Water Targeting Models for Simultaneous Flowsheet Optimization

- ESI meeting -

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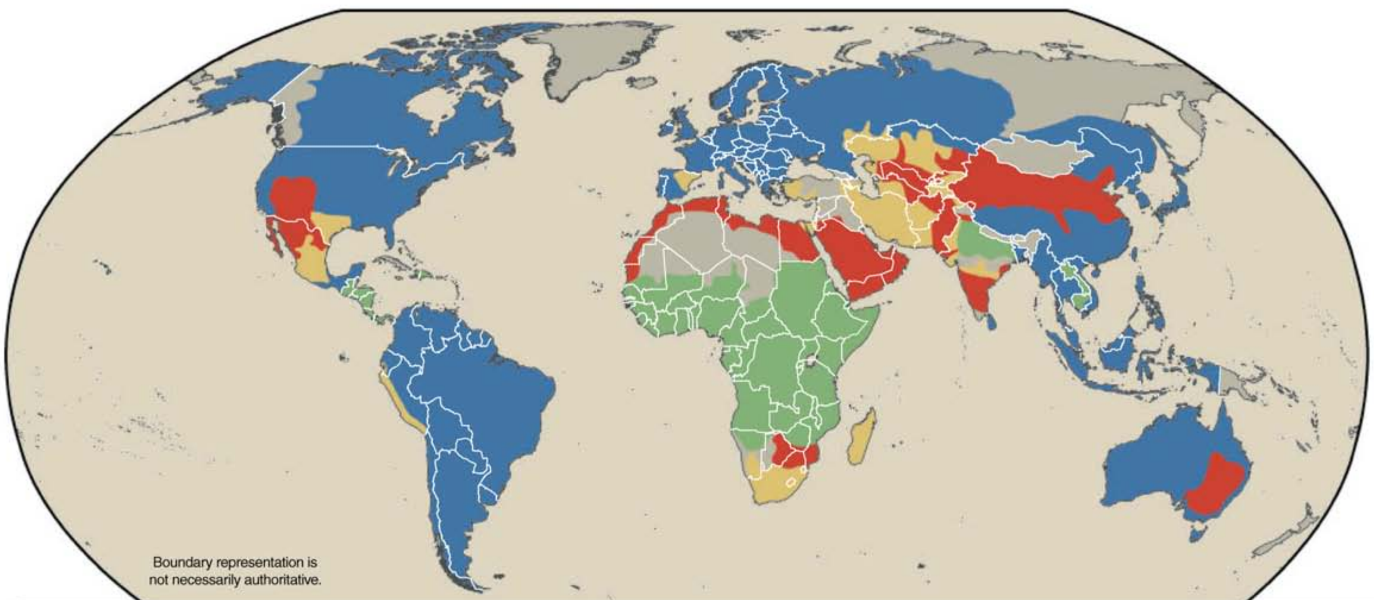
Water and energy are important resources in the process industries

"Water is the fastest growing market at the moment, with a size of $500 billion globally."

"If nothing is done, there will be a 40 percent gap between supply and demand by 2030."

Projected Global Water Scarcity, 2025



Physical water scarcity: More than 75% of river flows are allocated to agriculture, industries, or domestic purposes. This definition of scarcity — relating water availability to water demand — implies that dry areas are not necessarily water-scarce.

Approaching physical water scarcity: More than 60% of river flows are allocated. These basins will experience physical water scarcity in the near future.

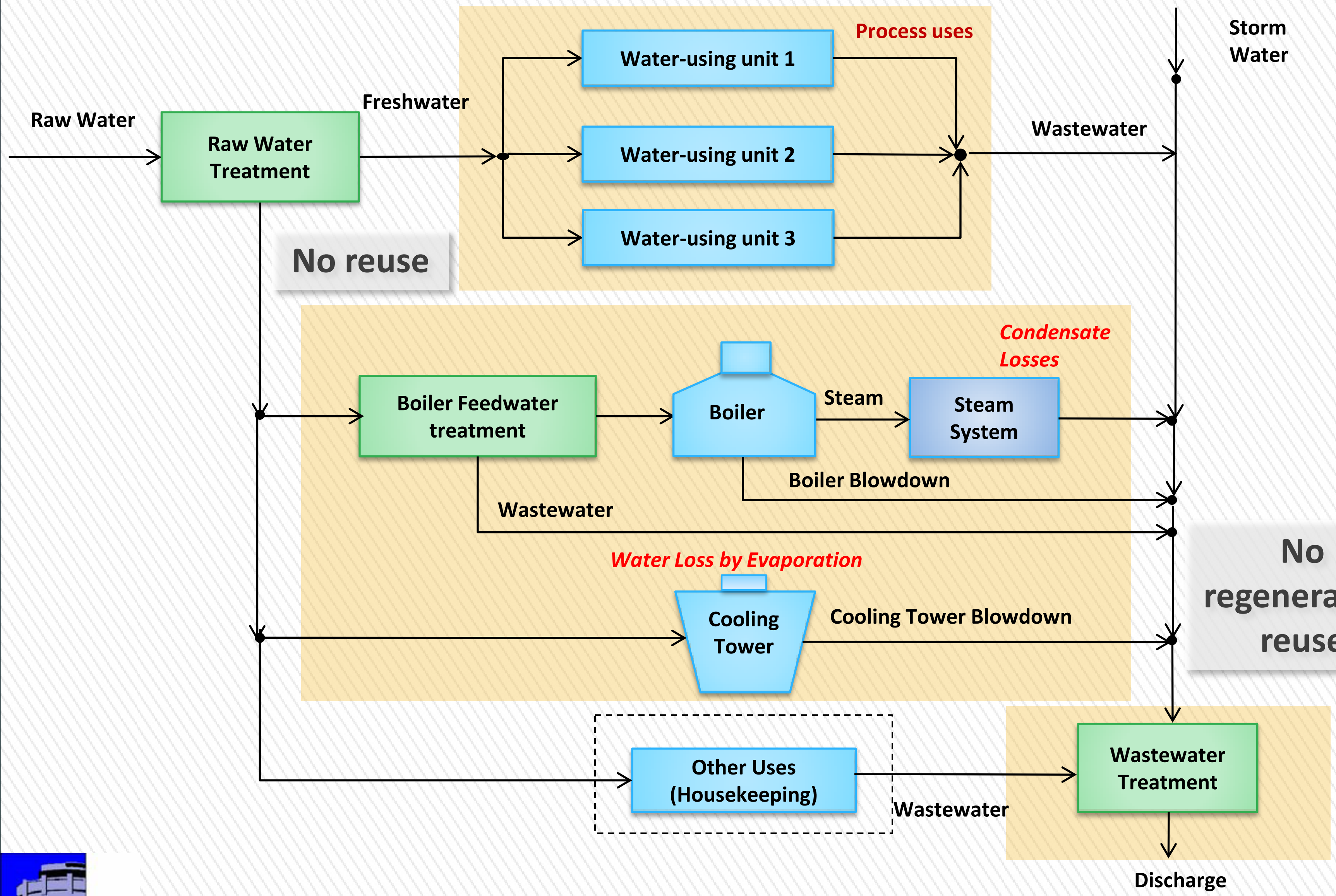
Economic water scarcity: Water resources are abundant relative to water use, with less than 25% of water from rivers withdrawn for human purposes, but malnutrition exists.

