Design of Cryogenic Systems for Advanced Power Plants using **Simultaneous Heat Integration** and **Process Optimization**

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Carnegie Mellon University

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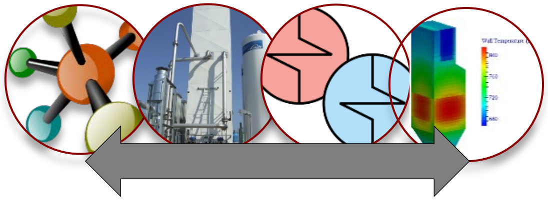
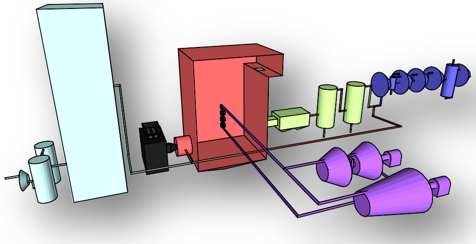
November 20th, 2014





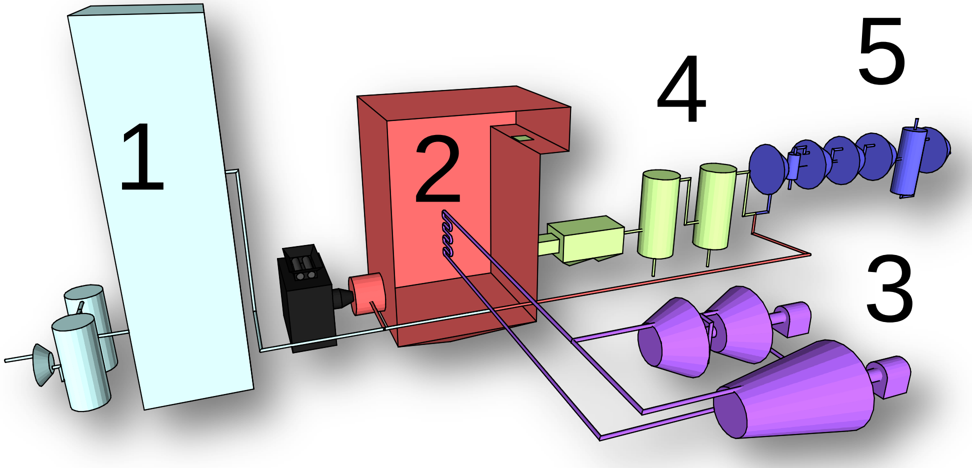
Motivation

Develop framework for full oxycombustion power plant optimization

- – Estimate *cost of electricity* with carbon capture
- – Balance trade-offs between systems

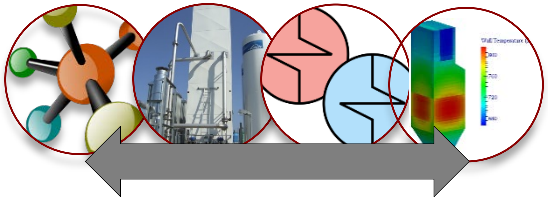
Oxycombustion Power Plant

1. Air Separation Unit
2. Boiler
3. Steam Turbines
4. Pollution Controls
5. CO_2 Compression Train

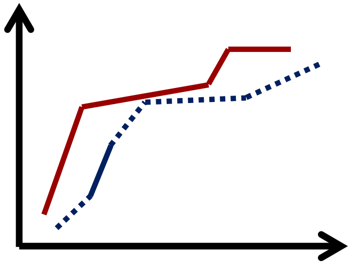


Agenda

1. Framework for **Equation Oriented** Flowsheet Optimization
    - Embedded pinch heat integration



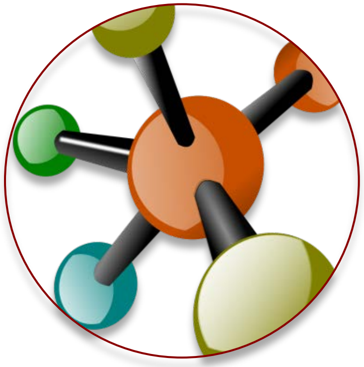
2. Case Study: Air Separation Unit
    - Multistream heat exchanger design



3. Driving Force Calculations
    - Extension of pinch methods

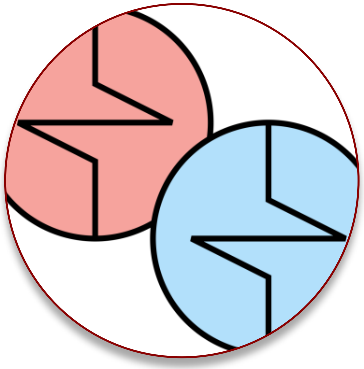
4. Case Study: CO_2 Process Unit

Framework for EO Flowsheet Optimization

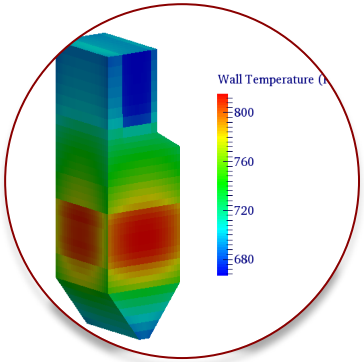


Thermodynamics
&
Flash Calculations

Distillation Cascades



Heat Integration

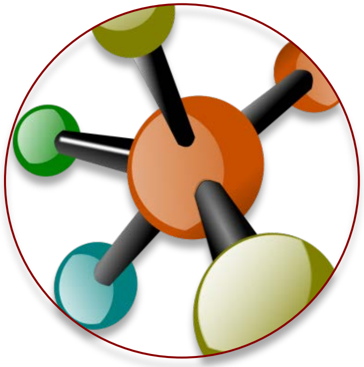


Complex Reactors
(*e.g.* CFD)

Trust Region Optimization with Filter

Dowling, A. W., & Biegler, L. T. (2015). A framework for efficient large scale equation-oriented flowsheet optimization. Computers & Chemical Engineering. 72 (2) 3-20.

