINABLE PROCESS ENGINEERING

BATCH PROCESSES:
Novel Scheduling Techniques

CONTINUOUS PROCESSES:
Utility Systems Debottlenecking

Heat Integration

Wastewater Minimization

Design, Synthesis and Optimization

Water & Energy Optimization

Cooling Water System Design

Clean Coal Technology: IGCC

Hot Utility System Design

Comprehensive Utility System Optimization

Outline

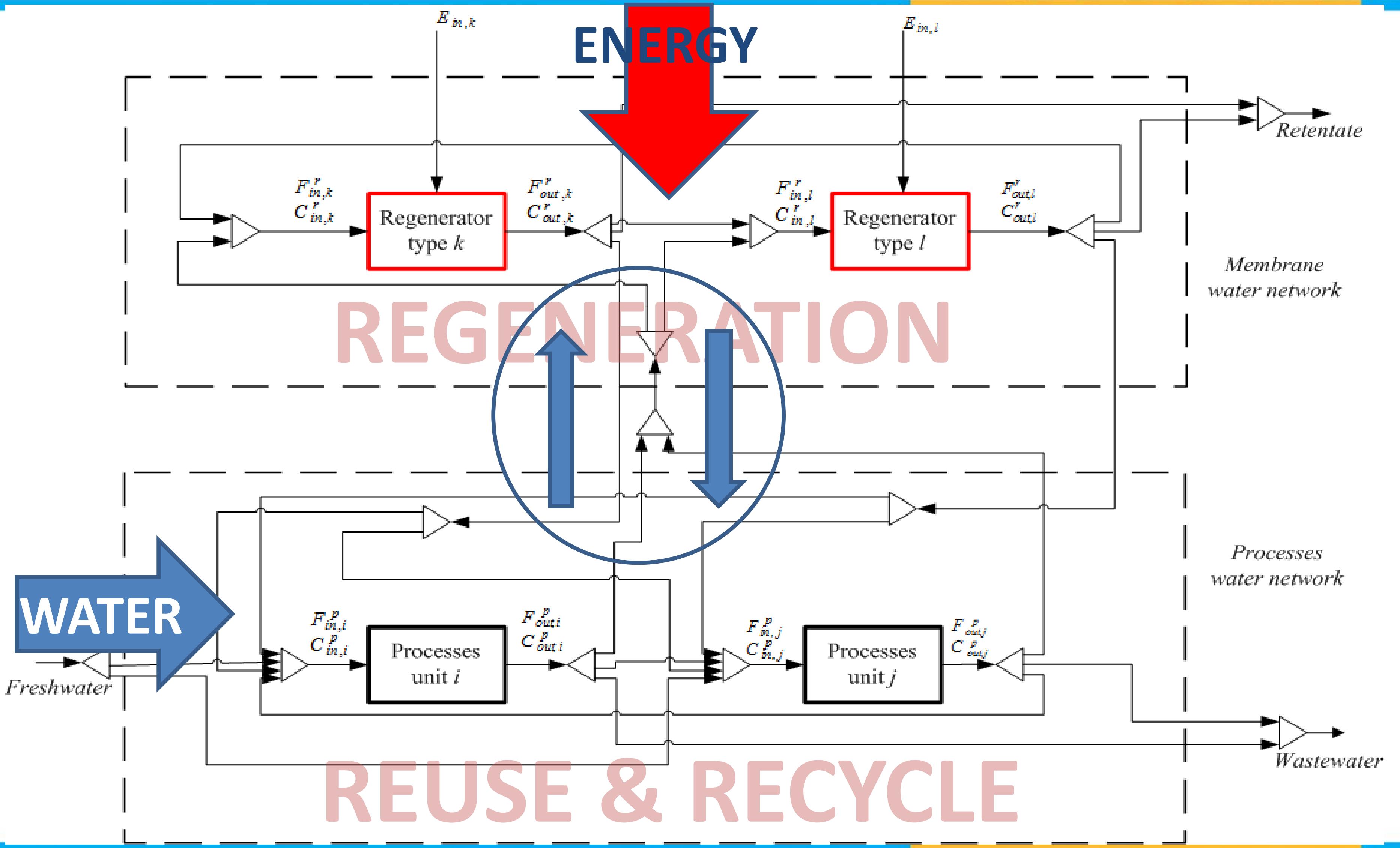
- Background & Motivation
- Problem Statement
- Model Development
- Illustrative Examples
- Case Study
- Results & Discussion
- Conclusion

Background

❑ Water and energy

- ❖ Each resource is consumed to produce the other
  - ➢ Hydroelectric
  - ➢ Geothermal
  - ➢ Steam turbines
  - ➢ Extraction
  - ➢ Production
  - ➢ Distribution
  - ➢ Treatment
- ❖ Water-energy-nexus
  - ➢ Considers the interdependence of water and energy resources and their effect on the environment
  - ➢ Increasing demand
  - ➢ Stricter environmental regulations
- ❖ Sustainable use of water and energy
  - ➢ Process integration techniques
    - ✓ Environmentally benign
    - ✓ Economically feasible