Little or no water scarcity: Abundant water resources relative to use. Less than 25% of water from rivers is withdrawn for human purposes.

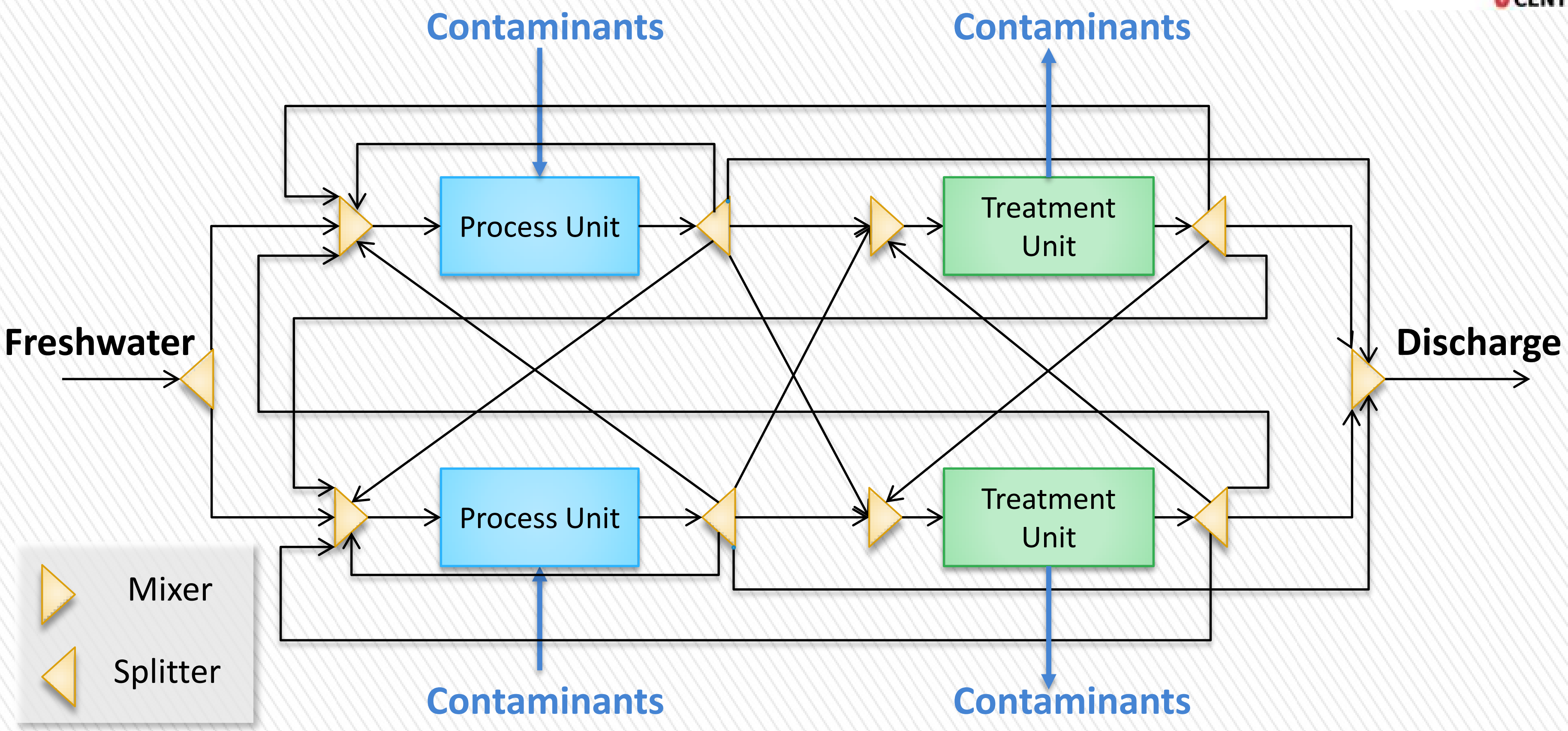
Not estimated

Source: International Water Management Institute.

Conventional water network



Superstructure based water network design



- Integrated water network with reuse, recycle, and regeneration schemes
- superstructure is formulated using a **nonconvex NLP** model

Karuppiah & Grossmann (2006); Ahmetovic & Grossmann (2010)

Freshwater targeting formulation

Goal: determine minimum freshwater consumption

(LP)

$$\min \quad Z = F_{fw}$$

$$\text{s.t.} \quad F^k = \sum_{i \in m_{in}} F^i \qquad \forall m \in MU, k \in m_{out}$$

$$F^k C_j^{k,\max} \geq \sum_{i \in m_{in}} (F^i C_j^{i,\max} + F_{fw}^i C_{fw}) \quad \forall j, \quad \forall m \in MU, k \in m_{out}$$

Mixer mass balances

$$F^k = \sum_{i \in s_{out}} F^i \qquad \forall s \in SU, k \in s_{in}$$

$$C_j^k = C_j^i \qquad \forall j, \quad \forall s \in SU, \qquad \forall i \in s_{out,} k \in s_{in}$$

Splitters mass balances

$$F^k = P_{in}^p \qquad \forall p \in PU, k \in p_{out}$$

$$F^i = P_{out}^p \qquad \forall p \in PU, i \in p_{in}$$

$$F^i C_j^i + L_j^p = F^k C_j^k \quad \forall j, \forall p \in PU, i \in p_{in}, k \in p_{out}$$