Framework for EO Flowsheet Optimization



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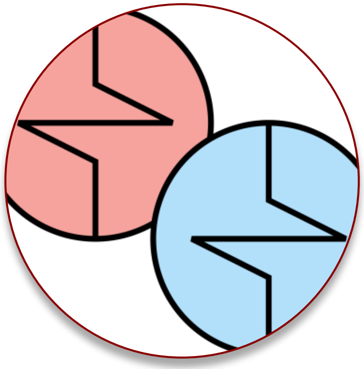
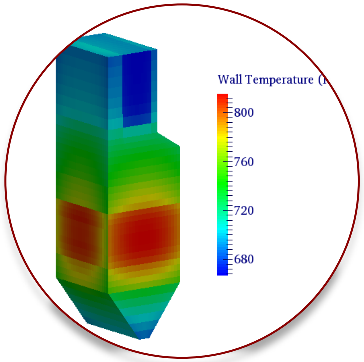


Heat Integration



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HENS Methodology Review

Two mathematical programming approaches for Heat Exchanger Network Synthesis:

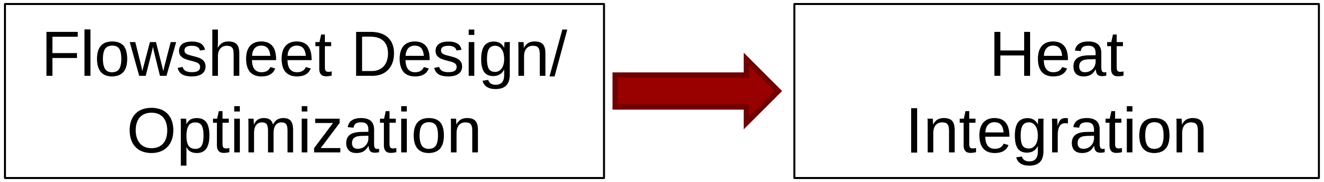
1. Sequential. LP → MILP → NLP

   Papoulias, S. A., & Grossmann, I. E. (1983)

2. Simultaneous. MINLP

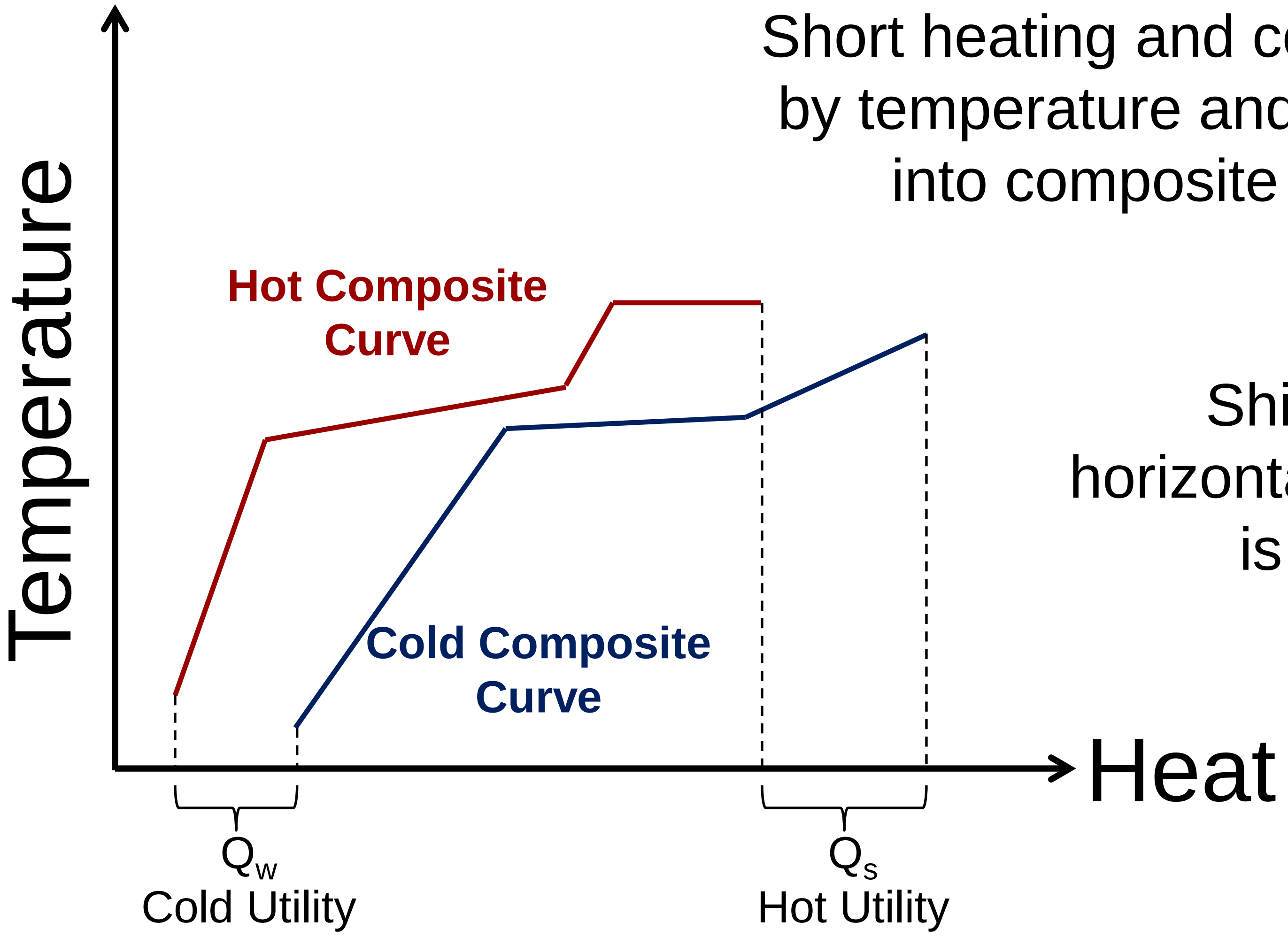
   Yee, T. F., Grossmann, I. E., & Kravanja, Z. (1990)

