A Mathematical Optimization Approach to Water-Energy Nexus

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Presentation Outline

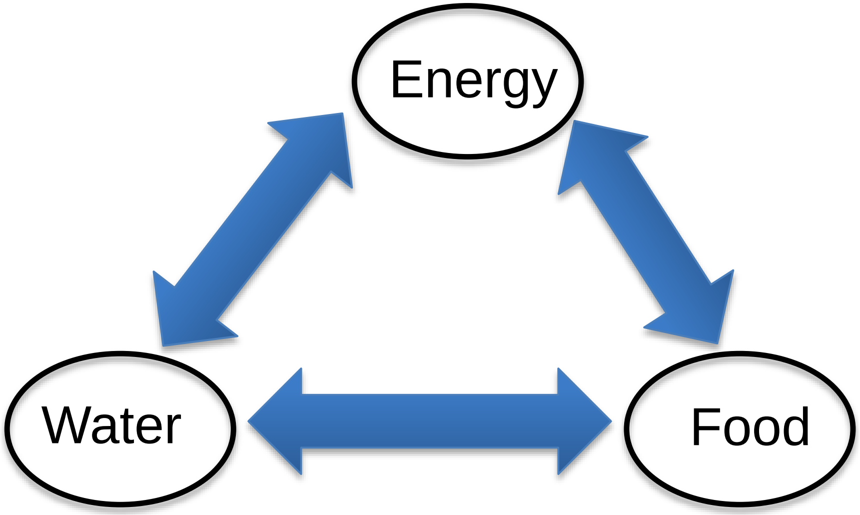
- Background
- Motivation for the study
- Objectives
- Problem statement
- Model development
- Results & Discussion
- Conclusion

Background

- Water and energy
  - Increasing demand for both resources
  - Existence of strict environmental regulations
- Sustainable use of water and energy
  - Process integration techniques
    - Analysis
    - Synthesis
    - Design & Optimization

