Mathematical Optimization of Process Flowsheet with Water Integration - PC Plant with CO_2 Capture

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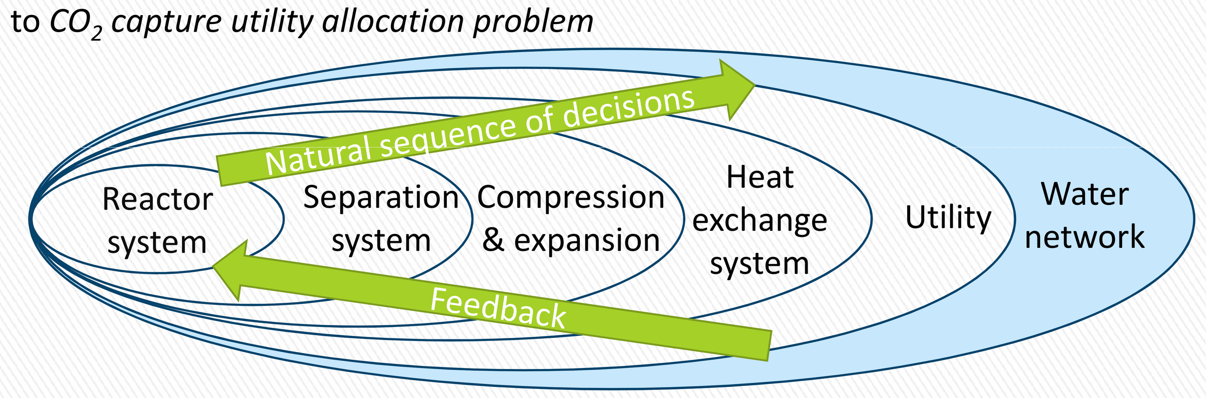
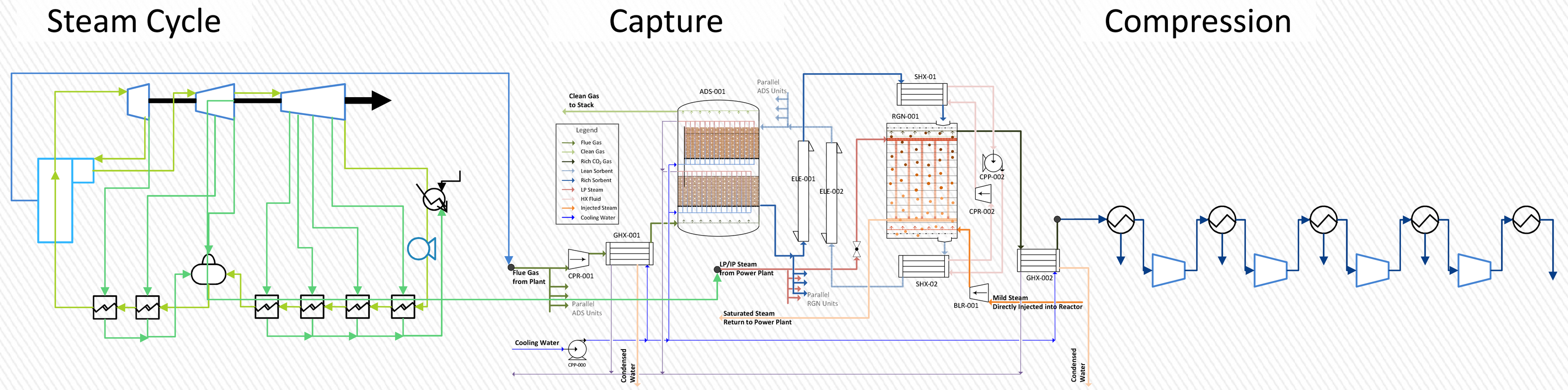
Motivation for Simultaneous Optimization

- In process synthesis, subsystems are designed after process flowsheet in a sequential fashion[5]
- **Simultaneous optimization** can capture tradeoffs among raw material, investment cost and operating cost
- Interest of this work to develop a method to perform simultaneous optimization to account for the feedbacks to the flowsheet from heat integration and **water integration**, and apply the method to *CO_2 capture utility allocation problem*