Assumption: **fixed** flowrates and temperatures


Flowsheet Design/ Optimization

Heat Integration

Pinch Based Heat Integration

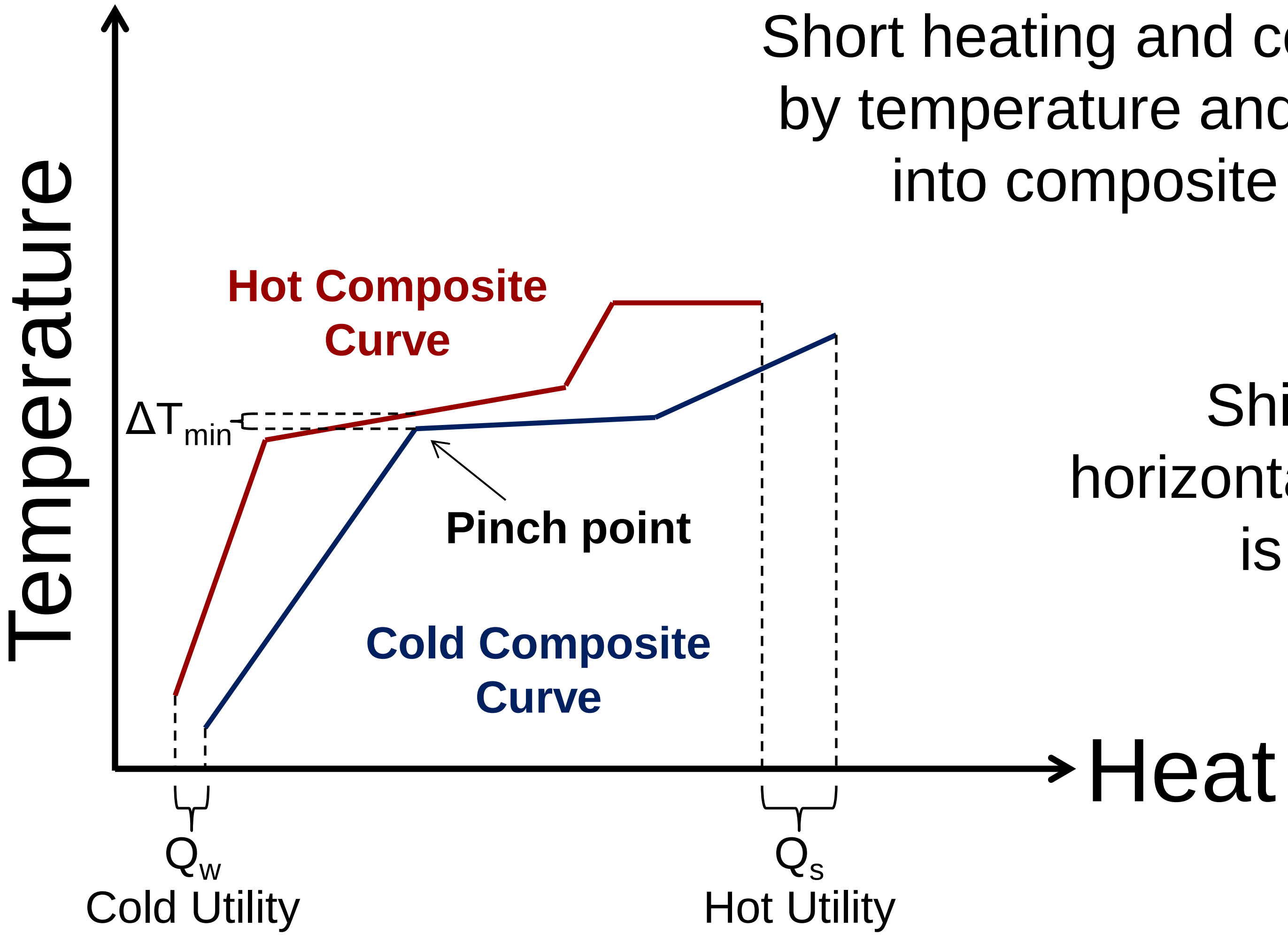


Short heating and cooling loads by temperature and aggregate into composite curves

Shift curves horizontally until ΔT_{min} is limiting

Hohmann, E.C. (1971). *Optimum Networks for Heat Exchangers.* PhD Thesis, University of So. Cal.
Linnhoff, B. (1993). Pinch analysis – A state-of-the-art overview. *Trans. IChemE.,* ***71****(A), 503.*

Pinch Based Heat Integration



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Duran-Grossmann Formulation

Pinch candidates

$$T^p = \begin{cases} T_p^{in} & \text{if candidate } p \text{ is a hot stream} \\ T_p^{in} + \Delta T_{min} & \text{if candidate } p \text{ is a cold stream} \end{cases}$$

Available heating and cooling above pinch

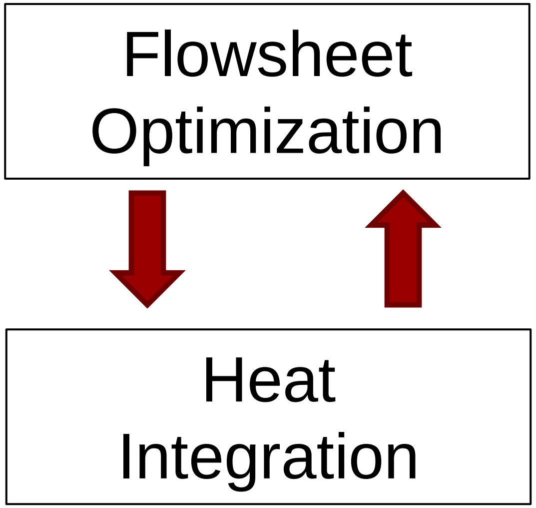
$$QA_H^p = \sum_{i \in \{Hot\}} FCp_i[\tilde{\max}(T_i^{in} - T^p) - \tilde{\max}(T_i^{out} - T^p)]$$

$$QA_C^p = \sum_{j \in \{Cold\}} FCp_j[\tilde{\max}(T_j^{out} - T^p + \Delta T_{min}) - \tilde{\max}(T_j^{in} - T^p + \Delta T_{min})]$$

Utility calculations

$$Q_s \geq QA_C^p - QA_H^p \quad \text{for all } p$$

$$Q_w = Q_s + \sum_{j \in \{Cold\}} Q_j^{in} - \sum_{i \in \{Hot\}} Q_i^{out}$$



Flowsheet Optimization

Heat Integration

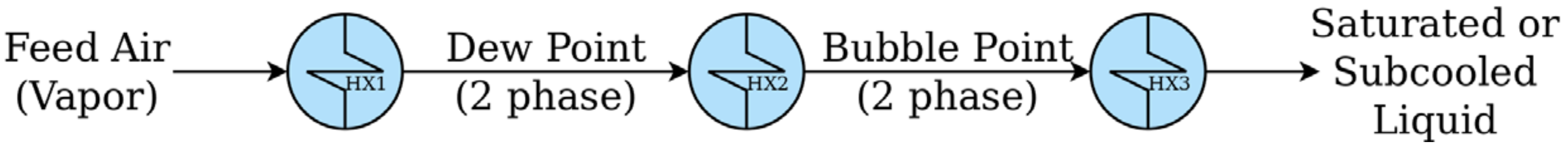
Duran, M. A., & Grossmann, I. E. (1986). Simultaneous optimization and heat integration of chemical processes. *AIChE Journal*, *32*(1), 123–138.