Motivation



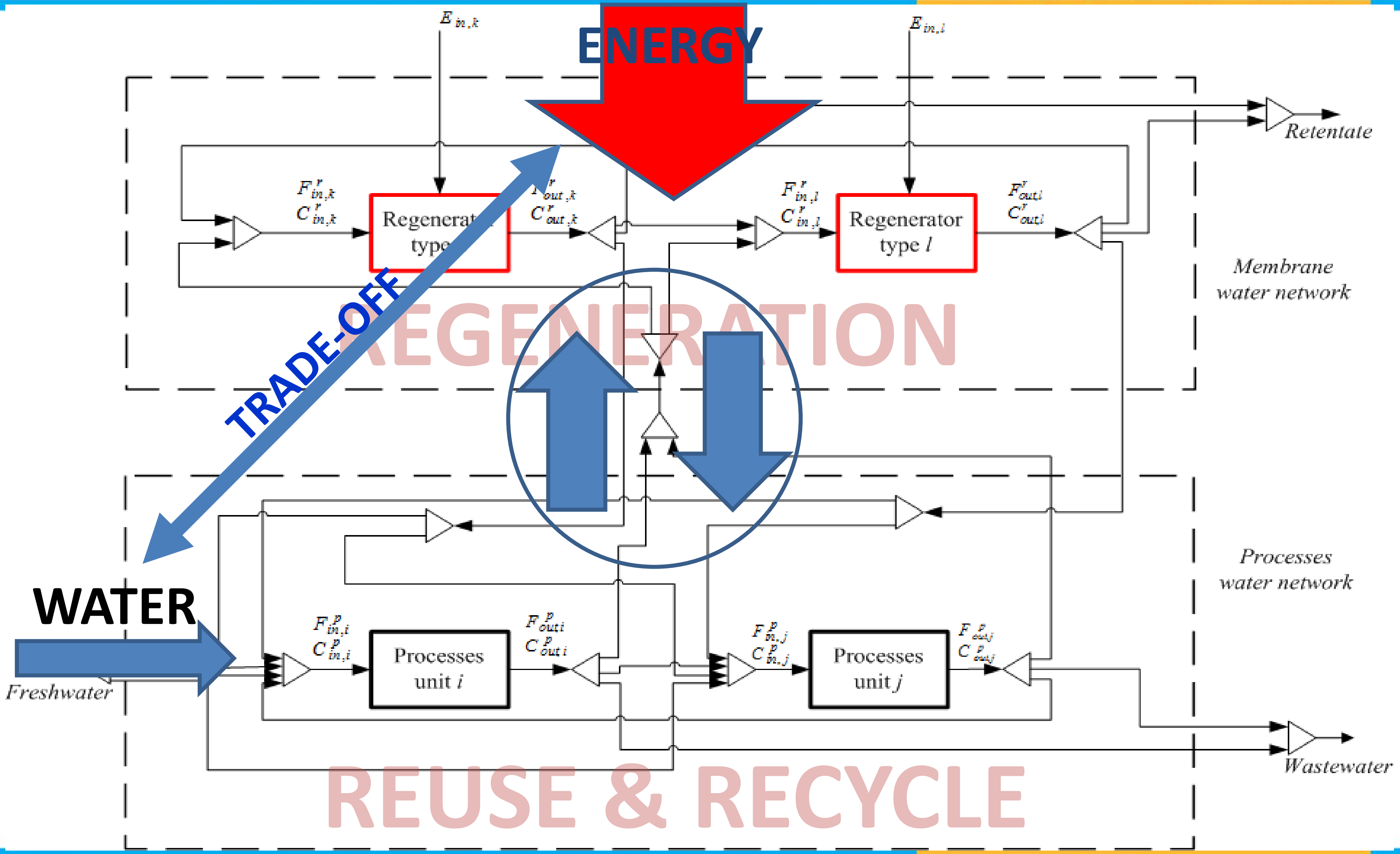
ENERGY

REGENERATION

WATER

REUSE & RECYCLE

Motivation



ENERGY

TRADE-OFF

REGENERATION

WATER

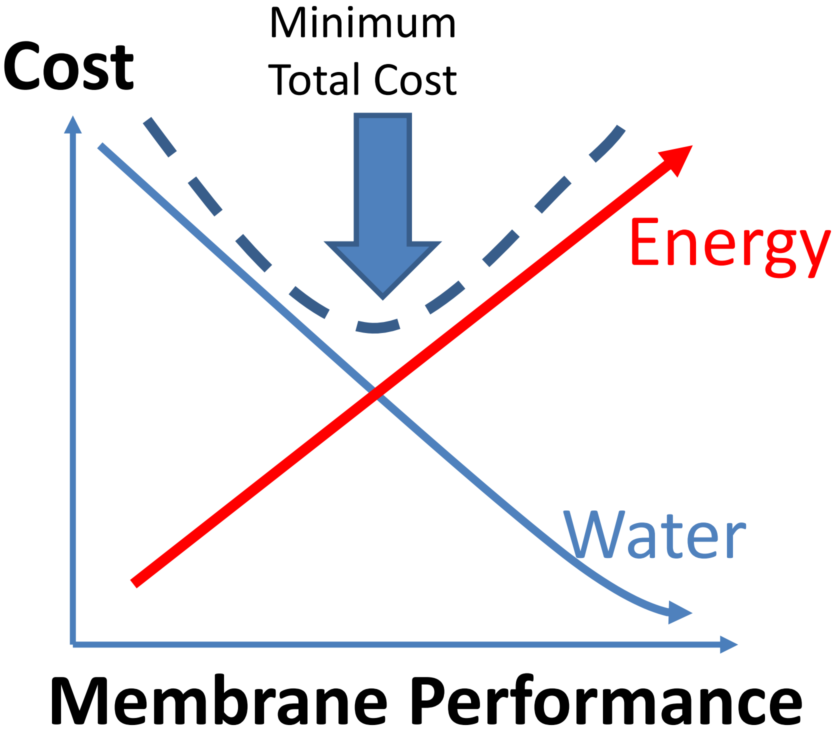
REUSE & RECYCLE

Motivation

ENERGY

TRADE-OFF

WATER



Problem Statement

❑ Given:

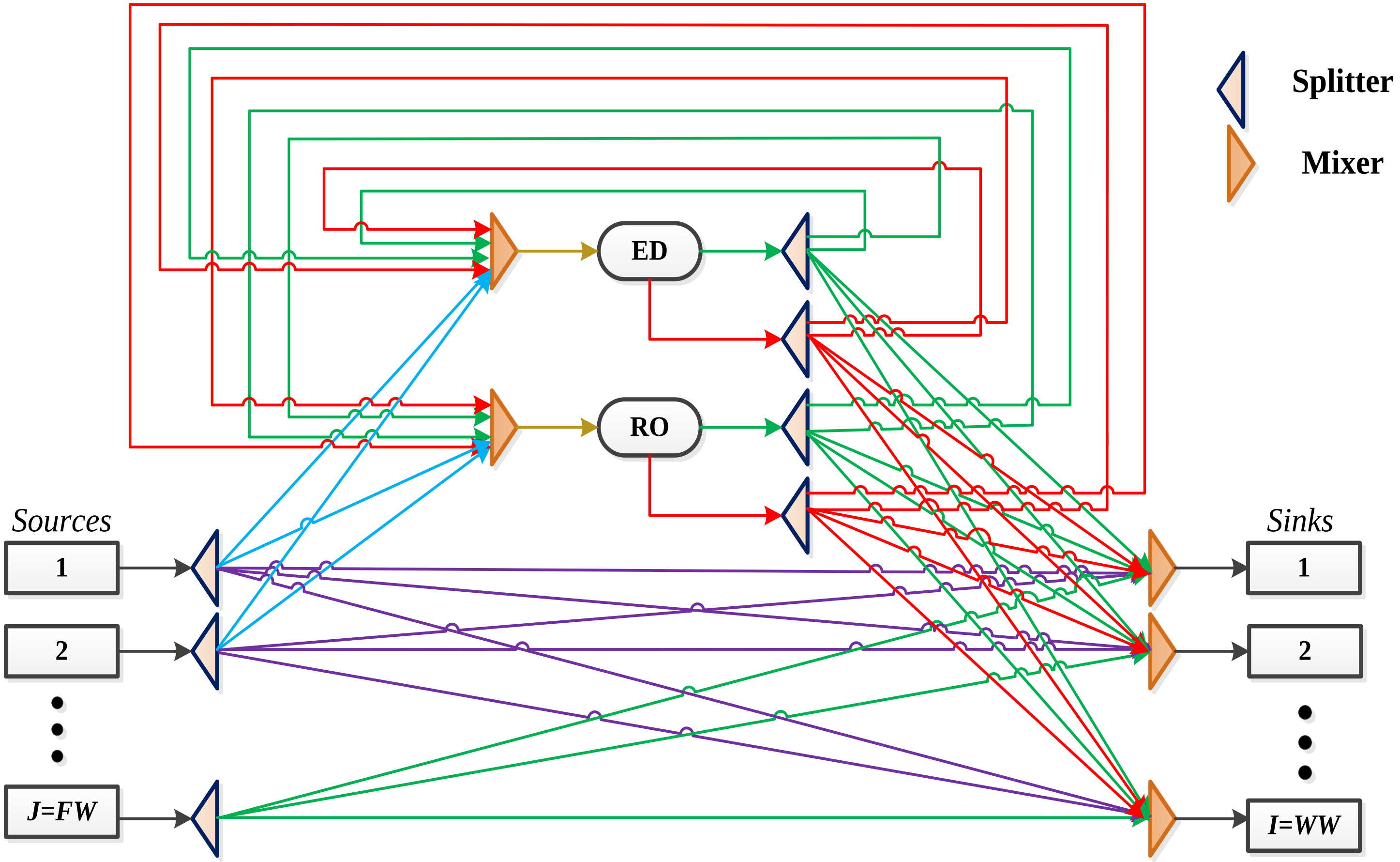
- Sources with known flowrates and contaminant concentrations
- Sinks with fixed flowrates and known maximum allowable concentration
- Water regeneration units (known design parameters)
- Freshwater source with known concentration and unlimited supply
- Wastewater sink with maximum allowable concentration and unlimited capacity