Steam Cycle | Capture | Compression



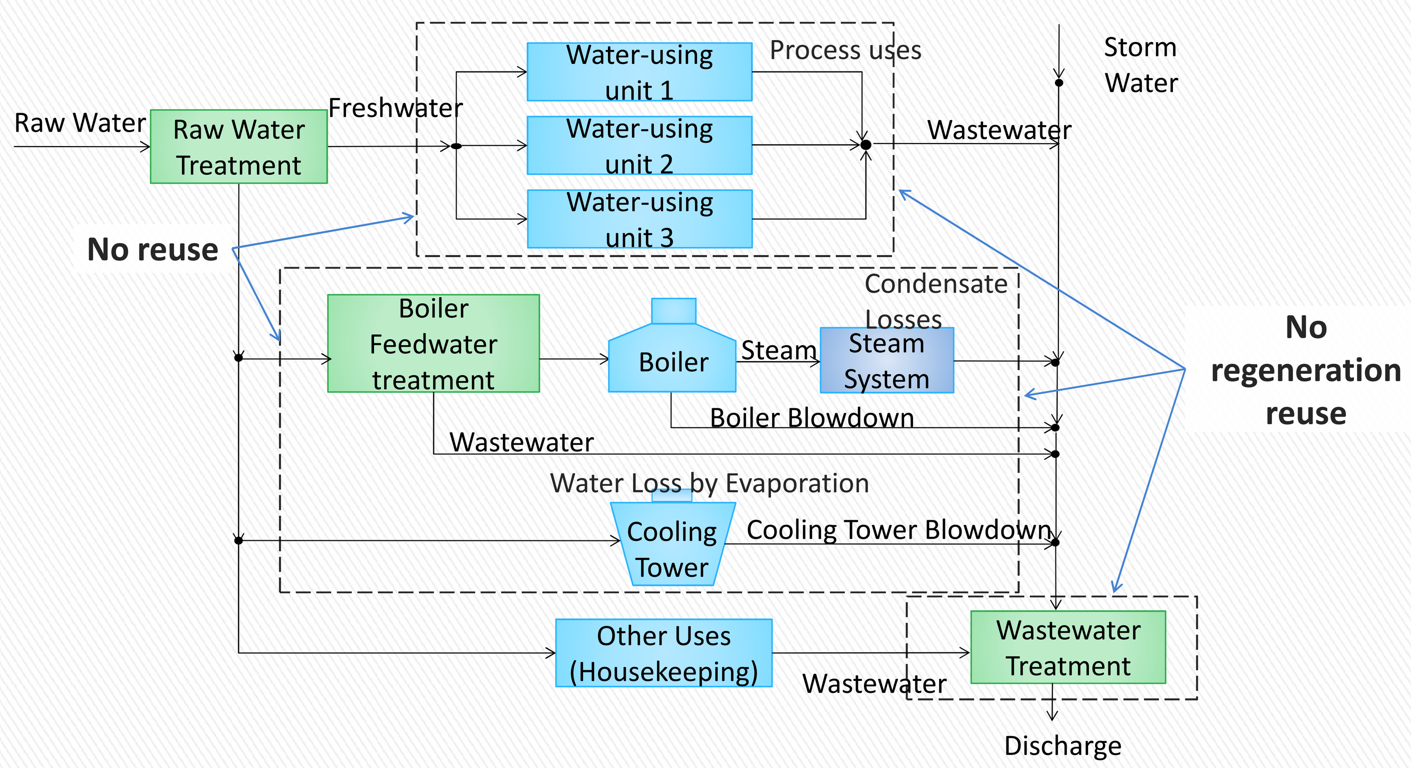
- Boiler feedwater
- Electricity required for FW pump
- Turbine generates electricity and steam
- Requires cooling water in the condenser

- Requires steam in the regenerator
- Requires cooling water

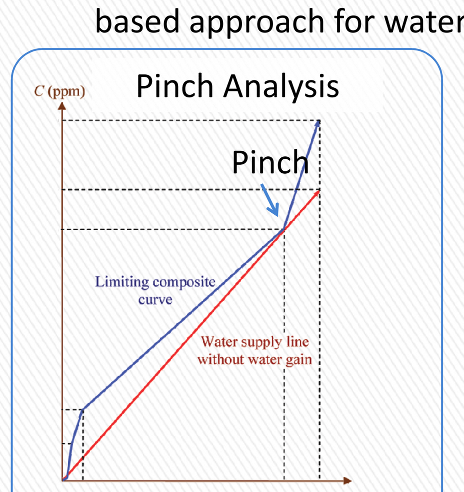
- Requires cooling water for isothermal compression
- Requires electricity for compression
- Generates wastewater from condensation