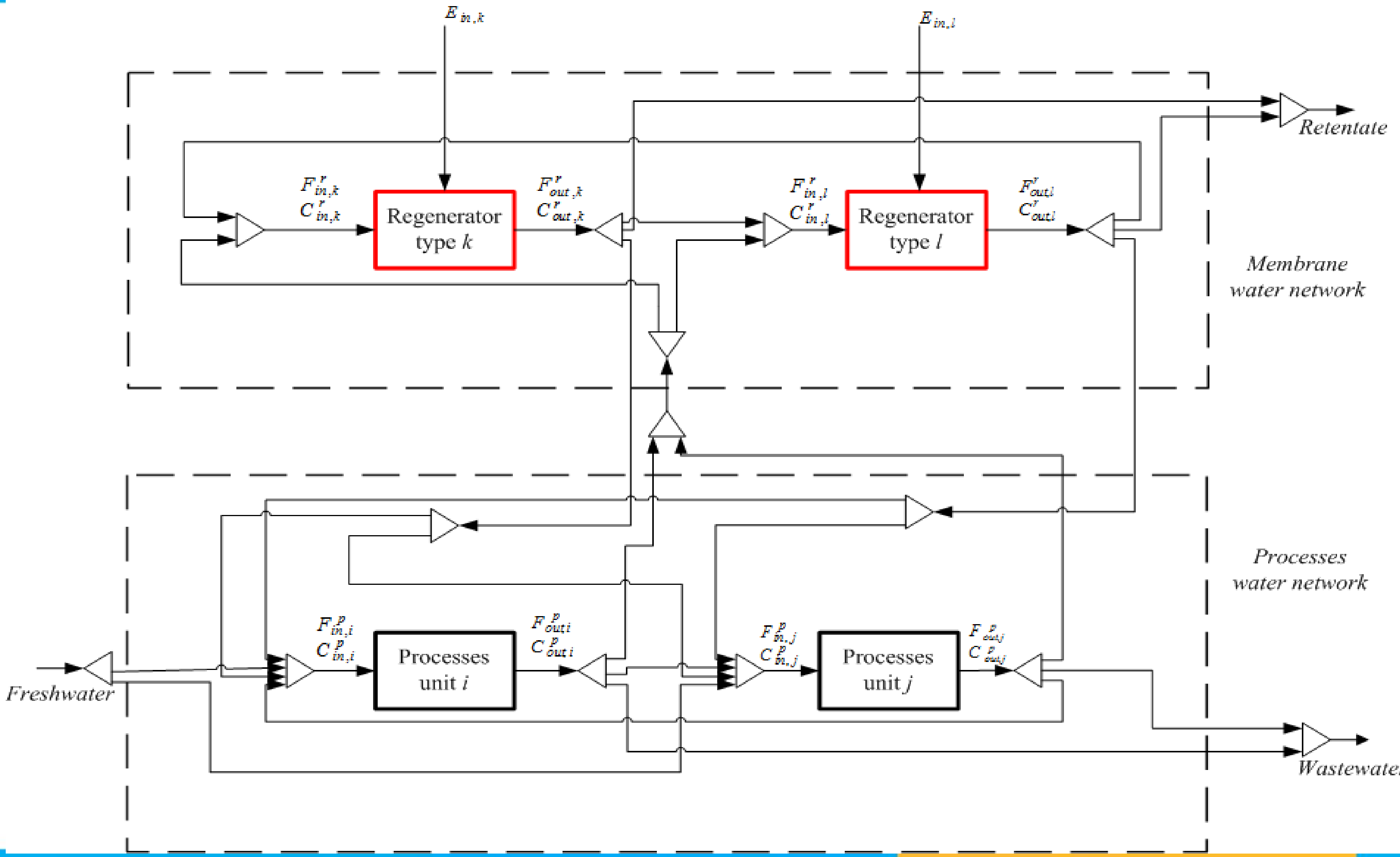
Background

- Water minimization
  - Process change
  - Reuse
  - Recycle
  - Regeneration-reuse
  - Regeneration-recycle



- **Energy requirements!!!!**

Motivation for the study



Motivation for the study

❑ Membrane technology

➢ Pressure driven

- ✓ Reverse osmosis
- ✓ Nanofiltration
- ✓ Ultrafiltration
- ✓ Microfiltration
- ✓ Vapour permeation
- ✓ Gas permeation
- ✓ Pervaporation

➢ Concentration Gradient

- ✓ Membrane extraction

➢ Electrical driven

- ✓ Electrodialysis
- ✓ Membrane electrolysis
- ✓ Electrosorption
- ✓ Electrofiltration
- ✓ Eelectrochemcial ion exchange

➢ Temperature Gradient

- ✓ Membrane distillation

➢ Combined driving forces

- ✓ Electro-osmofiltration

Motivation for the study

- Desalination and wastewater treatment (Tsiakis & Papageorgiou, 2005, El-Halwagi,1992)
  - No regeneration reuse/recycle
- "Blackbox" approach (Ng *et al.*, 2008, Tan *et al.*, 2009, Khor *et al.*, 2012)
  - Inaccurate costs representation
  - No design consideration
  - Treatment technology not identified
- Synthesis of membrane regeneration units (Khor *et al.*, 2011, Yang *et al.*, 2014)
  - Parallel configuration of regeneration units
  - No regeneration reuse/recycle
  - Short cut model with linear cost functions
- Detailed synthesis of multi-membrane regeneration network

Objectives

- Develop a water and membrane network superstructure
  - Membrane partitioning regenerator
  - Open reuse/recycle
- Develop mathematical model
  - Based on superstructure
  - Detailed model of regenerators
- Conduct a detail synthesis and design
  - Optimal operating variables: Minimum water and energy
  - Optimum design

Problem Statement

❑ Given:

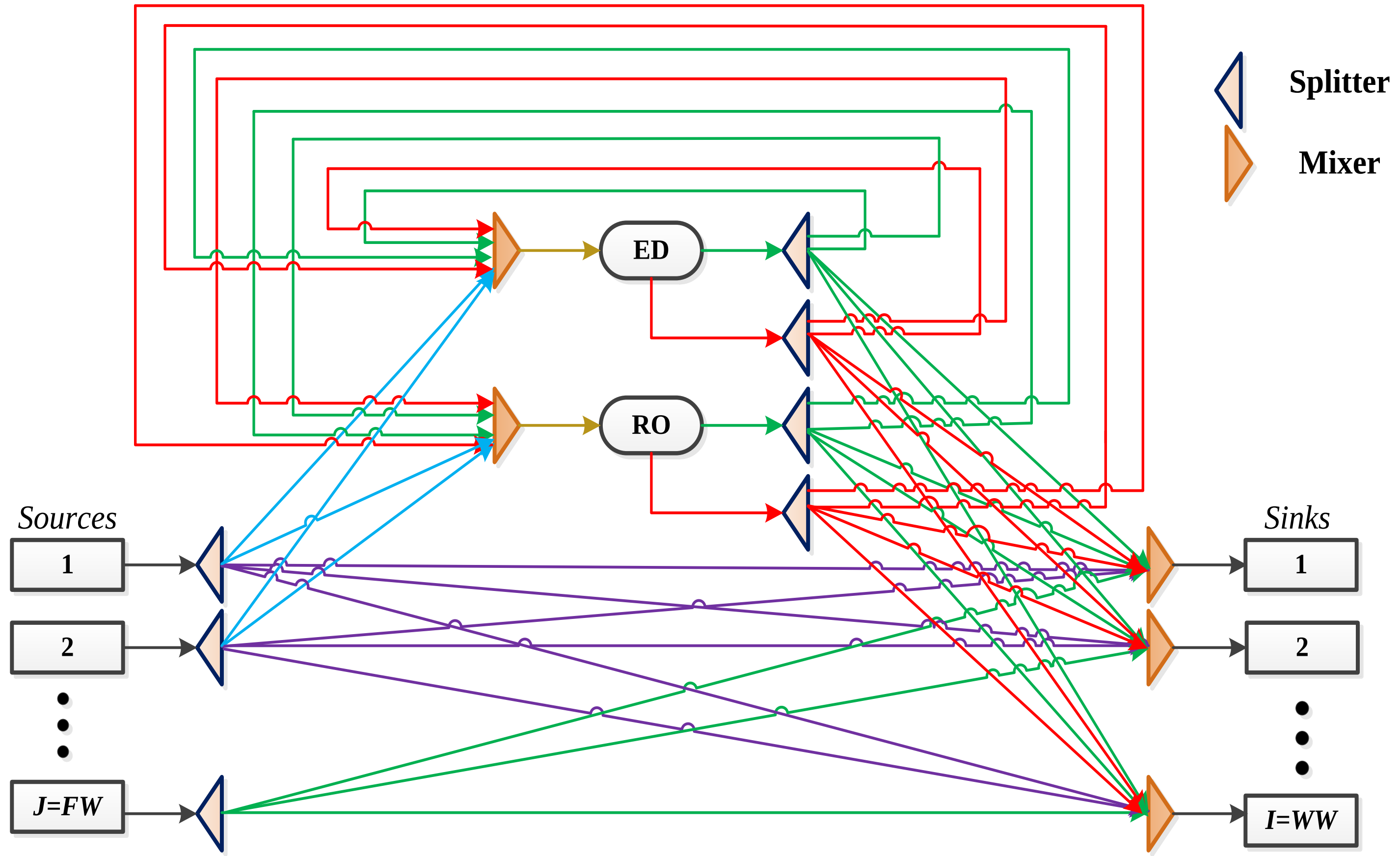
- Sources with known flowrates and contaminant concentrations
- Sinks with fixed flowrates and known maximum allowable concentration
- Water regeneration units (known design parameters)
- Freshwater source with known concentration