❑ Determine:

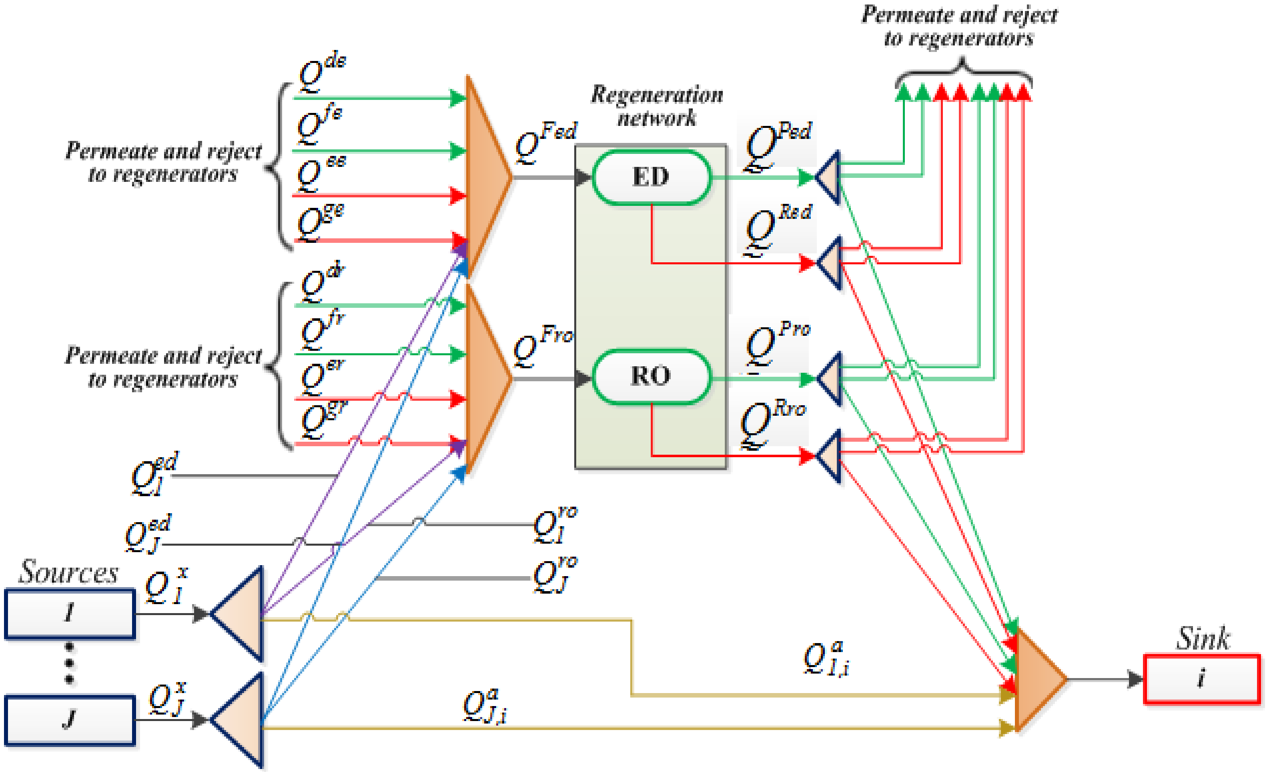
- Minimum flowrate of freshwater into sinks
- Minimum wastewater flowrate
- Optimum design variables of regenerators for minimal energy usage
- Optimum water network configuration

Model Development

❑ Superstructure



❑ Water balances for regeneration unit



$$\sum_{j\in J} Q_j^{ed} + Q^{de} + Q^{ee} + Q^{fe} + Q^{ge} = Q^{Fed}$$

$$\sum_{j\in J} Q_j^{ro} + Q^{dr} + Q^{er} + Q^{fr} + Q^{gr} = Q^{Fro}$$

Model Development

❑ Concentration balance for regeneration unit

- Max. allowable conc. into ED unit

$$\frac{\sum_{j\in J} Q_j^{ed} C_{j,co}^{x} + Q^{ed} C_{co}^{Ped} + Q^{ee} C_{co}^{Red} + Q^{fe} C_{co}^{Pro} + Q^{ge} C_{co}^{Rro}}{Q^{Fro}} \le C_{co}^{Ue} \qquad \forall co \in CO$$

- Max. allowable conc. into RO unit

$$\frac{\sum_{j\in J} Q_j^{ro} C_{j,co}^{x} + Q^{dr} C_{co}^{Ped} + Q^{er} C_{co}^{Red} + Q^{fr} C_{co}^{Pro} + Q^{ge} C_{co}^{Rro}}{Q^{Fro}} \le C_{co}^{Ur} \qquad \forall co \in CO$$