Water Network Synthesis Methods

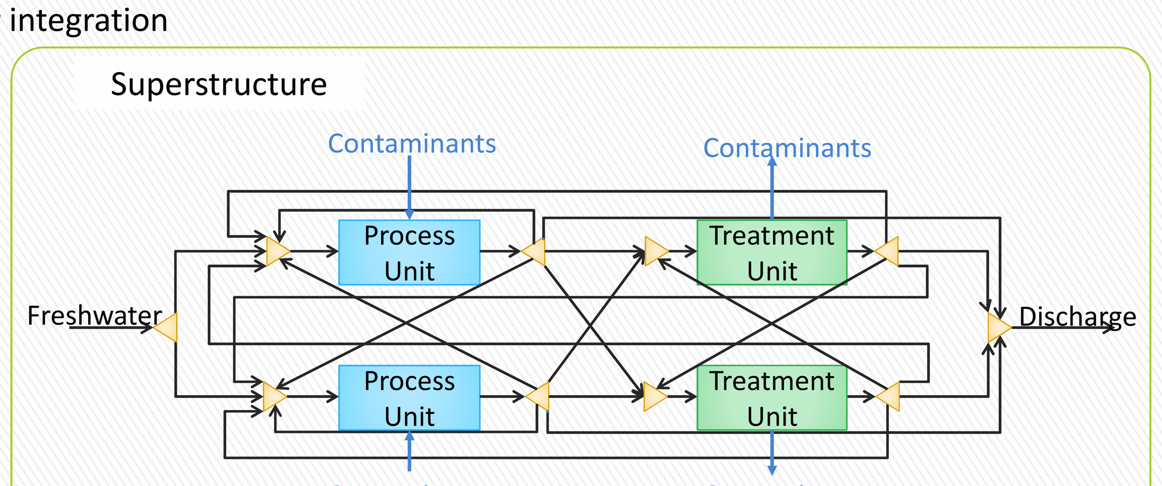
Conventional water network in the process industry does not allow for reuse of water streams



There are two general approaches to perform water network synthesis, this work uses the superstructure-based approach for water integration



- Linear formulation
- Valid only for single-contaminant system

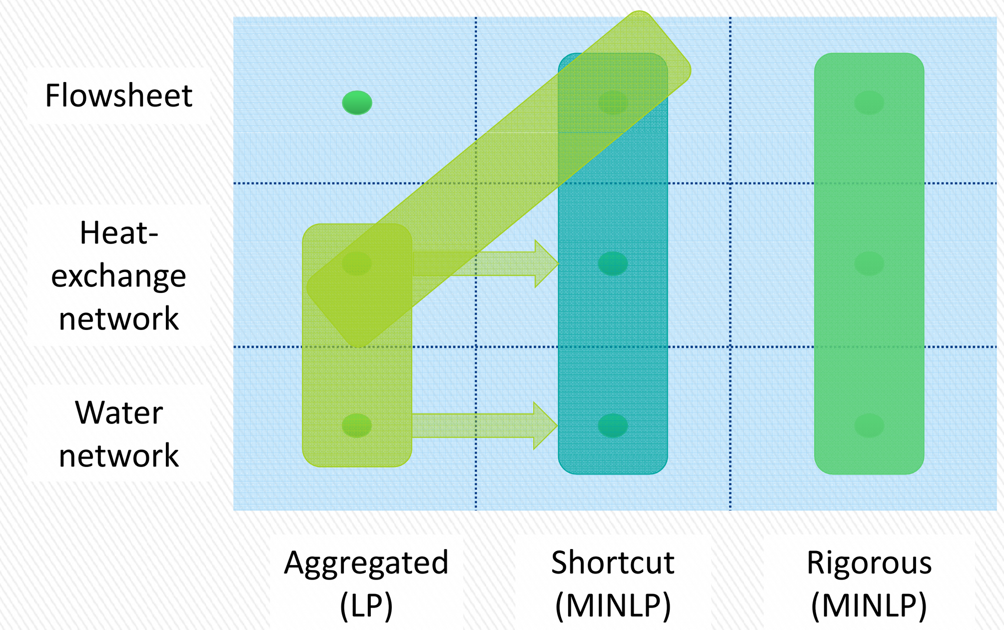


- Nonlinear formulation
- Guarantees global optimality[3]