❑ Determine:

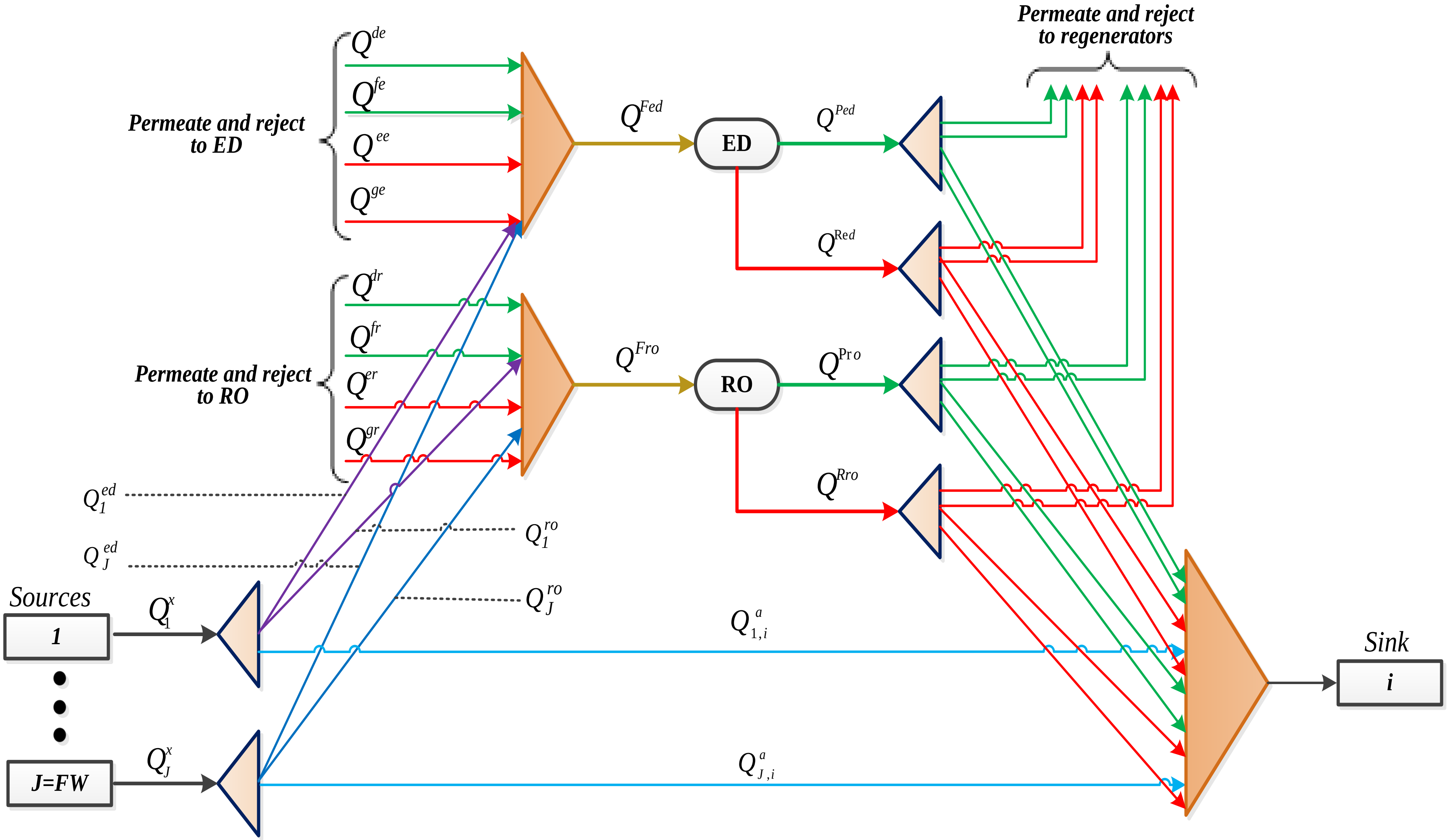
- Minimum flowrate of freshwater into sinks
- Minimum wastewater flowrate
- Optimum design variables of regenerators for minimal energy usage
- Optimal water network configuration