Model Development

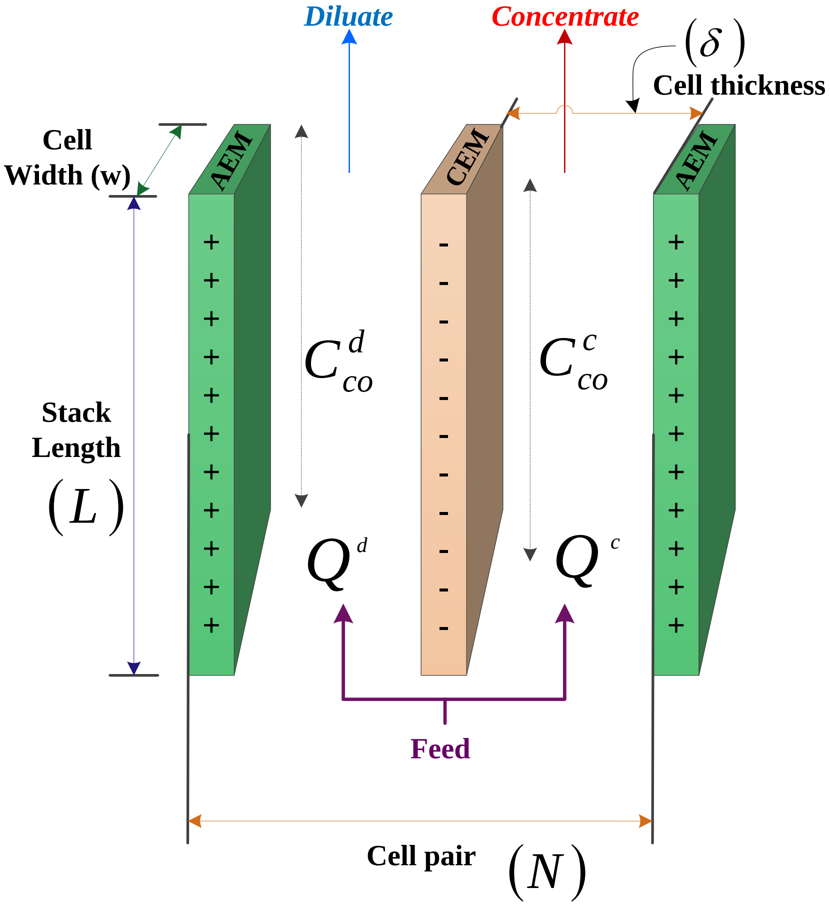
☐ Modelling the ED unit

- ❖ **Electric current**

$$I = \frac{Q^{d} C_{co}^{\Delta} F z}{\zeta N} \qquad \forall co \in CO$$

- ❖ **Stack length**

$$L = \frac{A}{2wN}$$



Model Development

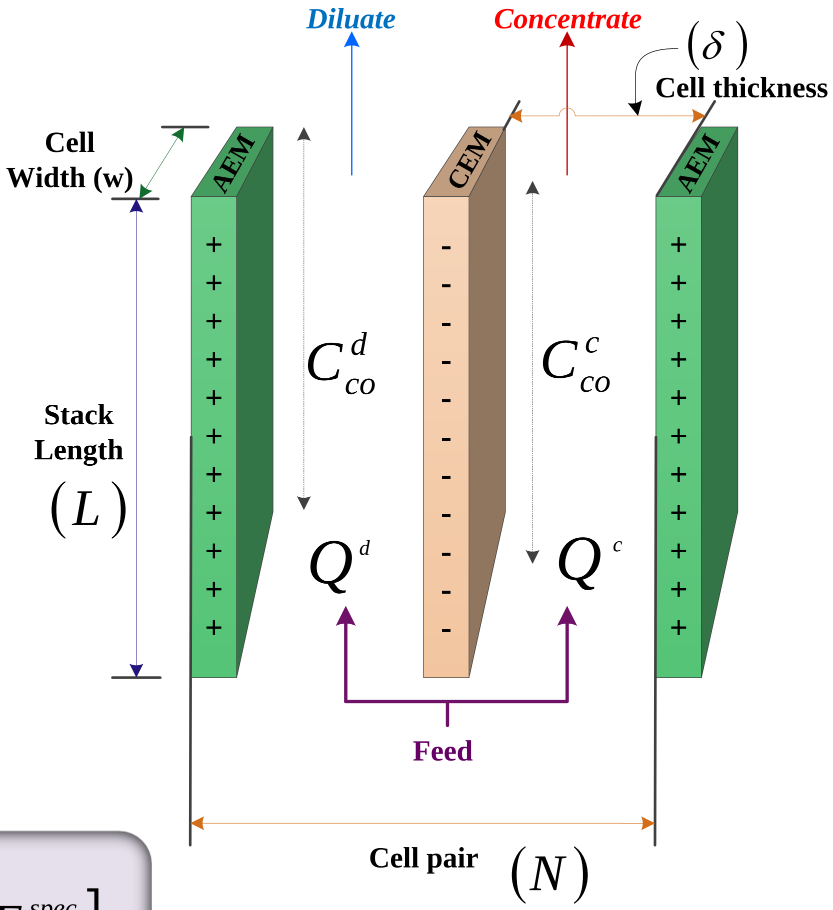
❖ Pressure drop

- ➢ Rectangular pipe channel
- ➢ Fluid is Newtonian & behaves like a continuum
- ➢ Flow is steady, laminar, fully developed & incompressible

$$\Delta P = \frac{12 v \mu L}{\delta^{2}}$$

❖ Total annualised cost

$$TAC_{e} = \frac{K^{mb} A}{t^{max}} + (AOT) K^{el} Q^{Ped} \left[E^{pump} + E^{spec} \right]$$

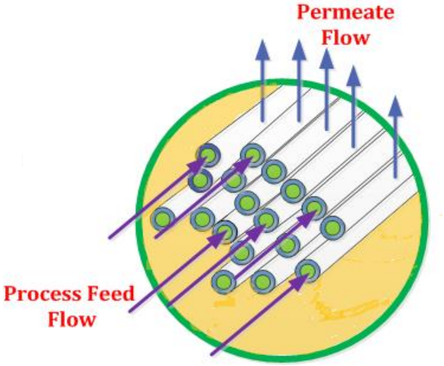


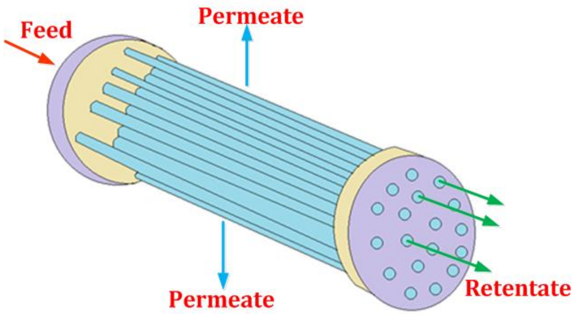
Model Development

❑ Modelling the RO unit

❖ Feed pressure

$$P_F = \Delta P + \left[\frac{\Delta P_{shell}}{2} + P_P \right]$$





❖ Water flux

$$N_{water} = A_p \left[\Delta P - \frac{\pi_F}{C_{co}^{Fro}} C_S \right] \gamma \quad \forall co \in CO$$

Model Development

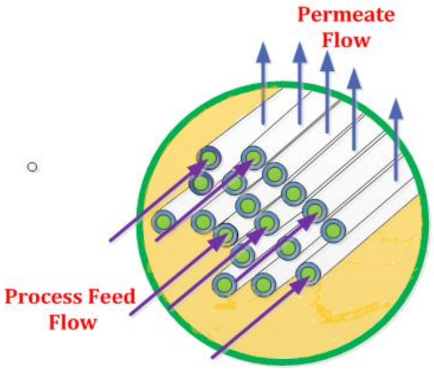
- Number of RO modules

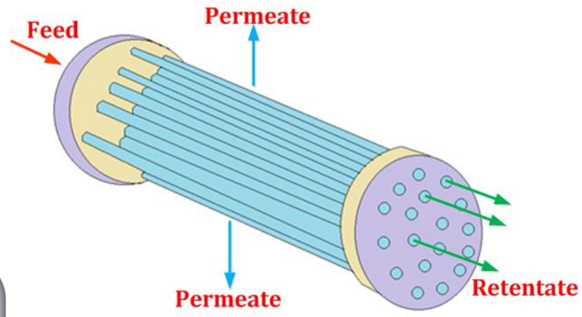
$$N_m = \frac{Q^{Pro}}{A_P S_m \gamma\left[\Delta P - OSC_{co}^{Fro}\right]}$$

$$\forall co \in CO$$

- Total annualised cost

$$TAC_r = K_{mod} N_m + K_{Pump}(P_{pump})^{0.65} + K_{turb}(P_{turb})^{0.43} + \frac{P_{Pump} K_{elec} AOT}{\eta_{Pump}}$$
$$+ Q^{Fro} K_{chemicals} AOT - P_{turbine} \eta_{turb} K_{elec} AOT$$





Model Development

❑ Performance of regeneration units

- Removal ratio

$$RR_{ed} = \frac{Q^{Red} C_{co}^{Red}}{Q^{Fed} C_{co}^{Fed}} \quad \forall co \in CO$$

$$RR_{ro} = \frac{Q^{Rro} C_{co}^{Rro}}{Q^{Fro} C_{co}^{Fro}} \quad \forall co \in CO$$