Comments on DG

1. Algebraic form of the pinch method
2. Temperature intervals and stream ordering not assumed *a prior*
3. Discrete decisions (ordering) accommodated with smoothed max

$$\widetilde{\max}(x) \overset{\text{def}}{=} x + \sqrt{x^2 + \varepsilon^2} \approx \max(x, 0)$$

Heat Exchanger Decomposition



Feed Air (Vapor) → Dew Point (2 phase) → Bubble Point (2 phase) → Saturated or Subcooled Liquid

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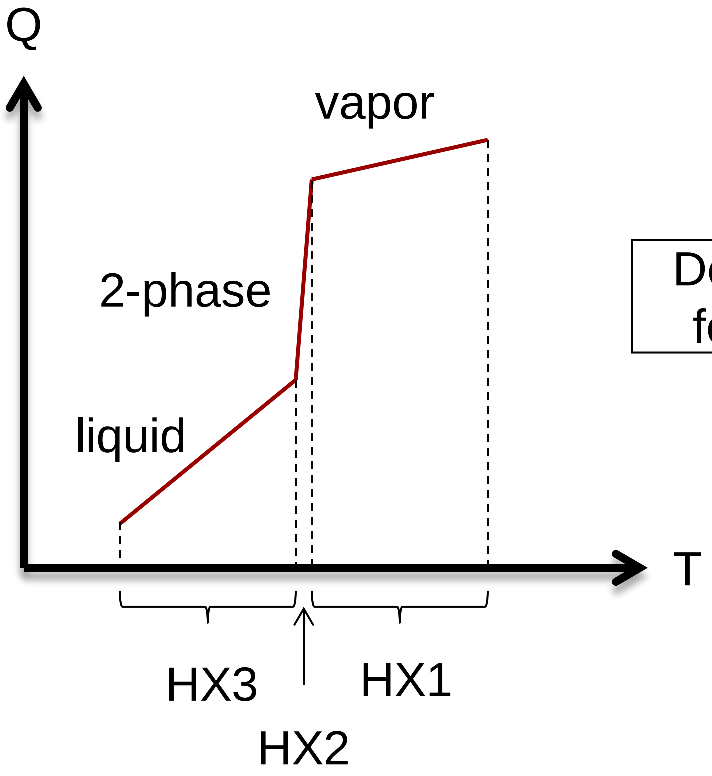
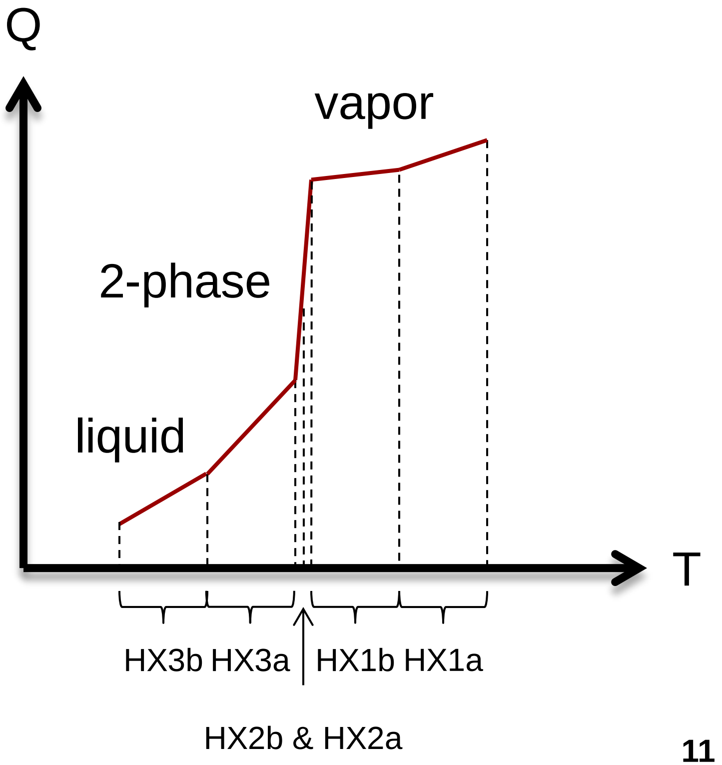
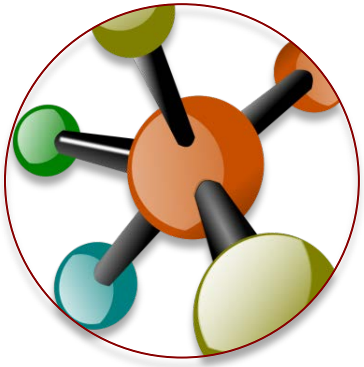


Decomposition for Validation



Framework for EO Flowsheet Optimization



Thermodynamics
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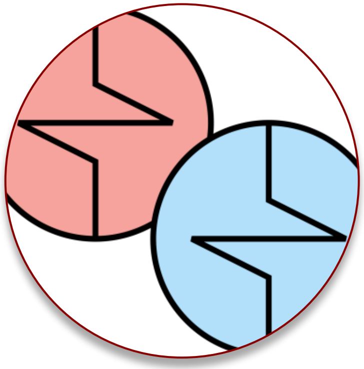
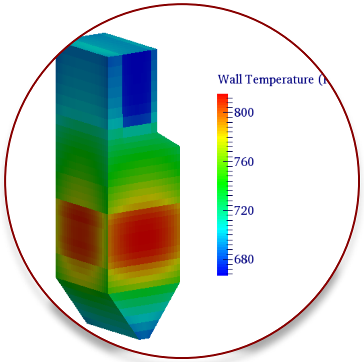