Model Development

Superstructure development



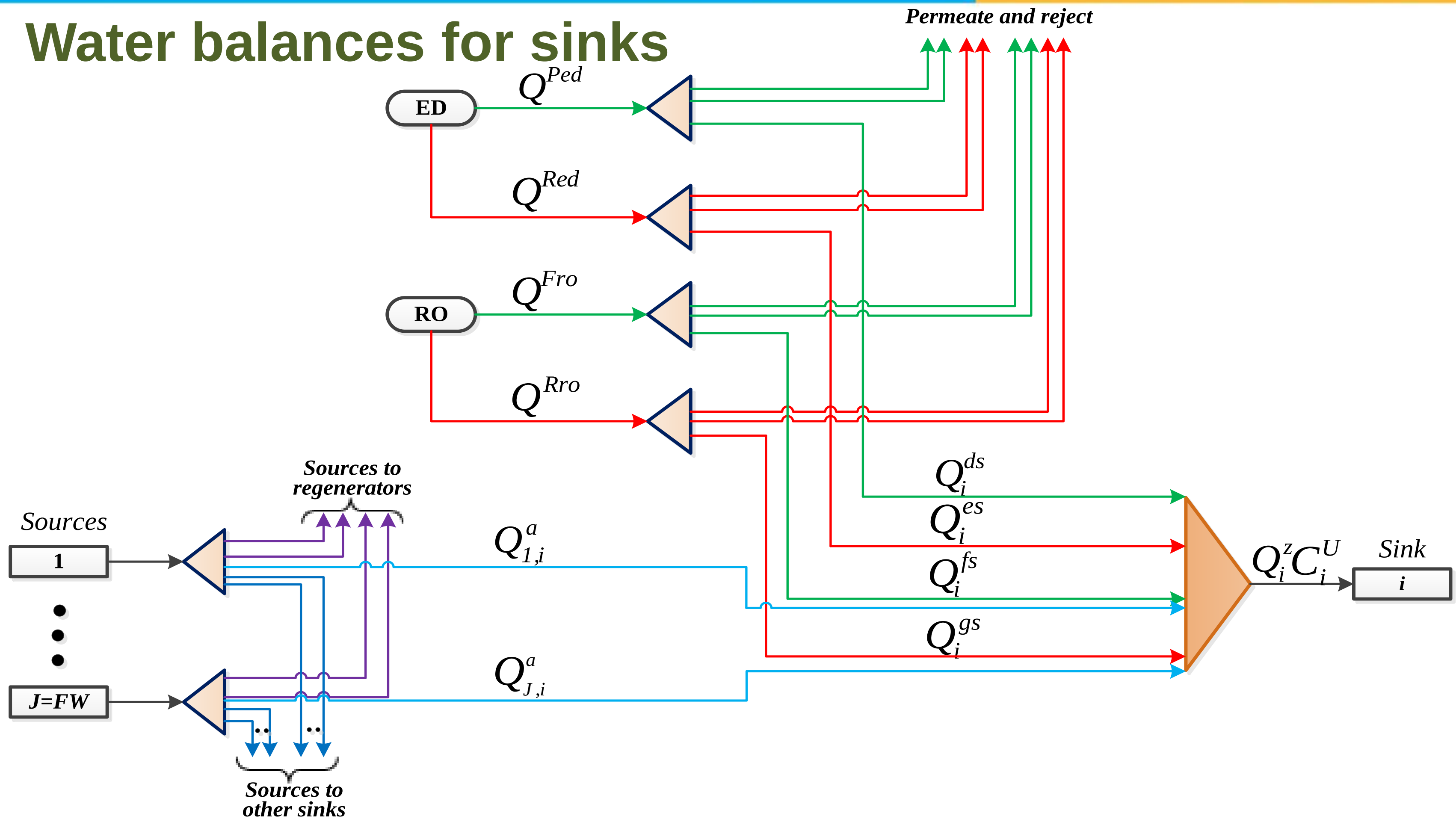
Water balances for regeneration unit



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

Model Development

Water balances for sinks



$$\sum_{j \in J} Q^{a}_{j,i} + Q_i^{ds} + Q_i^{es} + Q_i^{fs} + Q_i^{gs} = Q_i^{z} \qquad \forall i \in I$$

Model Development

Concentration balances for sinks

$$\frac{\sum_{j \in J} Q^{a}_{(j,i)} C_j + Q_i^{ds} C^{Ped} + Q_i^{es} C^{Red} + Q_i^{fs} C^{Pro} + Q_i^{gs} C^{Rro}}{Q_i^{z}} \leq C_i^{U} \qquad \forall i \in I$$