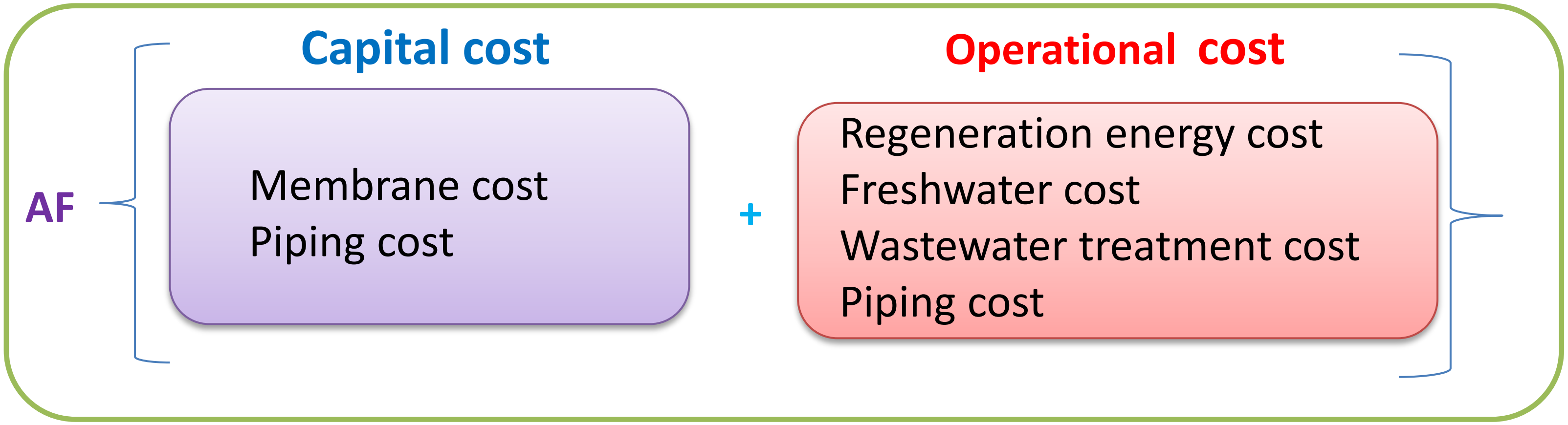
- Liquid recovery

$$LR_{ed} = \frac{Q^{Ped}}{Q^{Fed}}$$

$$LR_{ro} = \frac{Q^{Rro}}{Q^{Fro}}$$

Model Development

❑ Objective function



Min **AF**

Capital cost

Membrane cost
Piping cost

\+

Operational cost

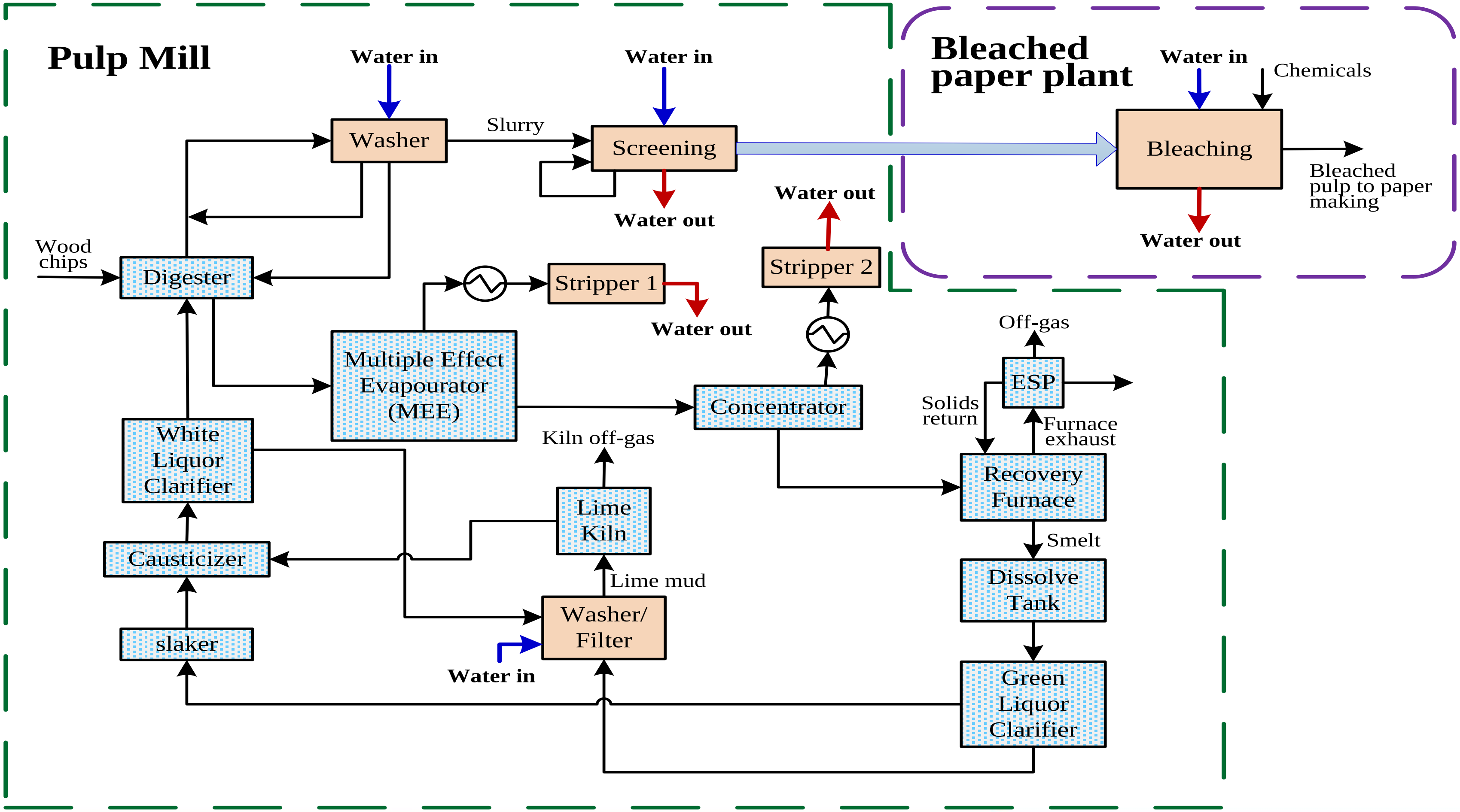
Regeneration energy cost
Freshwater cost
Wastewater treatment cost
Piping cost

❑ Model structure

- MINLP
  - Continuous and integer variables
  - Nonlinear constraints
- GAMS
  - **BARON**

Illustrative Example I

- ❑ **Typical pulp and paper plant**



Pulp Mill

Water in

Water in

Washer

Slurry

Screening

Water out

Water out

Bleached paper plant

Water in

Chemicals

Bleaching

Bleached pulp to paper making

Water out

Wood chips

Digester

Stripper 1

Water out

Stripper 2

Multiple Effect Evapourator (MEE)

Concentrator

Off-gas

ESP

Solids return

Furnace exhaust

Kiln off-gas

White Liquor Clarifier

Recovery Furnace

Lime Kiln

Smelt

Causticizer

Lime mud

Dissolve Tank

Washer/ Filter

slaker

Water in

Green Liquor Clarifier

Illustrative Example I

❑ Source/Sink identification

Sources	Process units	Sinks	Process units
1	Stripper 1	**1**	Washer
2	Screening	**2**	Screening
3	Stripper 2	**3**	Washer/Filter
4	Bleaching	**4**	Bleaching
FW	*FW*	***WW***	*WW*

Illustrative Example I

❑ Pulp and paper case study

Sources, *j*			Sinks, *i*		
j	**Flowrate (t/h)**	**Concentration (mg/L)**	***i***	**Flowrate (t/h)**	**Max. concentration (mg/L)**
1	2.07	89.4	**1**	3.26	34.0
2	0.34	272	**2**	0.34	84.0
3	0.024	18.3	**3**	1.34	50.0
4	7.22	36.0	**4**	7.22	6.30
FW	∞	0	***WW***	∞	600