Simultaneous Process Flowsheet / HEN / WN Integration

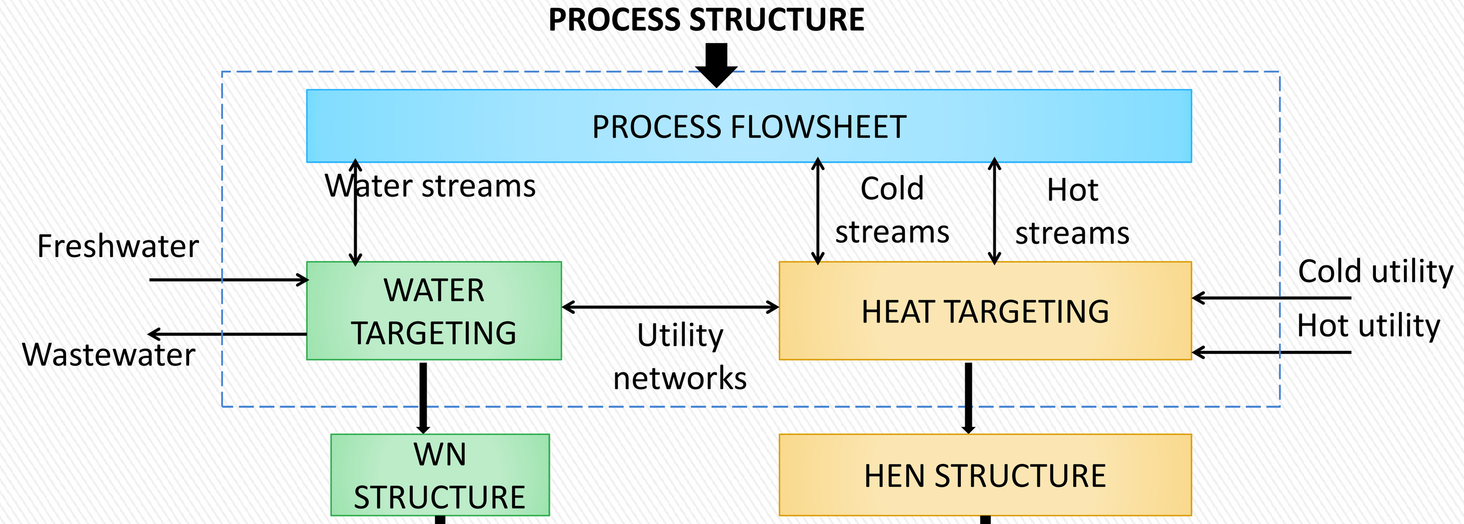
Targeting approach is used to **evaluate system performance** without commitment to detailed design. It is used to avoid solving a large nonconvex MINLP network models

Path 0: Unrealistic to solve (large MINLP)
Path 1: Very difficult to solve (MINLP)
Path 2: Can we avoid solving that MINLP but still get to the same optimal solution?



The strategy is to first optimize flowsheet operating conditions and the target requirement, then in the subsequent step determine the WN and HEN structures

PROCESS STRUCTURE



PROCESS FLOWSHEET WITH HEN AND WN

$$\min.\ \phi = F(x,u,v) + \sum_{i \in HU} c_H^i Q_H^i + \sum_{j \in CU} c_C^j Q_C^j + c_{fw} F_{fw}$$