Removal ratio

$$RR_e = \frac{Q^{Red} C^{Red}}{Q^{Fed} C^{Fed}}$$

Model Development

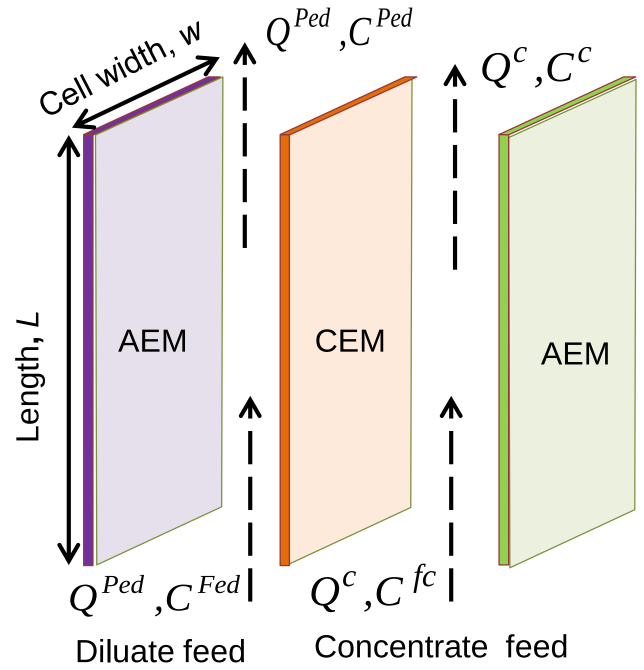
❑ Modelling of the ED unit

❖ Electric current

$$I = \frac{Q^{Ped} F\, C^{\Delta} z}{\zeta N}$$

❖ Membrane area

$$A = 2NLw$$



❖ Annualised cost equation

$$TAC_e = \frac{K^{mb} A}{t^{max}} (AOT) K^{el} Q^{Ped} \left[E^{Pump} + E^{Spec} \right]$$

❖ Pressure drop

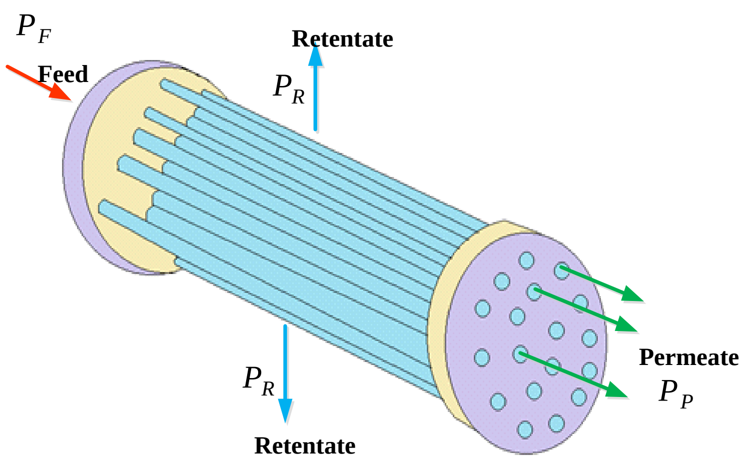
$$\frac{\Delta P}{L} = \frac{12\, \mu \bar{v}}{h^2}$$