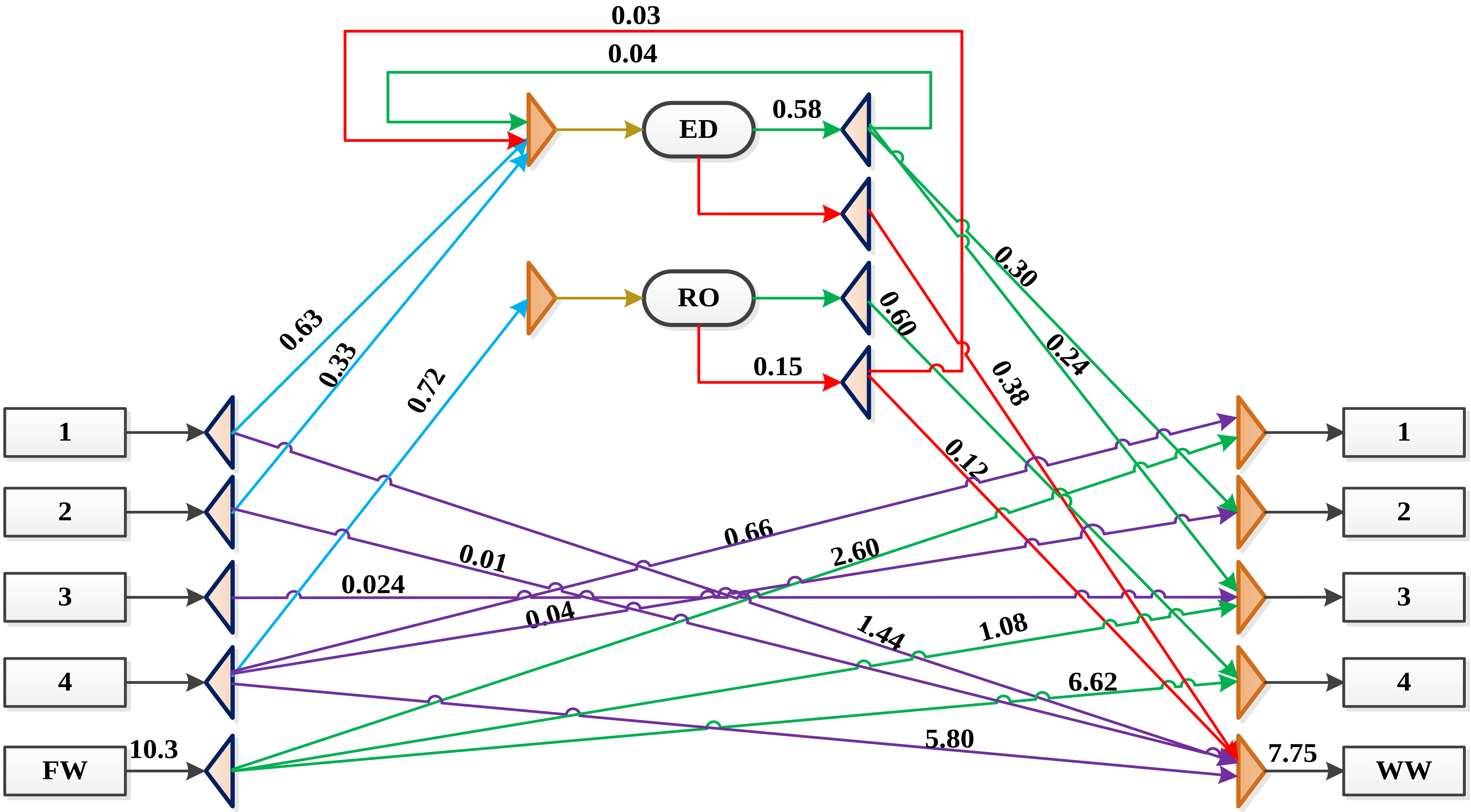
- ❖ Design parameters of ED and RO units
- ❖ Economic data for the case study
- ❖ Data for Manhattan distances

Results

		Scenario 1	Scenario 2		Scenario 3	
		Base case	Fixed RR	Variable RR	Fixed RR	Variable RR
Removal ratio	RR_e		0.70	0.75	0.70	**0.78**
	RR_r		0.70	0.85	0.70	**0.84**
Total freshwater use (t/h)		18.30	11.42	9.83	11.64	**10.30**
Freshwater savings			37.50%	46.30%	36.40%	**43.70%**
Total wastewater generated		15.8	8.89	7.30	9.11	**7.75**
Wastewater saved			43.70%	53.70%	42.30%	**50.90%**
Total cost of water network millions($/year)		1.17	0.84	0.81	0.63	**0.62**
CPU time (s)		0.06	688	2764	865	**16710**