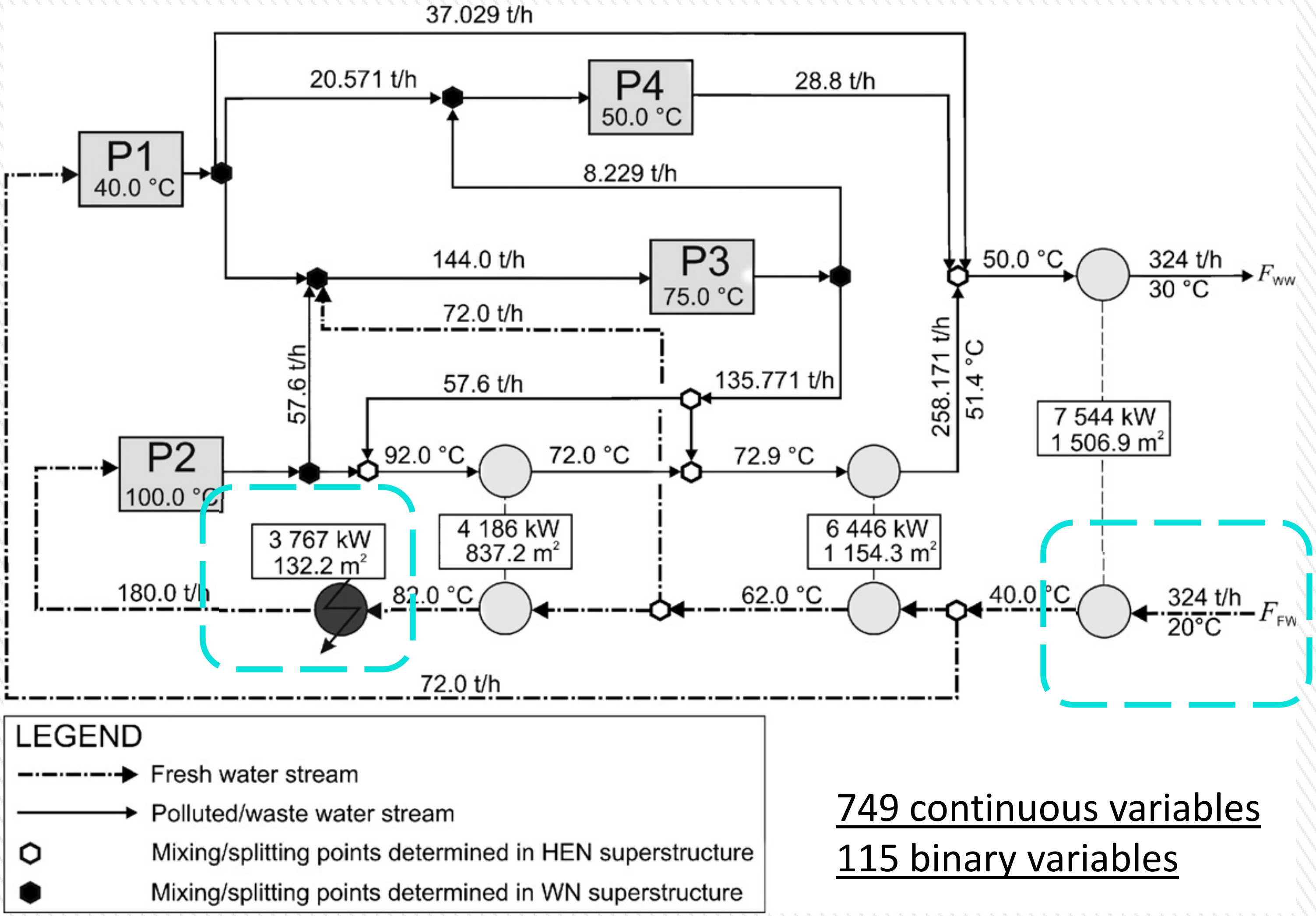
Process unit mass balances

This formulation provides target for a network consists of a set of water-using process units using linear constraints

Assumption: for some contaminant j that reaches its concentration upper bound at a given unit, it also reaches the upper bound at all other process units from which reuse streams have non-zero flowrate

Heat-integrated WN reported in the literature

Use heat and water network formulation **(MINLP model)** to obtain network structure

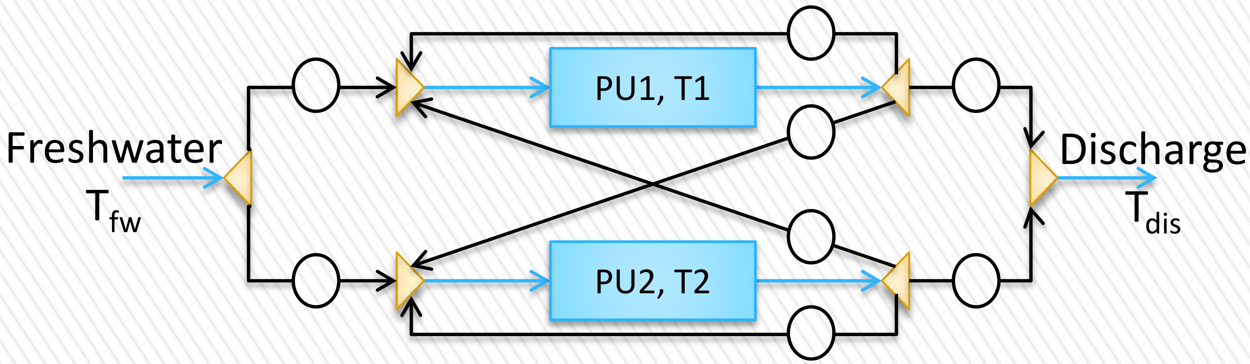


749 continuous variables

115 binary variables

Bogataj & Bagajewicz (2007)

Extension: heat-integrated water network



All black streams can participate in heat integration

Objective fcn

$$\min.\ \phi = c_H Q_H + c_C Q_C + c_{fw} F_{fw}$$

Water targeting (LP)

$$F^k = \sum_{i \in m_{in}} F^i \qquad \forall m \in MU, k \in m_{out}$$

$$F^k C_j^{k,\max} \geq \sum_{i \in m_{in}} (F^i C_j^{i,\max} + F^i_{fw} C_{fw})$$

$$\forall j, \quad \forall m \in MU, k \in m_{out}$$

$$F^k = \sum_{i \in s_{out}} F^i \qquad \forall s \in SU, k \in s_{in}$$

$$C_j^k = C_j^i \qquad \forall j, \quad \forall s \in SU, \qquad \forall i \in s_{out}, k \in s_{in}$$

$$F^k = P_{in}^p \qquad \forall p \in PU, k \in p_{out}$$

$$F^i = P_{out}^p \qquad \forall p \in PU, i \in p_{in}$$

$$F^i C_j^i + L_j^p = F^k C_j^k$$

$$\forall j, \forall p \in PU, i \in p_{in}, k \in p_{out}$$

Heat targeting (LP)

$$Q_H \geq \sum_{js \in C \cup s_{out}} f_{js} c_{js} [\max\{0, t_{js}^{out} - (T^p - \Delta T_m)\}$$