Model Development

Modelling of the RO unit

Feed pressure

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



Total annual cost of RO unit

$$TAC_r = C_{mod} N_m + C_{Pump}(P_{pump})^{0.65} + C_{turb}(P_{turb})^{0.43}$$

$$+ \frac{P_{Pump} C_{elec} AOT}{\eta_{Pump}} - P_{turbine}\, \eta_{turb} C_{chemicals} AOT$$

Model Development

Objective function

- Minimize capital and operating cost of the water network
  - Total annual cost of RO and ED unit
  - Cost of freshwater (*FW*)
  - Cost of wastewater treatment (*WW*)
  - Capital and operating cost of the piping interconnections

Case Study

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	0.0002	1	3.26	0.00057
2	0.34	0.0051	2	0.34	0
3	0.024	0	3	1.34	6.16×10^{-6}
4	7.22	0.0083	4	7.22	0
FW	∞	0	*WW*	∞	0.01

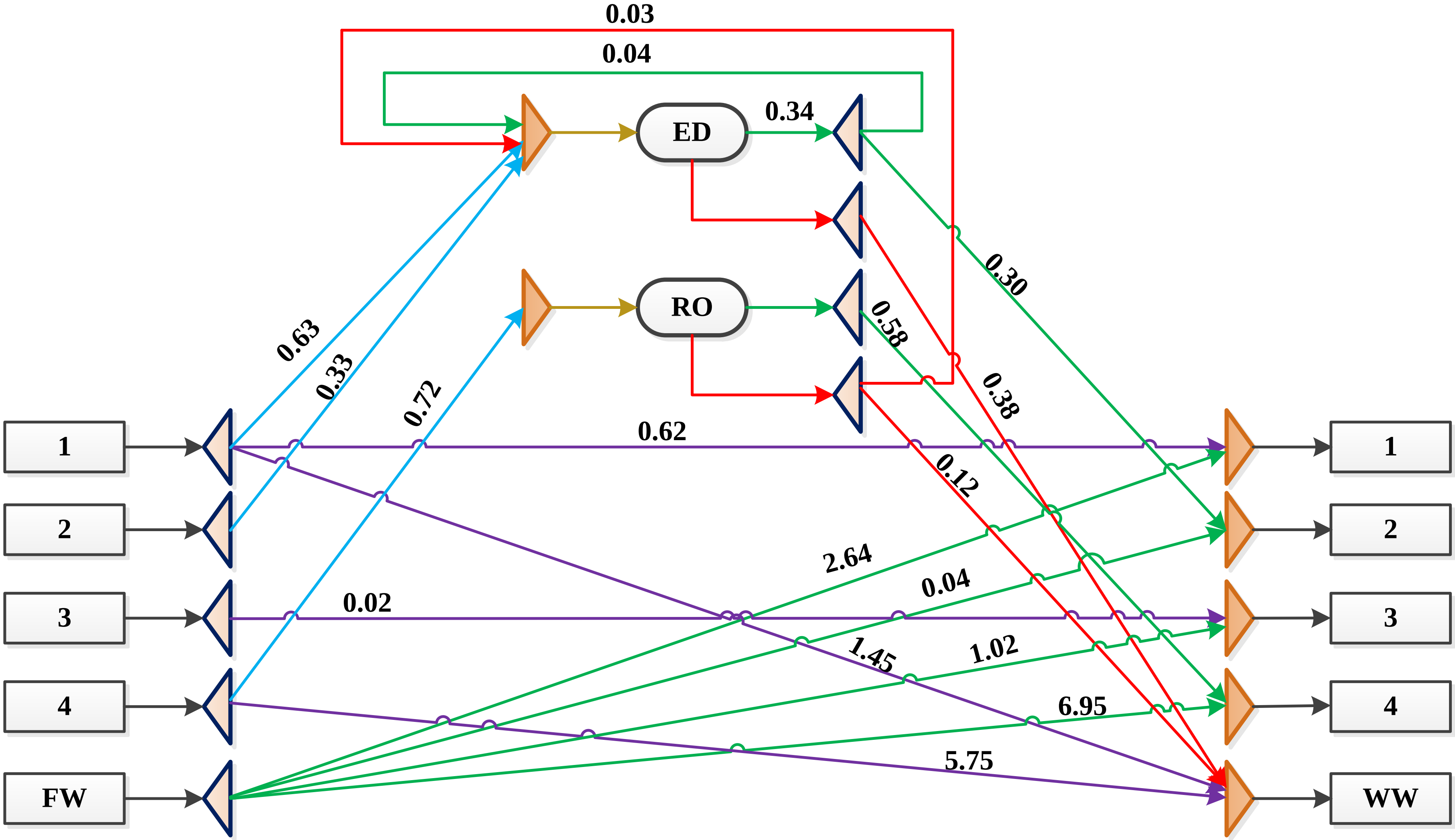
- Design parameters of ED and RO units
- Economic data for the case study
- Data for manhattan distances