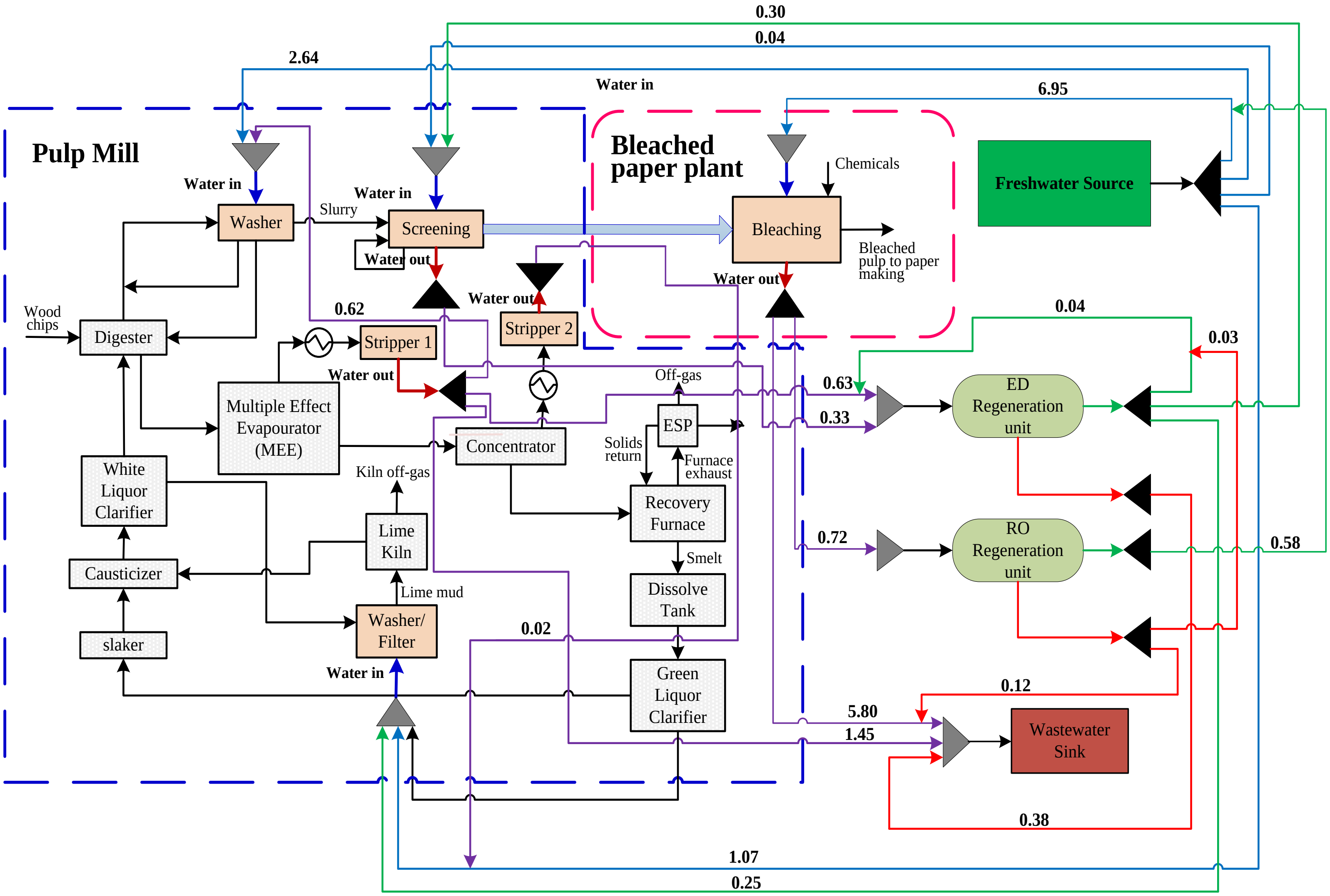
❑ Results

❖ Optimal results for case 3 variable RR



❑ Results

❖ Optimum water flowsheet for scenario 3 (Variable RR)



Results

❑ Optimal design results of ED and RO unit

Variable	Value
Area of ED	54m^2
Number of cell pairs in the ED unit	50
Number of RO modules	20
Length of ED unit	0.82 m
Specific Energy	0.021 J/s
Pumping Energy	0.004 J/s
Electric Current	12 A
Voltage across the ED unit	30 V
Pressure drop on the shell side	4.5x10^5 kPa
Osmotic pressure	1.6 kPa
Feed pressure	5.7x10^5 kPa

Results

- ❑ **Energy savings for ED and RO units**
  - ❖ Variable RR case

	Scenario2 (“Black-box”)	Scenario3 (Detailed)
Energy requirement of RO unit kWh/annum	**37452**	17280
ED Desalination Energy kWh/annum		15552
Total		**32832**

>12% savings in energy

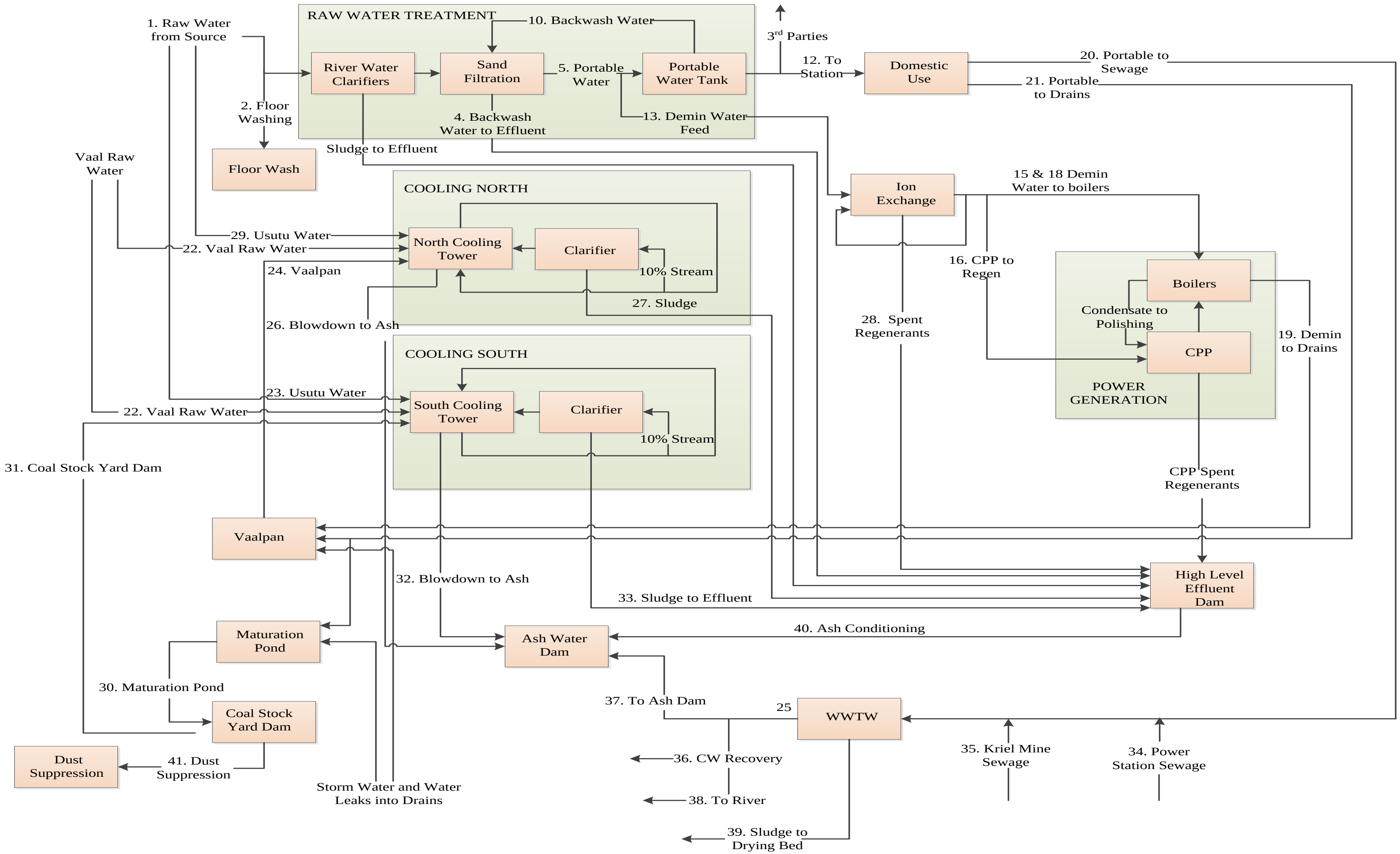
Case Study

Application to Eskom Kriel Power Station


3.6 GW
[43 GW]

❑ Case Study

❖ Current water utilisation network flowsheet at Kriel power plant



❖ Identified sources and sinks for the case study

Unit Operations	Sources	Sinks	Variables
Usutu raw water			X
Vaal raw water supply			X
Floor washing		X	
3rd Parties		X	
Sand filter backwash water		X	
Dirty sand filter backwash water	X		
Power station potable water use (bathrooms, kitchen etc)		X	
Power station potable water leaking into drains	X		
Power generation: Demin water		X	
Power generation: Demin water to drains-mostly tanks overflows	X		
Power generation: CPP spend regenerants	X		
Ion exchange: Spent regenerants	X		
Effluent dam	X		
North cooling Tower	X	X	
South cooling tower	X	X	
WWTW	X		
Ash dam/Ash conditioning		X	
Dust suppression		X	
Vaalpan – mostly from leaks from process units	X		