$$- \max\{0, t_{js}^{in} - (T^p - \Delta T_m\}]$$

$$- \sum_{is \in H \cup s_{out}} F_{is} C_{is} [\max\{0, T_{is}^{in} - T^p)\}$$

$$- \max\{0, T_{is}^{out} - T^p\}]$$

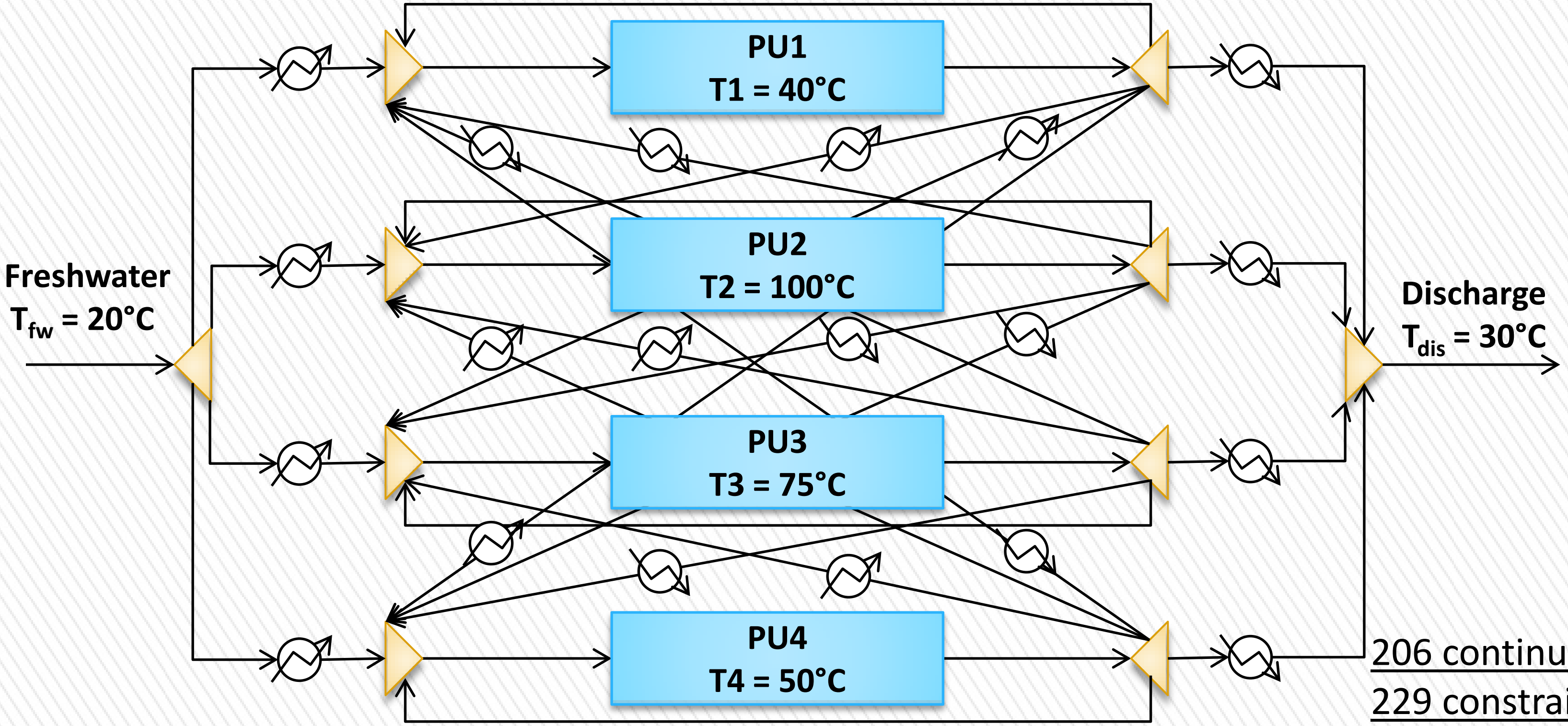
$$Qc = Q_H + \sum_{is \in H \cup s_{out}} F_{is} C_{is} (T_{is}^{in} - T_{is}^{out})$$

$$- \sum_{js \in C \cup s_{out}} f_{js} c_{js} (t_{js}^{out} - t_{js}^{in})$$

$$T^p = T_{is}^{in} \qquad \forall p = is \in H \cup s_{out} \qquad \forall s \in SU$$

$$T^p = (t_{js}^{in} + \Delta T_m) \qquad \forall p = js \in C \cup s_{out} \qquad \forall s \in SU$$

Revisit: heat-integrated water network utility targeting



206 continuous variables
229 constraints

Parameter			
C_{HU} (\$/kW a)	260	T_{HU}^{in} (°C)	126
C_{CU} (\$/kW a)	150	T_{HU}^{out} (°C)	126
C_{FW} (\$/t)	2.5	T_{CU}^{in} (°C)	15
HRAT (°C)	10	T_{CU}^{out} (°C)	20

Use heat and water targeting formulation:

Minimum heating utility: 3767 kW
Minimum cooling utility : No cooling utility required
Minimum freshwater consumption: 324 ton/h