$$\text{s.t. } h^P(x,u,v) = 0$$

$$g^P(x,u,v) \le 0$$

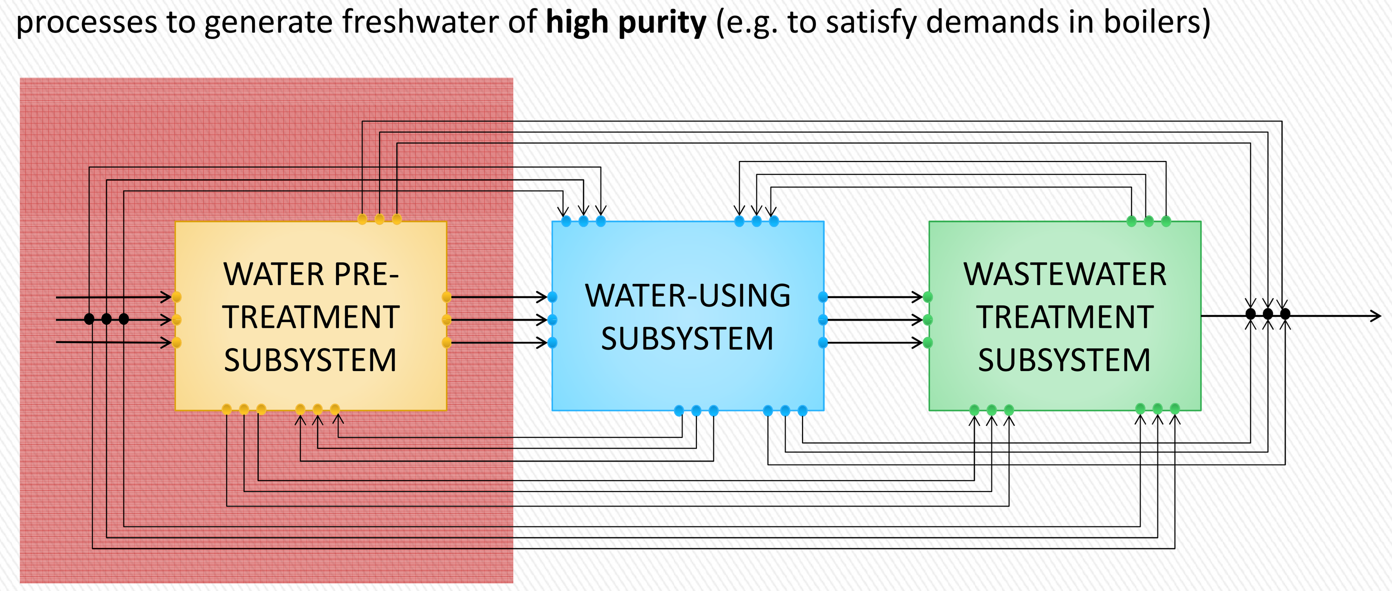
$$g^{HEN}(u, Q_H, Q_C) \le 0$$

$$g^{WN}(v, F_{fw}) \le 0 \quad \text{Need to derive this targeting formulation}$$