Heat Integration



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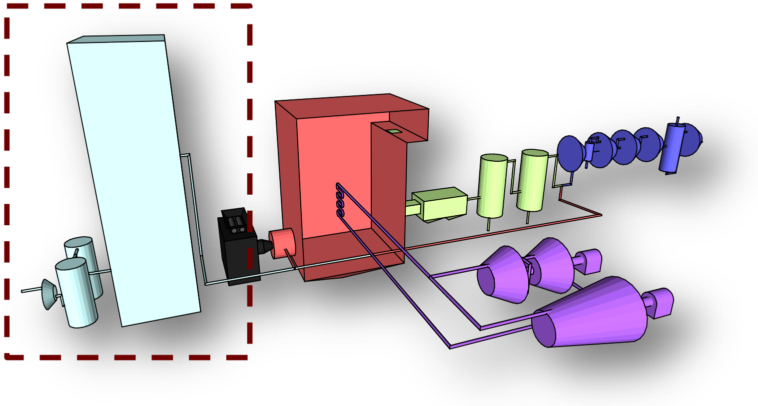
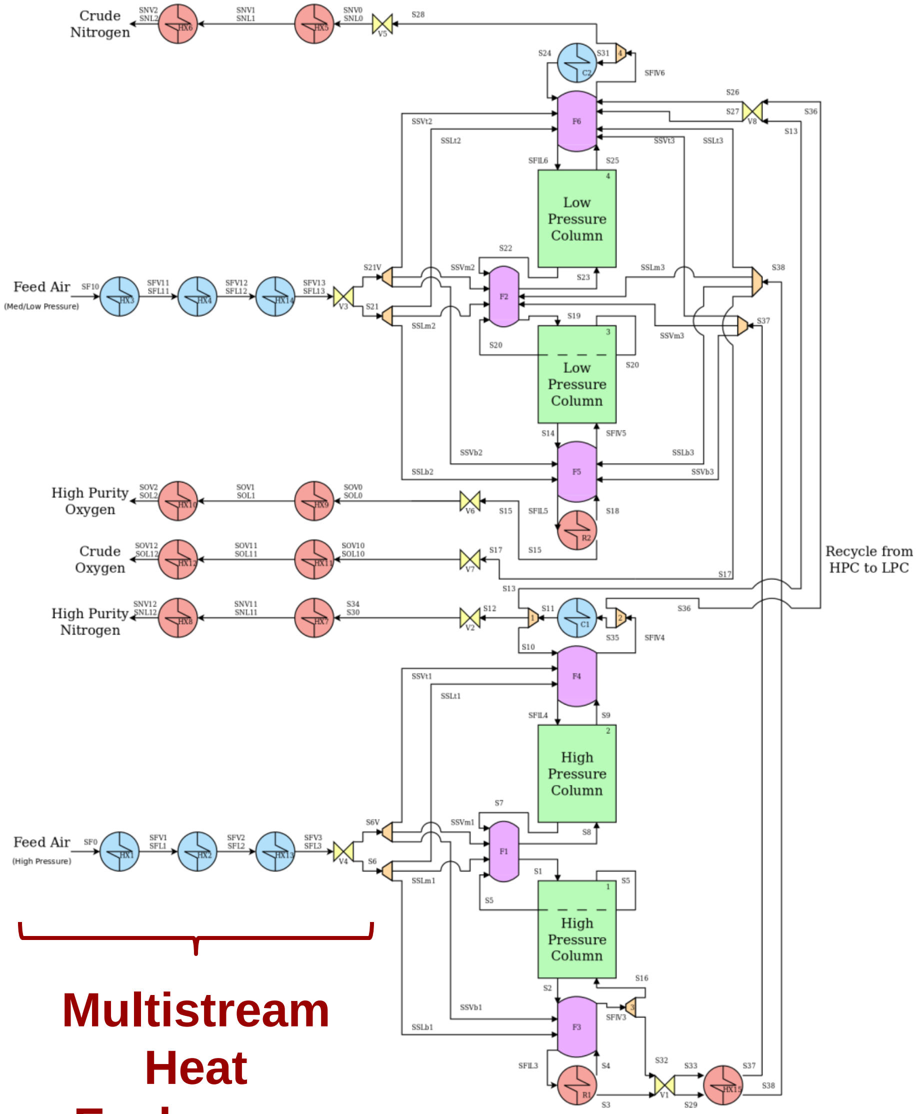
ASU Superstructure



- *__Many__* different column configurations realizable

- NLP optimizer selects the best configuration



Multistream Heat Exchanger

Optimization Formulation

min ASU Compression Energy (kWh / kg O_2 product)

s.t.

Flowsheet Superstructure

Peng-Robinson Thermodynamics

Unit Operation Models

Distillation Model

Heat Integration

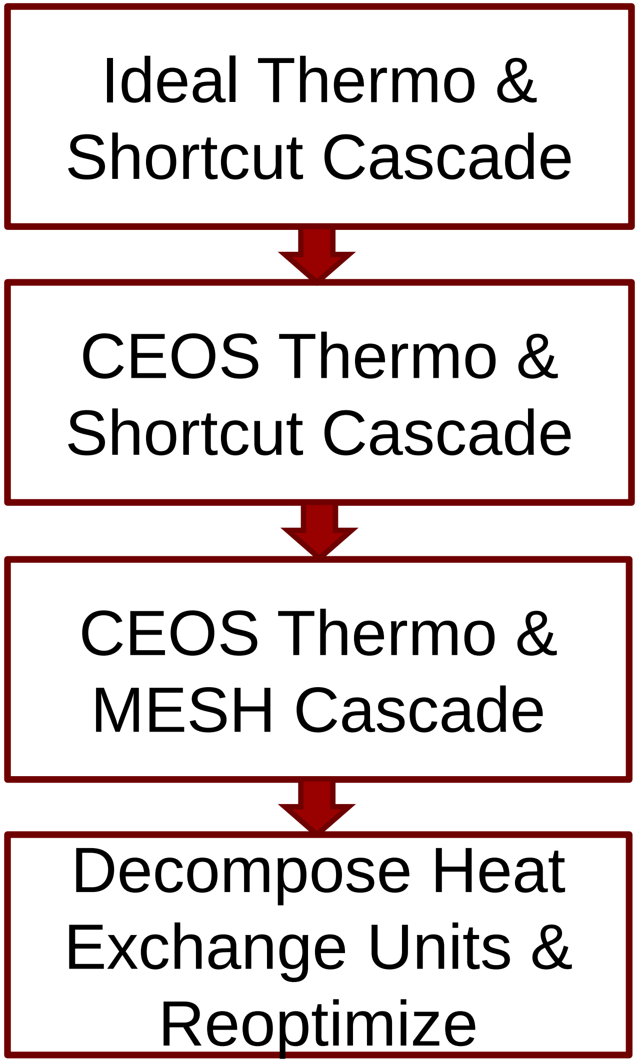
O_2 product purity ≥ 95 mol%

Complementarity Constraints (thermo, etc.)