Same result as network approach

Simultaneous optimization strategy

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

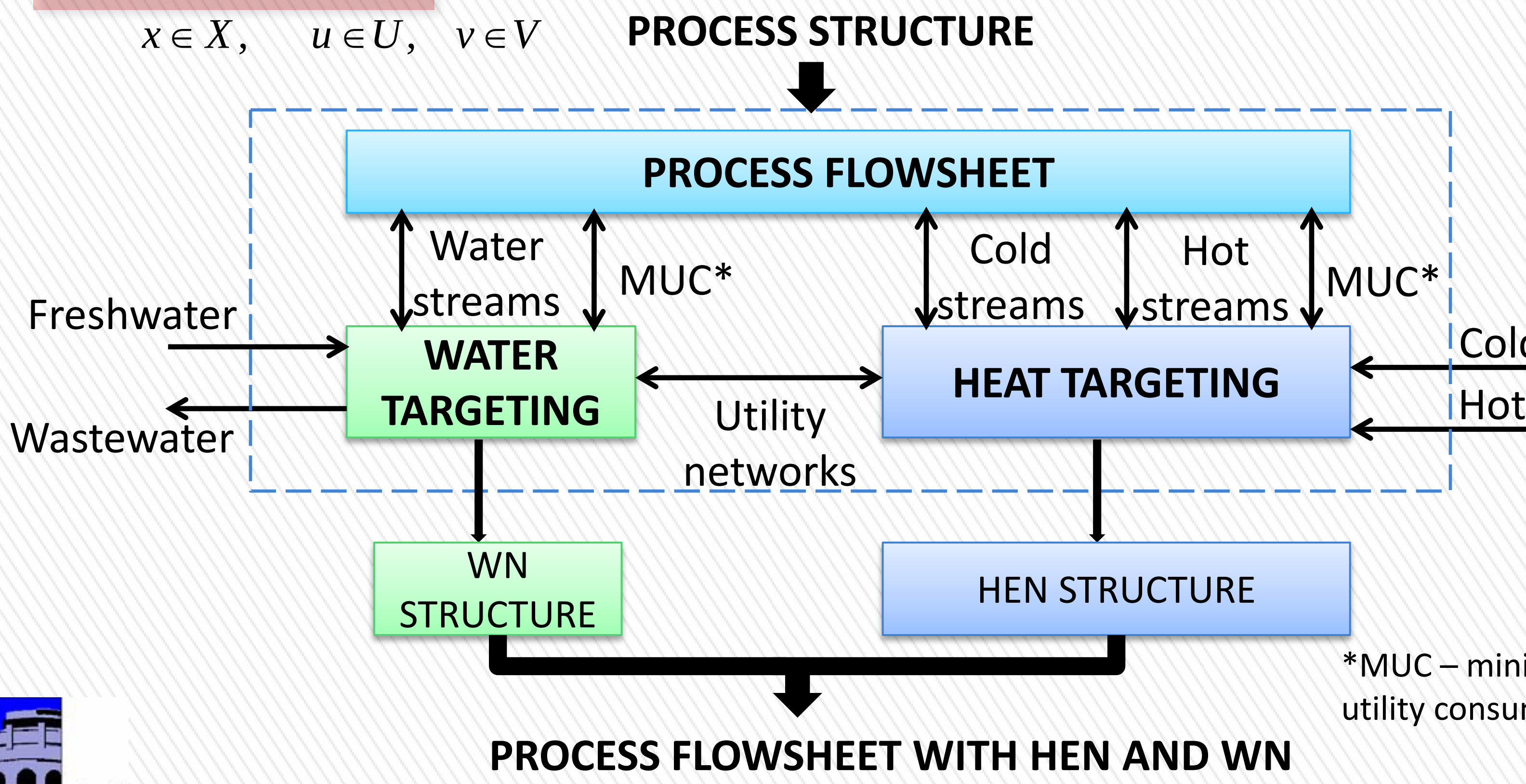
$$\text{s.t. } h(x,u,v) = 0$$

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

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

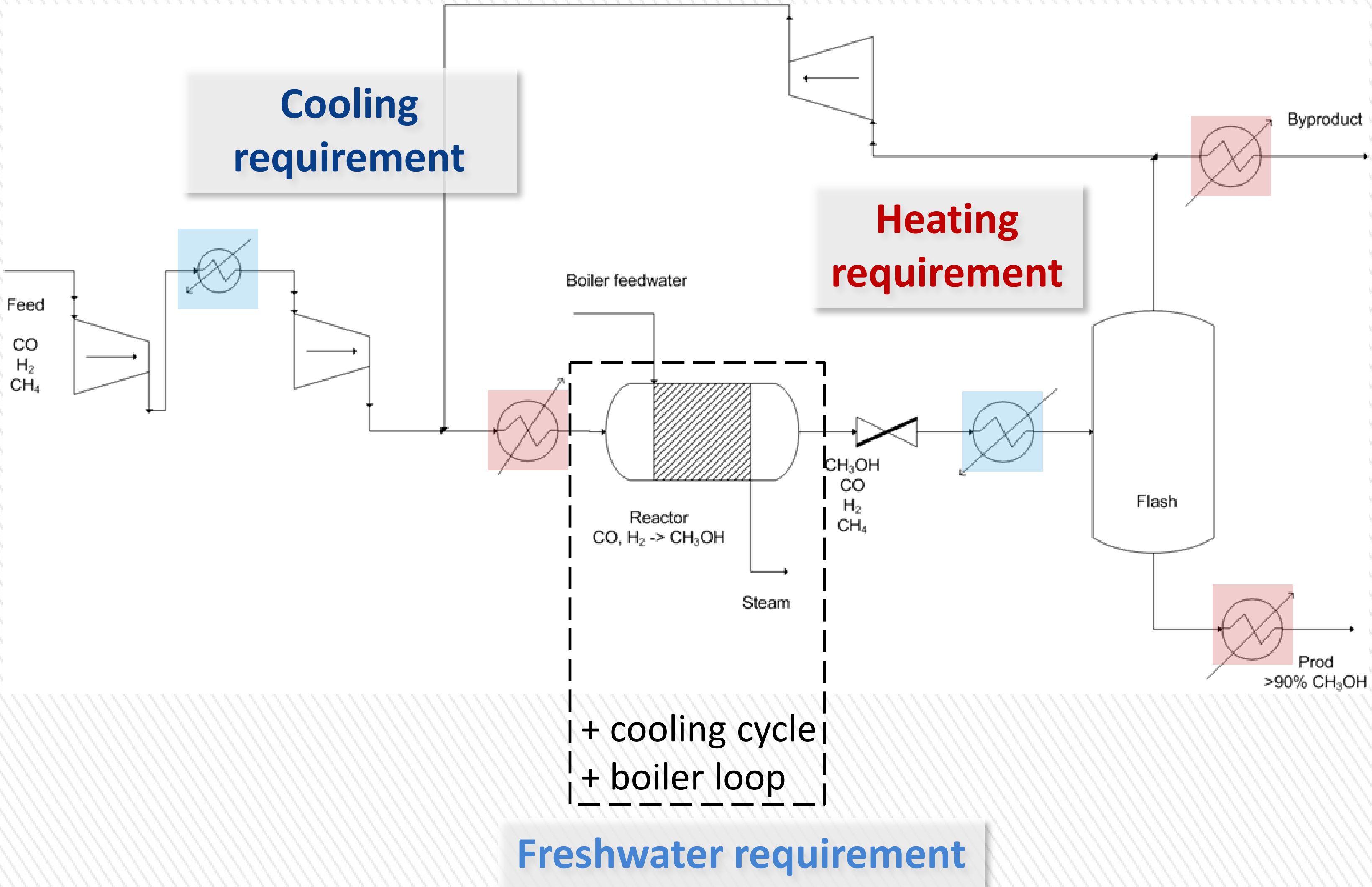
$$g^{WN}(v,F_{fw}) \le 0$$

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



*MUC – minimum utility consumption

Simultaneous optimization: methanol synthesis from syngas



Duran & Grossmann (1987)