$$x \in X, \quad u \in U, \quad v \in V$$

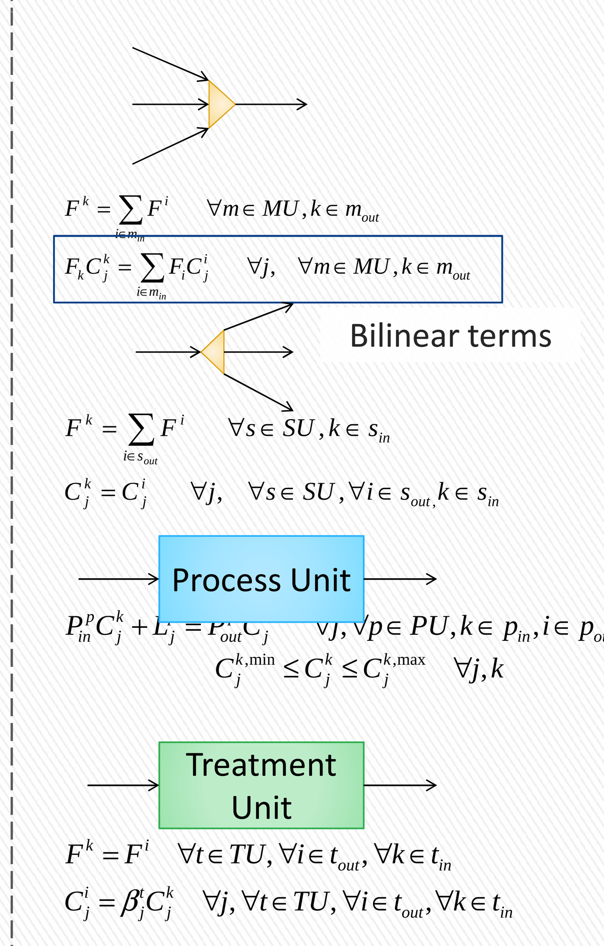
Rethinking Water Network Architecture

- We cannot take it for granted that freshwater is of high purity
- Need to design the **proper architecture** of water network[1] such that it contains pretreatment processes to generate freshwater of **high purity** (e.g. to satisfy demands in boilers)

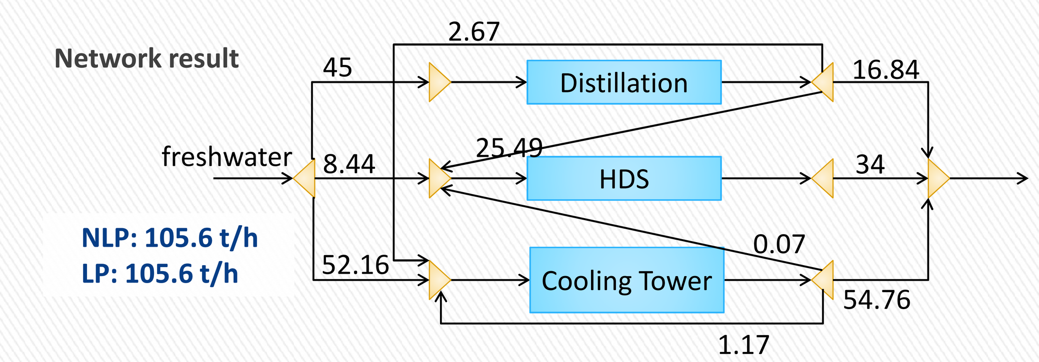


Water Targeting Method for Process Use

We have developed a water targeting formulation that relaxes the *nonlinear* water network formulation into *linear* formulation. The proposed LP model predicts the *exact* target for minimum freshwater consumption of a set of water-using processes under some assumptions.



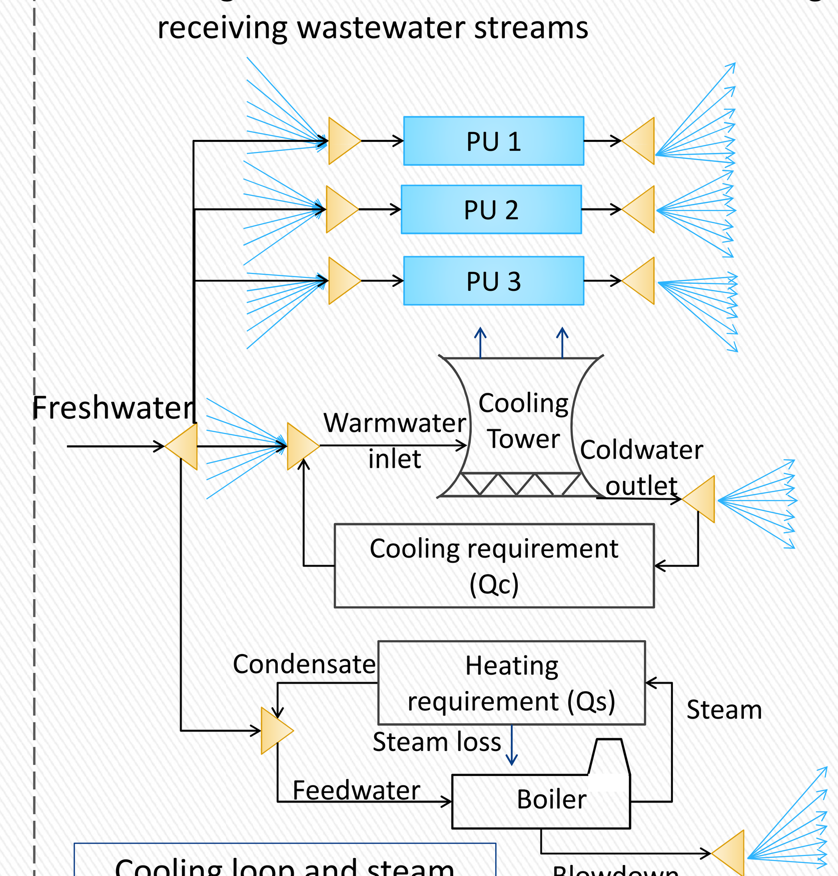
	Distillation			HDS			Cooling Tower		
	$C_j^{pin,max}$ (ppm)	Load (kg/h)	F (ton/h)	$C_j^{pin,max}$ (ppm)	Load (kg/h)	F (ton/h)	$C_j^{pin,max}$ (ppm)	Load (kg/h)	F (ton/h)
HC	0	0.675		20	3.4		120	5.6	
H_2S	0	18	45	300	414.8	34	20	1.4	56
Salt	0	1.575		45	4.59		200	520.8	