Note: **Upper and lower bounds not shown above** are considered for many variables including stream/equipment temperatures and pressures.

Implementation Details

- Non-convex problem
  - 16,000 variables & constraints
- Penalty formulation for *complementarity constraints*
- Automated initialization
  - Simple → complex models
  - Custom multistart procedure
- Solved using **CONOPT3** in GAMS
  - **16 CPU minutes** average for single initial point



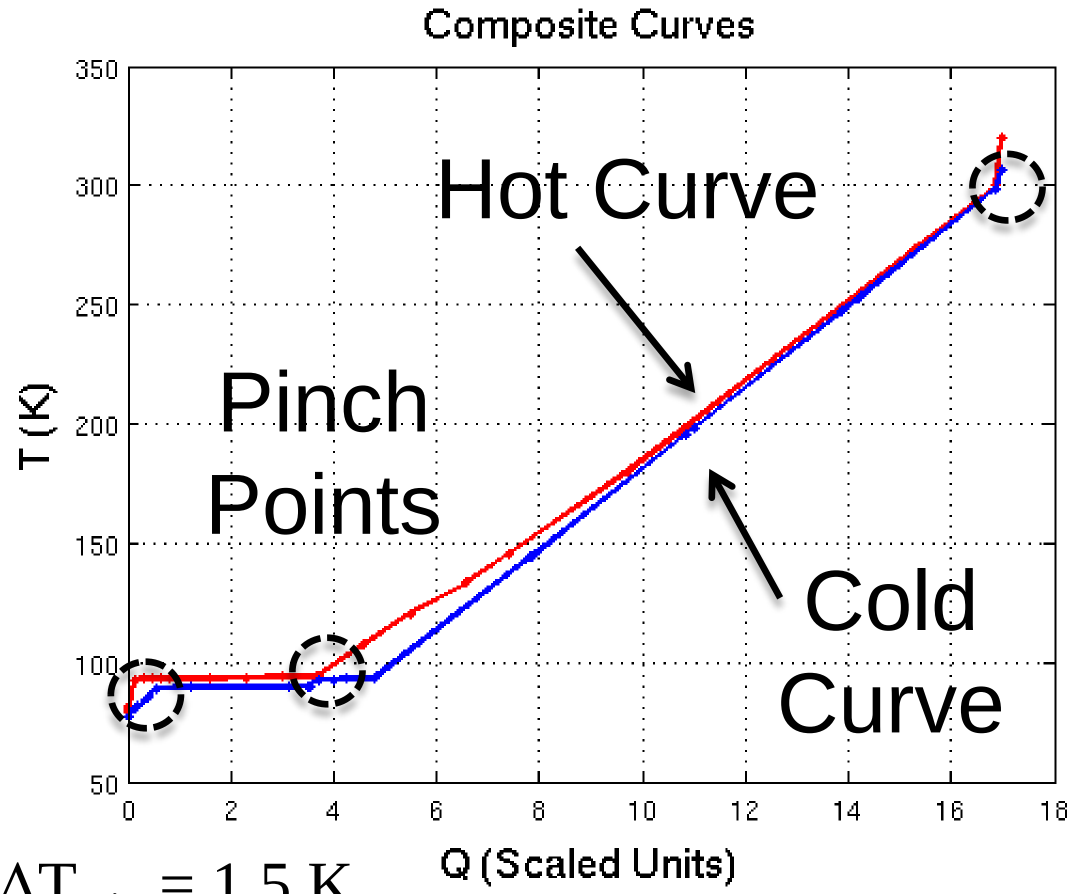
Ideal Thermo & Shortcut Cascade

CEOS Thermo & Shortcut Cascade

CEOS Thermo & MESH Cascade

Decompose Heat Exchange Units & Reoptimize

Heat Integration Results

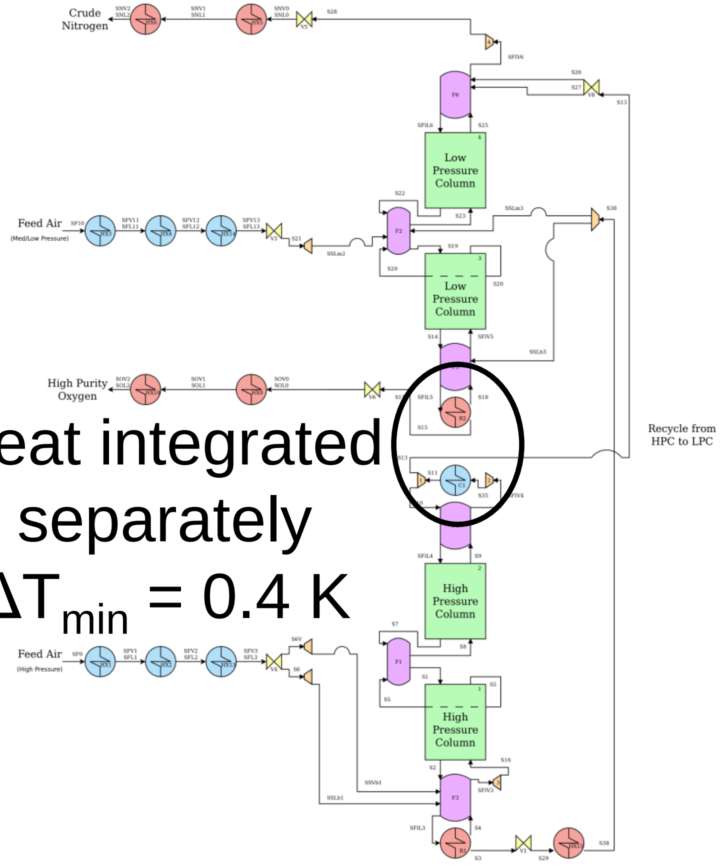


Hot Curve

Pinch Points

Cold Curve

$\Delta T_{min} = 1.5$ K

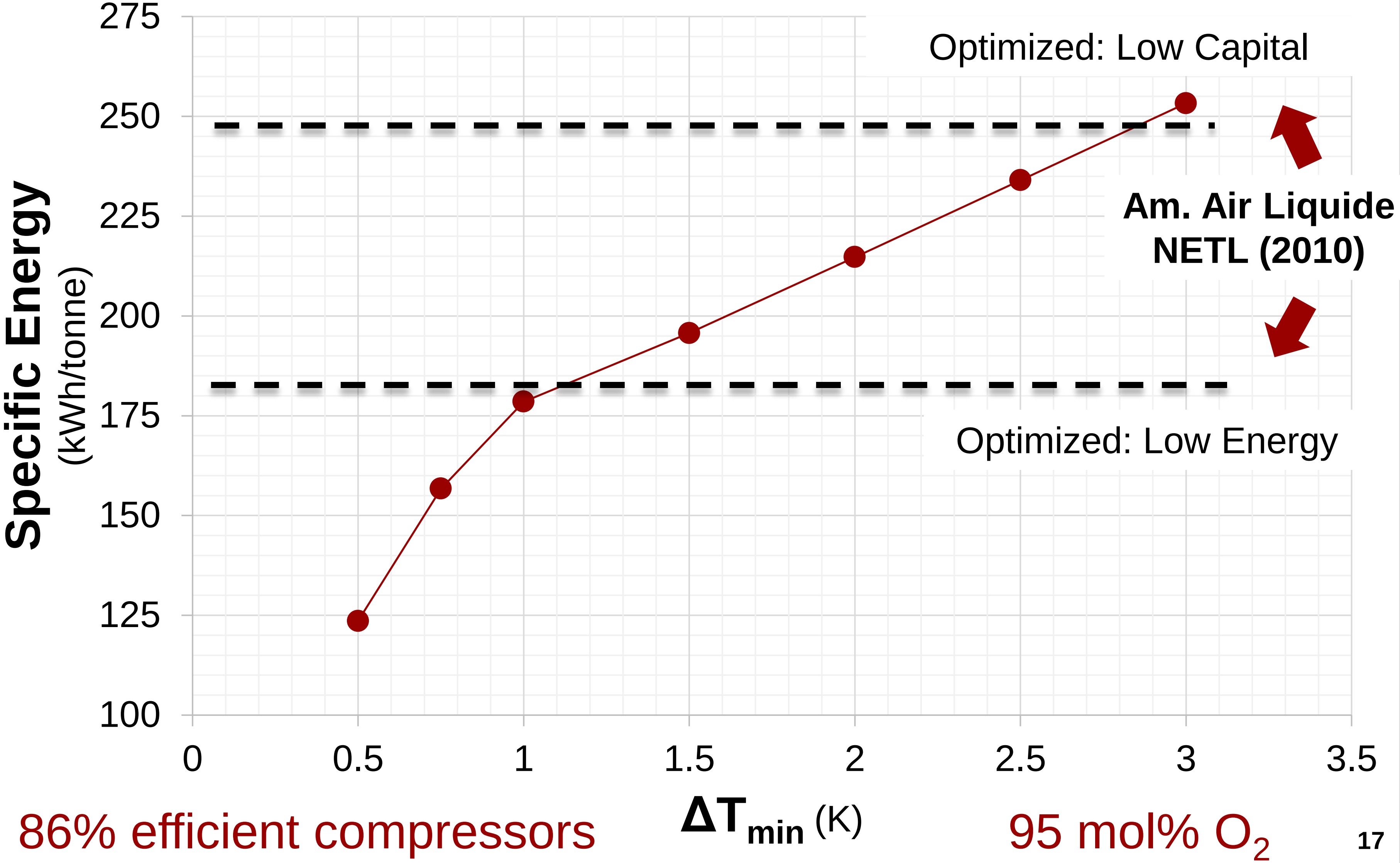


Heat integrated separately

$\Delta T_{min} = 0.4$ K

Tight heat integration with multiple pinch points