Sequential vs. simultaneous result comparison

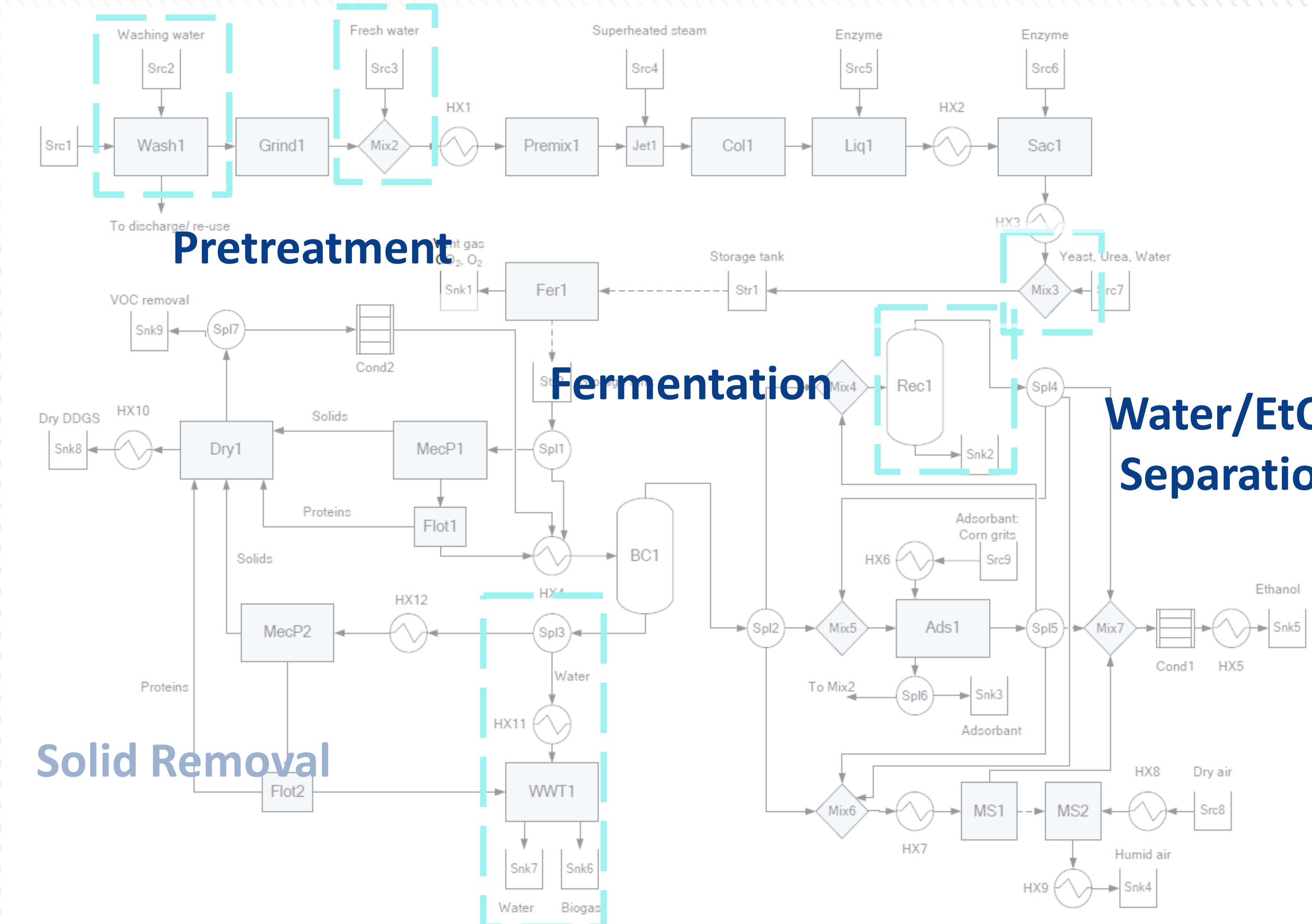
		SEQUENTIAL	SIMULTANEOUS
Profit	**(1000 $/yr)**	**62,695**	**73,416**
Investment cost	(1000 $)	1,891	1,174
Operating parameters			
	electricity (KW)	6.59	1.84
	freshwater (kg/s)	36.43	29.25
	heating utility (10^9 KJ/yr)	0.293	0
	cooling utility (10^9 KJ/yr)	67.3	72.7
	Steam generated (10^9 kJ/yr)	2448	1965
	overall conversion	0.68	0.88
Material flowrate (10^6 kmol/yr)			
	feedstock	48.04	37.13
	product	10.89	10.89