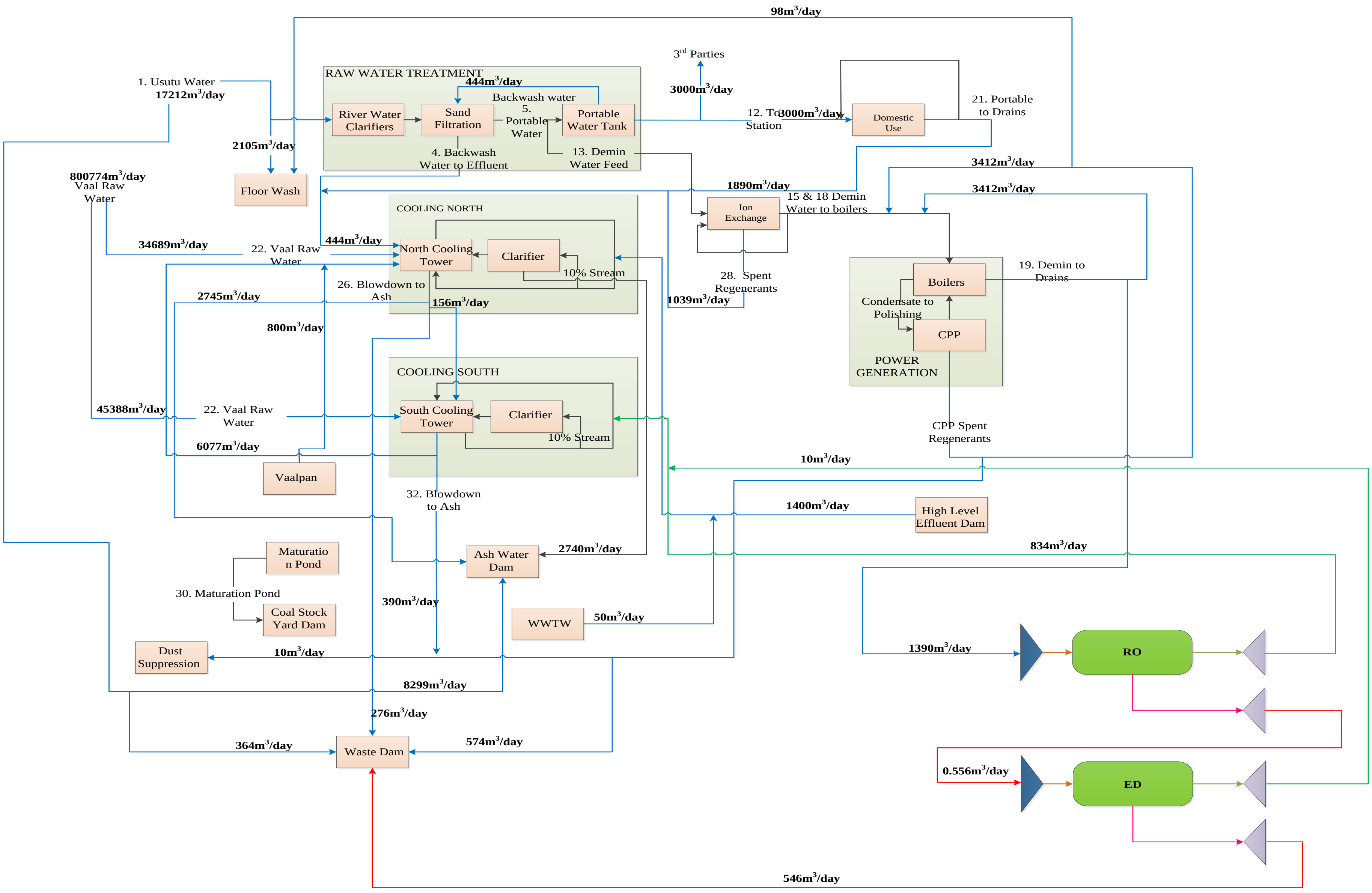
❑ Limiting data for case study

Sources				Sinks			
No	**Name**	**Flowrate m^3/d**	**Conc. mg/l**	**No**	**Name**	**Flowrate m^3/d**	**Conc. mg/l**
1	SF backwash	444	48	***1***	F Washing	2203	43
2	PS to Drains	1890	58	***2***	3rd Parties	3000	45
3	PG to Drains	3412	0	***3***	SF Backwash	444	45
4	CPP Regents	4094	0	***4***	PS Potable	3000	45
5	Spent Regents	1039	127	***5***	PG Demin	6824	0
6	NC Tower	3177	2548	***6***	NC Tower	46389	826
7	SC Tower	6467	2548	***7***	SC Tower	46389	130
8	Effluent Dam	1400	6369	***8***	Ash Dam	11044	6369
9	WWTW	50	249	***9***	D Suppression	400	2548
10	Vaalpan	800	732	***10***	Waste Dam	∞	10000
11	Freshwater	∞	45				

Results

	Current Practice	Direct Reuse and Recycle	"Black-box" Model	Detailed Model
Freshwater m^3/d	119693 (3.1 l/uso)	102718 (2.1 l/uso)	96920	**97290** **(1.9 l/uso)**
FW Savings %		14.2	19	**18.7**
Wastewater m^3/d	10000	5789	0	**1760**
WW Savings %		42	100	**82.4**

❑ Optimal water network flowsheet configuration



Results

❖ Regeneration cost analysis

	"Black-box" Model		Detailed Model
	Estimated cost	**True cost**	
Total reg. feed (m^3/d)	3,768	3,768	1,390
Regeneration cost (ZAR)	59,246	729,906	269,156
Total cost (ZAR)	**588,129**	**1,256,789**	**597,419**

❖ Energy Savings within the Regeneration units

	"Black-Box"	Detailed
Combined desalination and pumping Energy in kWh/annum	5,211.10	**2,933.30**

❖ 43.7% savings in both desalination and pumping energy

Results

❑ Summary of model characteristics

	Direct Reuse and Recycle	“Black-box” Model	Detailed Model
No. of constraints	283	350	500
No. of continuous variables	244	309	445
No. of discrete variables	110	140	181
Tolerance	0	0.01	0.01
CPU time (s)	0.063	18	3280

- Size of model
  - Increasing number of constraints
    - ✓ Integer
    - ✓ Nonlinear terms
  - Computational intensity

Conclusion

- Mathematical model was developed
  - Based on a superstructure
    - ✓regeneration reuse/recycle
  - Detailed regeneration units (ED & RO)
- The proposed model was applied to
  - Illustrative example involving single contaminant
  - Case study involving single contaminant
- Results showed
  - 43.7% freshwater savings and 50.9% reduction in wastewater
  - 18.7% freshwater savings and 82.4% reduction in wastewater
  - Accurate cost representation
  - Optimal operating parameters and design configurations
  - Minimum network cost and Energy Savings

Conclusion

❑ Recent publications

1. Buabeng-Baidoo, E., Majozi, T., 2015, Effective synthesis and optimization framework for integrated water and membrane networks: A focus on Reverse Osmosis membranes**, *Industrial and Engineering Chemistry Research***, *54: 9394-9406* **(IF: 2.567)**.
2. Mafukidze, N.Y., Majozi, T., 2016, Synthesis and optimisation of an integrated water and membrane network framework with multiple electrodialysis regenerators**, *Computers & Chemical Engineering***, *85: 151-161* **(IF: 2.581)**.
3. Nezungai, C.D., Majozi, T., 2016, Optimum Synthesis of an Electrodialysis Framework with a Background Process. I: A Novel Electrodialysis Model, ***Chemical Engineering Science***, *147*: *180 – 188* **(IF: 2.570).**
4. Nezungai, C.D., Majozi, T., 2016, Optimum Synthesis of an Electrodialysis Framework with a Background Process. II: Optimization and Synthesis of a Water Network, ***Chemical Engineering Science***, *147*: *189 - 199* **(IF: 2.570)**.
5. Abass, M., Majozi, T., 2016, Optimization of integrated water and multiregenerator membrane systems, ***Industrial and Engineering Chemistry Research***, *55*: *1995 - 2007* **(IF: 2.567)**.

Acknowledgements

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Thank You

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