Results

	Case 1	Case 2		Case 3	
	Base case	Fixed RR	Variable RR	Fixed RR	Variable RR
Removal ratio RR_e		0.7	0.75	0.7	0.78
Removal ratio RR_r		0.7	0.85	0.7	0.84
Total freshwater use (t/h)	18.3	11.1	9.4	12	10.2
Freshwater savings		39.1%	48.6%	34.4%	44.3%
Total wastewater generated	15.8	8.96	7	9.6	7.7
Wastewater saved		43.2%	54%	37%	50.9%
Total cost of water network millions($/year)	1.17	0.59	0.58	0.63	0.60
CPU time (s)	0.06	688	2764	865	16710

Results

Optimal results for case 3 variable RR



Results

Model structure

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

	Case 1	Case 2		Case 3	
	Base Case	Fixed RR	Variable RR	Fixed RR	Variable RR
Number of constraints	31	232	232	281	281
Number of continuous variables	68	185	187	222	224
Number of discrete variables	25	67	67	69	69
Tolerance	0	0.001	0.001	0.001	0.001

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	0.0040 J/s
Electric Current	12 A
Voltage across the ED unit	30 V
Pressure drop on the shell side	$4.5x10^5$ k/Pa
Osmotic pressure	1.6 k/Pa
Feed pressure	$5.7x10^5$ k/Pa

Results

Energy savings for ED and RO units

	Scenario 2 (Blackbox)		Scenario 3 (Detailed)	
	Fixed RR	Variable RR	Fixed RR	Variable RR
Energy recovery of RO unit kWh/annum	22521.38	37452.34	21563.76	36696.87
% savings in energy recovery for RO unit	39.8		41	
Desalination energy kWh/annum	0.041	0.032	0.031	0.021
% savings in desalination energy	24		34	
Pumping Energy kWh/annum	0.0067	0.006	0.0043	0.004
% savings in energy for ED unit	35.8		33.3	

Conclusion

- Mathematical model was developed for multi membrane regenerators
- The developed model was used for the synthesis and optimization of water network.
- The proposed model was applied to a pulp and paper case study and showed 44.3% reduction in freshwater
  - Optimal design
  - Optimal operating variables
  - Minimum water network cost

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Thank You

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