Solved with BARON 9

17% improvement

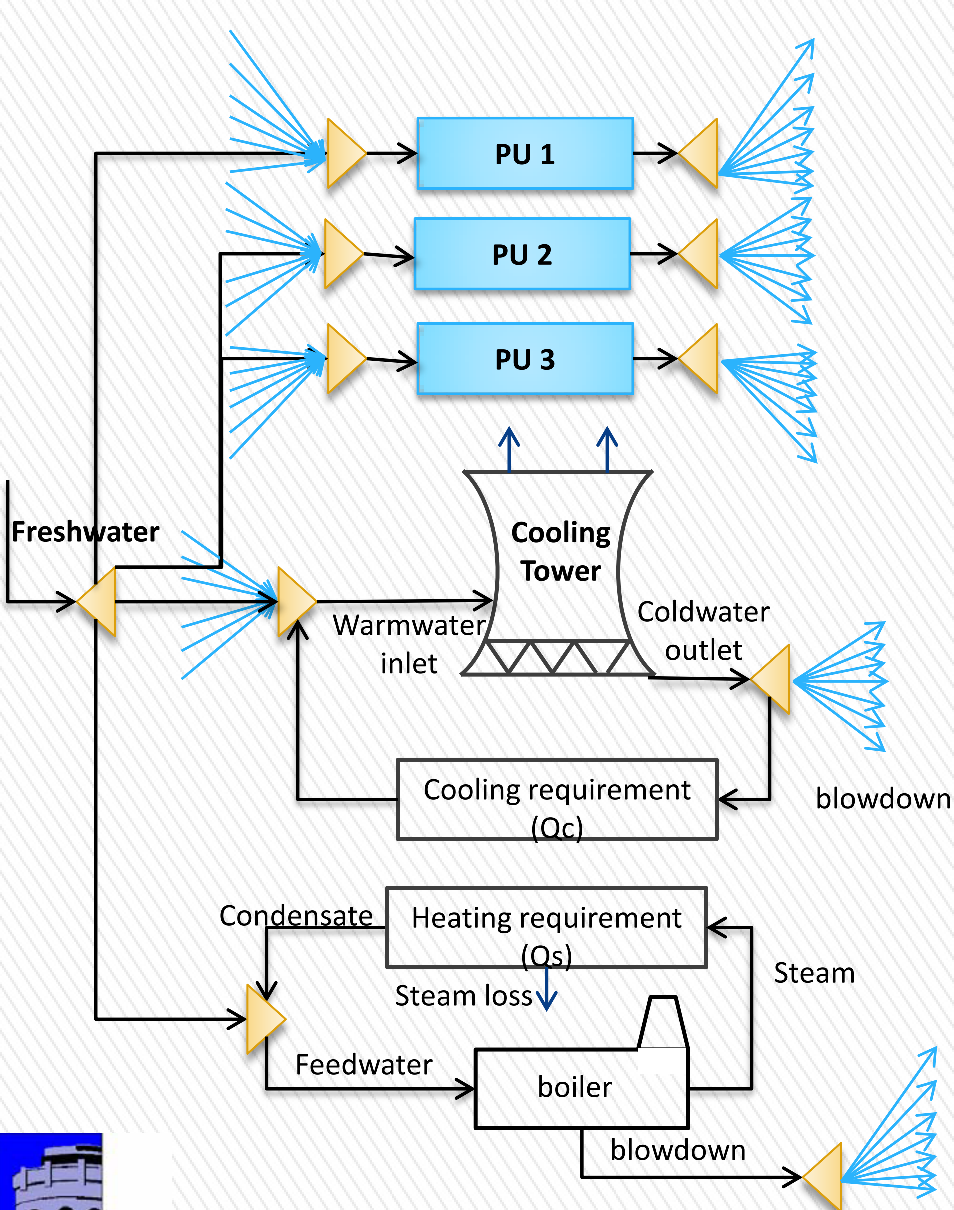
Example 2: Bioethanol production

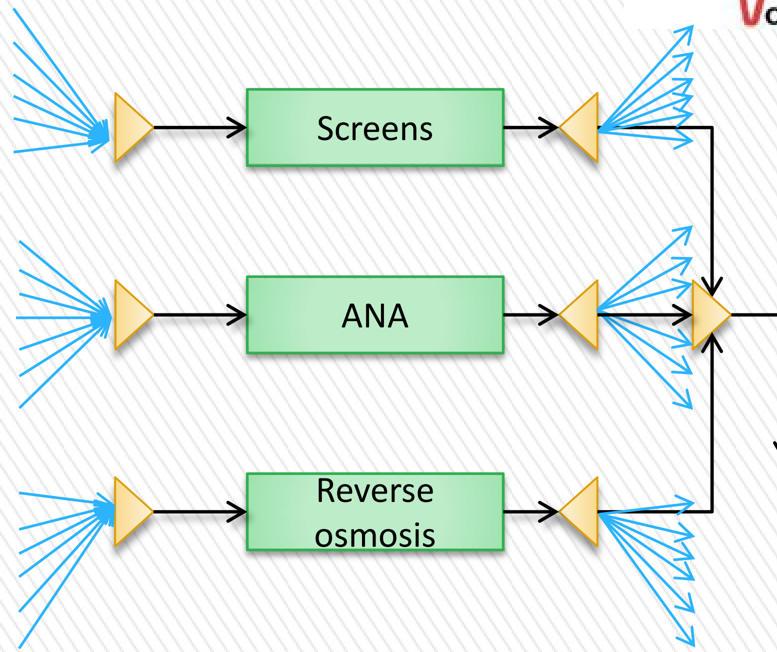
Water Consumption and generation



R. Karuppiah, A. Peschel, I. E. Grossmann, M. Martın, W. son, and L. Zullo, “Energy optimization for the design of corn-based ethanol plants,” AIChE Journal, vol. 54, no. 6, 2008, pp. 1499–1525.

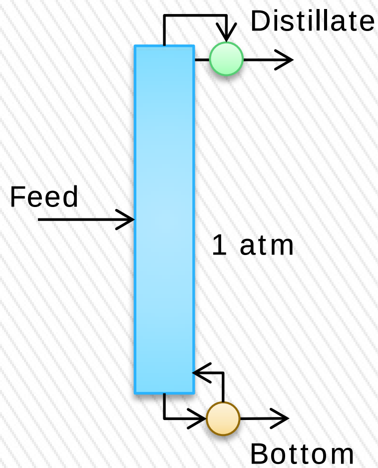
Water network superstructure

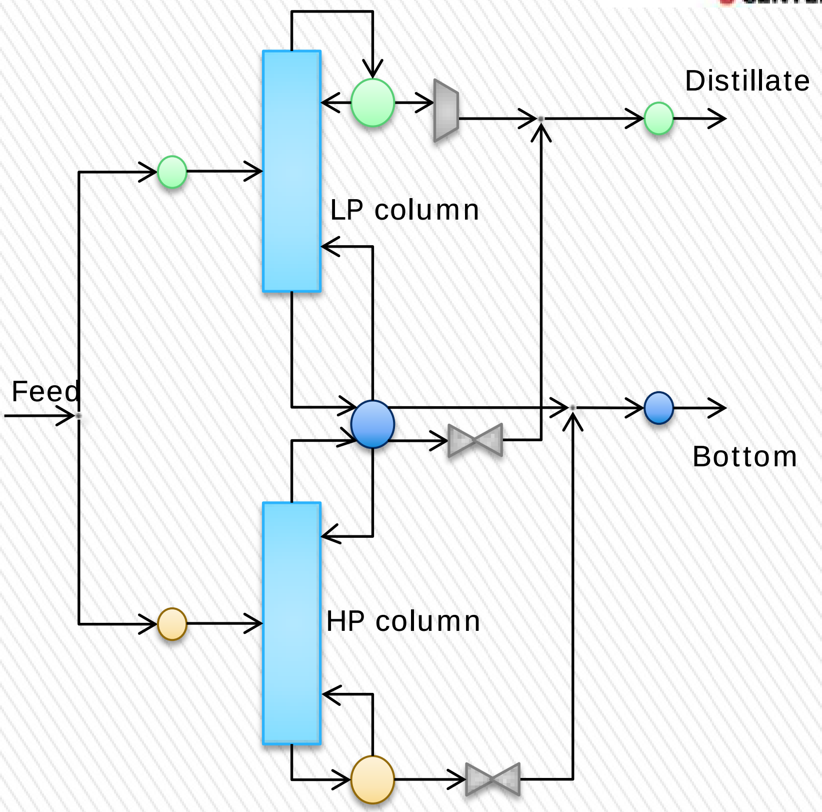




$C_j^{in,max}$ (ppm)	TSS	TDS	ORG
Boiler loop	2	100	10
Cooling cycle	10	500	10
$1-B_j^t$			
Screens	95%	0	0
Reverse osmosis	0	90%	0
Anaerobic tank	0	0	99%

Multieffect columns





Formulation

- Dew point equation - condenser temperature
- Bubble point equation - feed and reboiler temperature
- Fenske equation - # of trays
- Watson's equation – heat of vaporization
- Mass balance
- Energy balance

Assumptions

- Constant relative volatility
- Ideal solution
- Water is the only component contributing to heat of vaporization
- Temperature change due to pumps is negligible