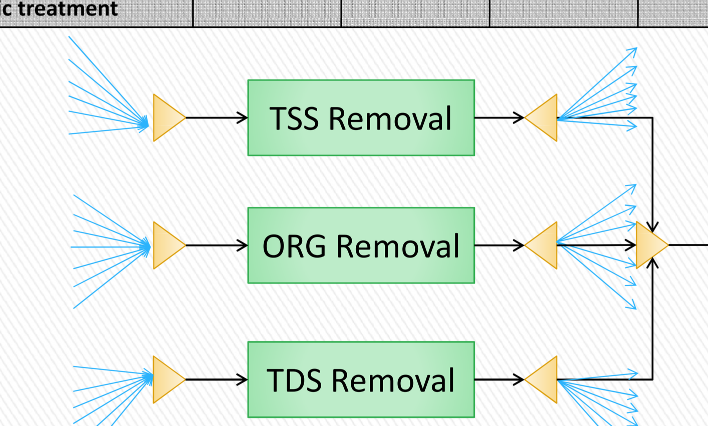
Using the targeting approach, the freshwater consumption is 105.6 ton/hr, which is a significant saving over 135 ton/hr required for conventional water network

Considerations for Process Units & Treatment Units

The goal is to select a subset of BAT technologies[6] and flowrates that best fit the treatment of the receiving wastewater streams



	Suspended Solids (TSS)	Heavy Metals (HM)	Inorganic Salt (TDS)	Organic (BOD)
Sedimentation	☑	☑		
Flotation	☑	☑		
Filtration	☑	☑		
Ultrafiltration	☑			
Precipitation		☑		
Ion exchange		☑	☑	
Reverse osmosis		☑	☑	
Evaporation			☑	
Bio. sulphate treatment			☑	
Anaerobic treatment				☑
Aerobic treatment				☑



Cooling loop and steam cycle are modeled with algebraic correlations

References:

[1] M. J. Bagajewicz, D. C. Faria, "On the appropriate architecture of the water/wastewater allocation problem in process plants," *Computer Aided Chemical Engineering,* Vol. 26, 2009, pp. 1-20.
[2] M. A. Duran and I. E. Grossmann, "Simultaneous optimization and heat integration of chemical processes," AIChE Journal, vol. 32, no. 1, 1986, pp. 123–138.
[3] R. Karuppiah and I. E. Grossmann, "Global optimization for the synthesis of integrated water systems in chemical processes," *Computers & Chemical Engineering*, vol. 30, no. 4, 2006, pp. 650 – 673.
[4] M. J. Savelski and M. J. Bagajewicz, "On the necessary conditions of optimality of water utilization systems in process plants with multiple contaminants". *Chem. Eng. Sci.* 2003, *58 (23-24), 5349-5362.*
[5] A. Wechsung, A. Aspelund, T. Gundersen, and P. I. Barton, "Synthesis of heat exchanger networks at subambient conditions with compression and expansion of process streams," *AIChE Journal*, vol. 57, no. 8, 2011, pp. 2090–2108.
[6] Integrated Pollution Prevention and Control Reference Document on Available Techniques in Common Waste Water and Waste Gas Treatment/Management Systems in the Chemical Sector, Tech. Rep., European Commission, BREF document, Current Draft, 2009.