Result

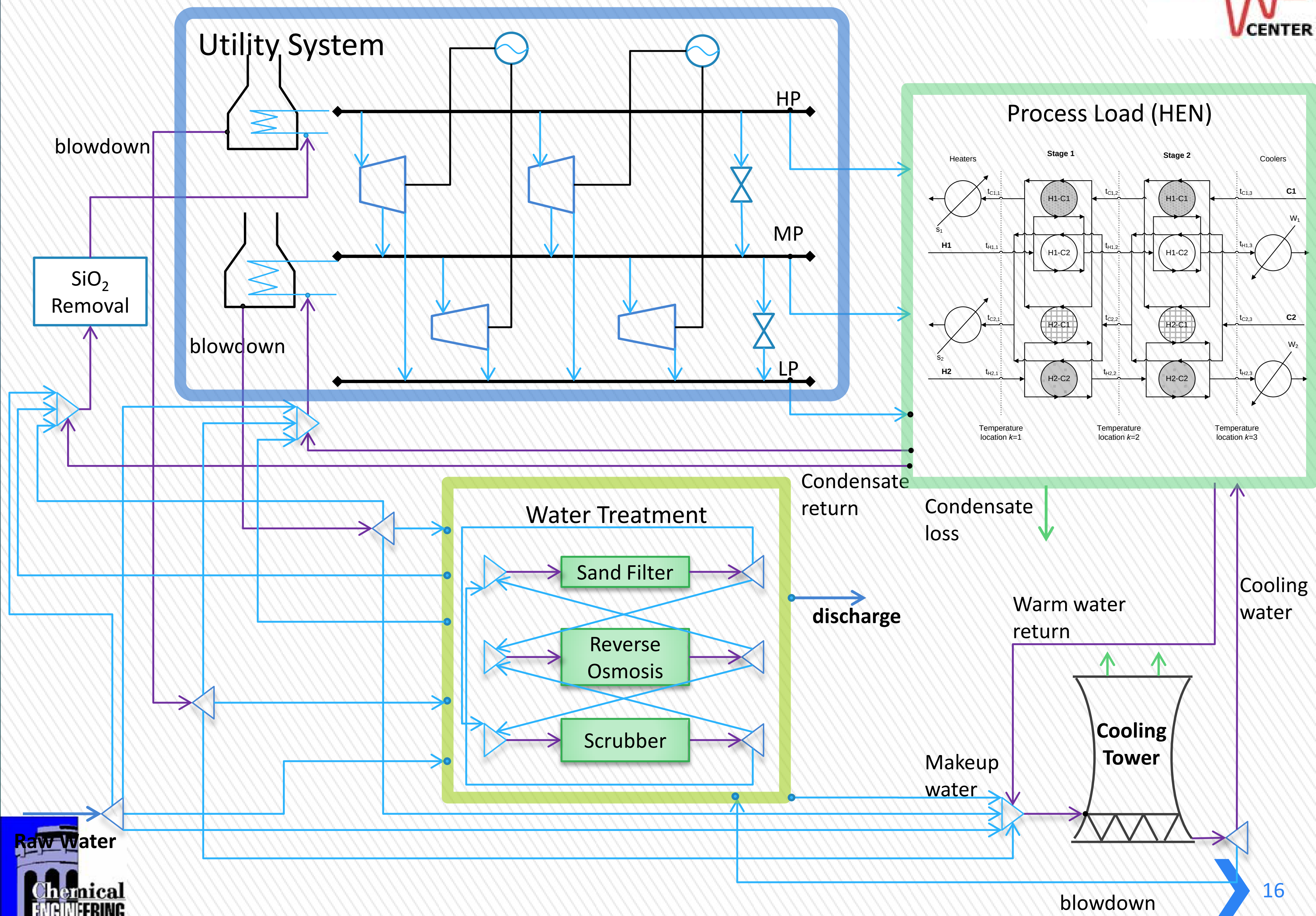
	No integration	Sequential single column	Sequential w/ multieffect	Simultaneous w/ Multieffect
Cost (MM$/yr)	**14.91**	**11.77**	**8.57**	**8.57**
Cooling water use (kg/s)	2895.6	1998.3	1127.3	1124.8
Freshwater use (kg/s)	40.8	127.6	90.0	90.0
Steam use (kg/s)	35.1	28.3	21.2	21.3
CPU(s)	387	387	470	563
# eqns	2,232	2,232	3,213	5,221
# cont var	2,921	2,921	3,914	5,392

NLP solver: CONOPT 3
MINLP solver: BARON 9
GAMS 23.7

Even though the objective function did not improve using simultaneous method, we can see that the solution time did not increase drastically

Reboiler duty reduced by ~36% by with multieffect column

Utility integration – power, water, & heat



Problem statement

Objective function

$$\phi = \sum_{st} c_b^{fix} Y_b^{st} + \sum_{st} c_b^{var} F_b^{st} + \sum_{st}\sum_{d} c_{tur}^{fix} Y_d^{st} + \sum_{d} c_{ext}^{fix} Y_d^{ext} + \sum_{st}\sum_{d} c_{tur}^{var} W_d^{st} + \sum_{s} c_s F_s + c_{fw} F_{fw}$$

Boiler cost | Turbine cost | Flowsheet stream cost | freshwater cost

HEN	Utility system	WN
• 2 hot streams/ 2 cold streams • Inlet and outlet temperature can vary within +/- 10 K • Heat capacity flowrate can vary within 20% • Two streams have assigned costs • Hot utility - HP, MP, and LP steam • Cold utility - cooling water	• Existence of boiler • Existence of turbine • Back pressure turbine • Extraction turbine (additional cost $20,000) • Flowsheet power demand (7500kW) • 70% condensate return	• HP boiler has more stringent feedwater requirement • HP boiler/MP boiler have different blowdown rates • RO consumes electricity • Raw water needs treatment • TSS, TDS, GAS present in freshwater • Discharge limit imposed

Multiple hot utility targeting (Duran & Grossmann)

- Heating utilities targets
- Cooling utility target

Utility system

- Logical constraints
- Demand constraints
- Power balances
- Mass balances

Water network

- Mass balances
- Power demand constraint

Result

	Sequential		Simultaneous	
Cost (1000 $ / yr)		**884.2**		**641.5**
Utility				
HP boiler flowrate (kg/s)	Yes	17.66	Yes	18.20
MP boiler flowrate (kg/s)	No		No	
Power demand external (kW)	HP → LP	7500	Extraction	7500
Reverse osmosis power demand (kW)	MP → LP	62.0	MP → LP	63.89
HEN Utility (kW)				
Cooling		1463.8		751.1
HP steam		3820.2		5727.2
MP steam		13628.2		21065.7
LP steam		4743.4		19110.2
Fcp,H1 (kW/K)		48		32
Fcp,C2 (kW/K)		144		216
WN flowrate (kg/s)				
Freshwater		7.26		6.47
Sand filter		7.2		6.4
Reverse osmosis		5.6		5.8
Scrubber		2.4		1.2

Conclusion

- Developed LP formulations for targeting minimum freshwater consumption for a set of water-using process units under a specific condition
- Extended the water targeting formulation to nonisothermal water network
- **Targeting method can be used to improve objective function and computational effort under the simultaneous approach for flowsheet optimization**
- **The interaction among power use, heat use, and water use can be exploited to achieve better flowsheet design**

Thank you!

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