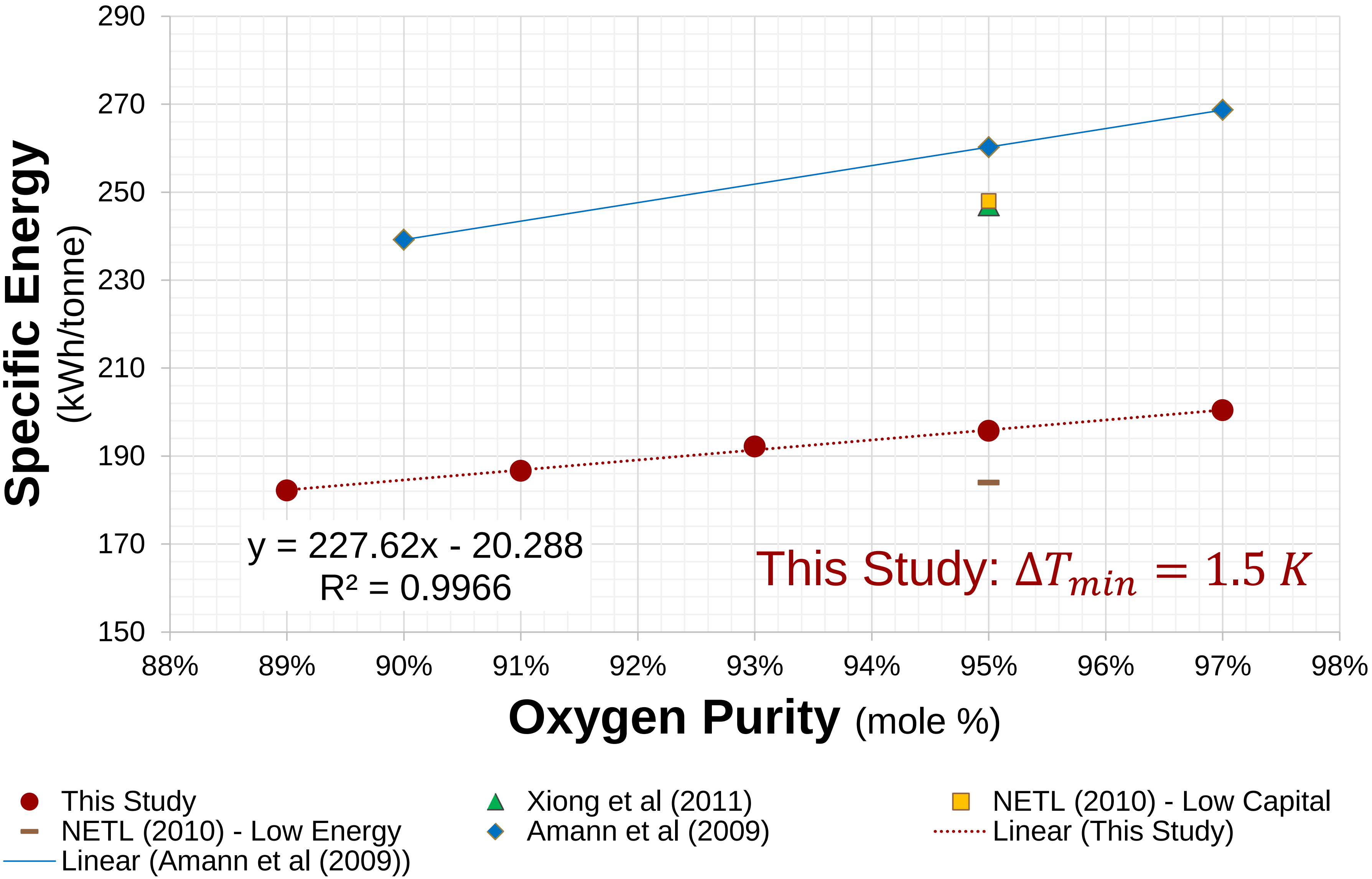
Heat Integration Sensitivity



86% efficient compressors

95 mol% O_2

O_2 Purity Sensitivity



This Study: $\Delta T_{min} = 1.5\ K$

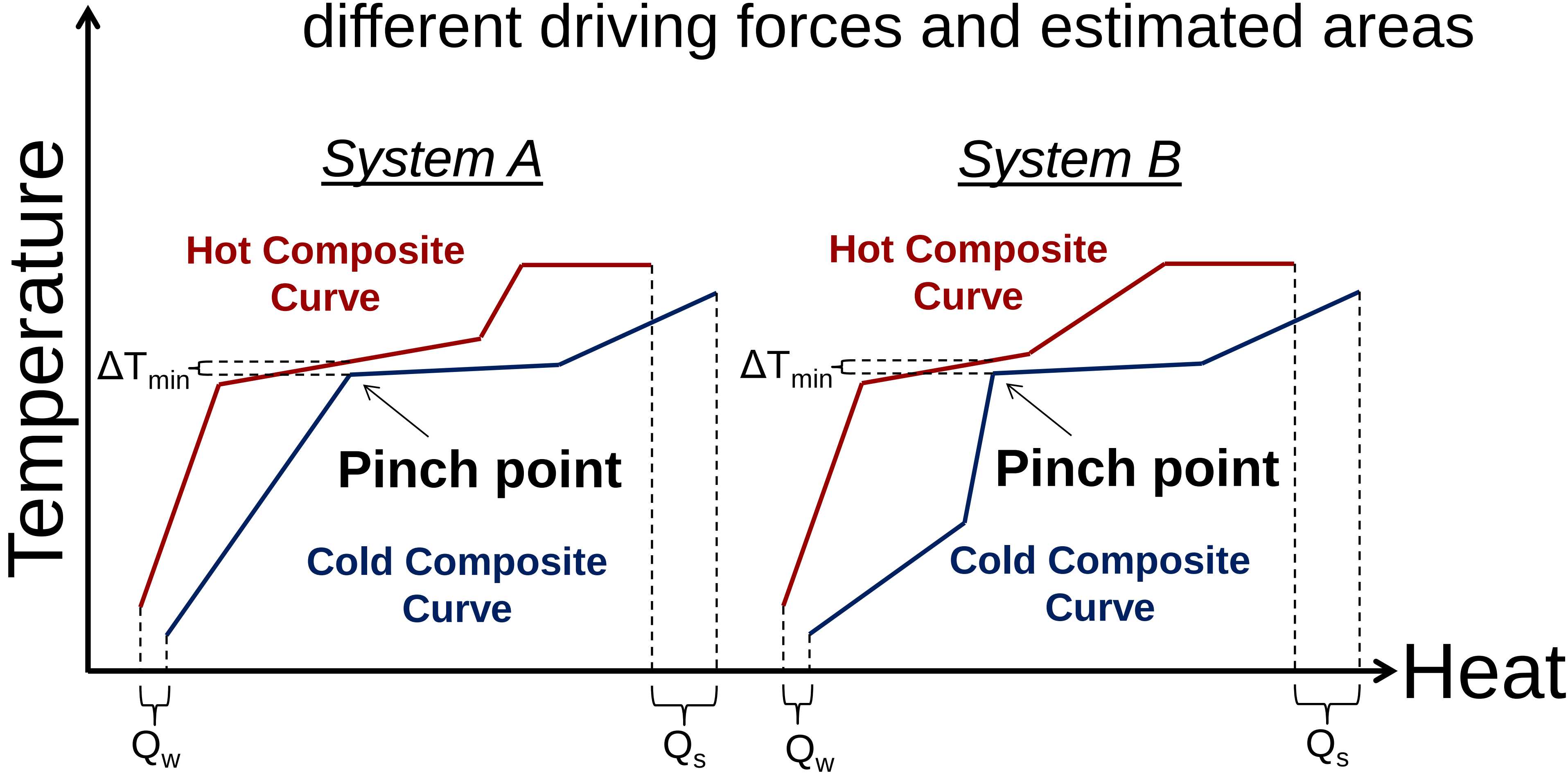
HEN Costs

	Fixed Stream Data	Utility Costs	Area Costs	Number of Exchangers
Sequential HENS (LP → MILP → NLP)	No	Yes	Yes	Yes
Simultaneous HENS (MINLP)	No	Yes	Yes	Yes
Duran-Grossmann Formulation (NLP)	Yes	Yes	No	No

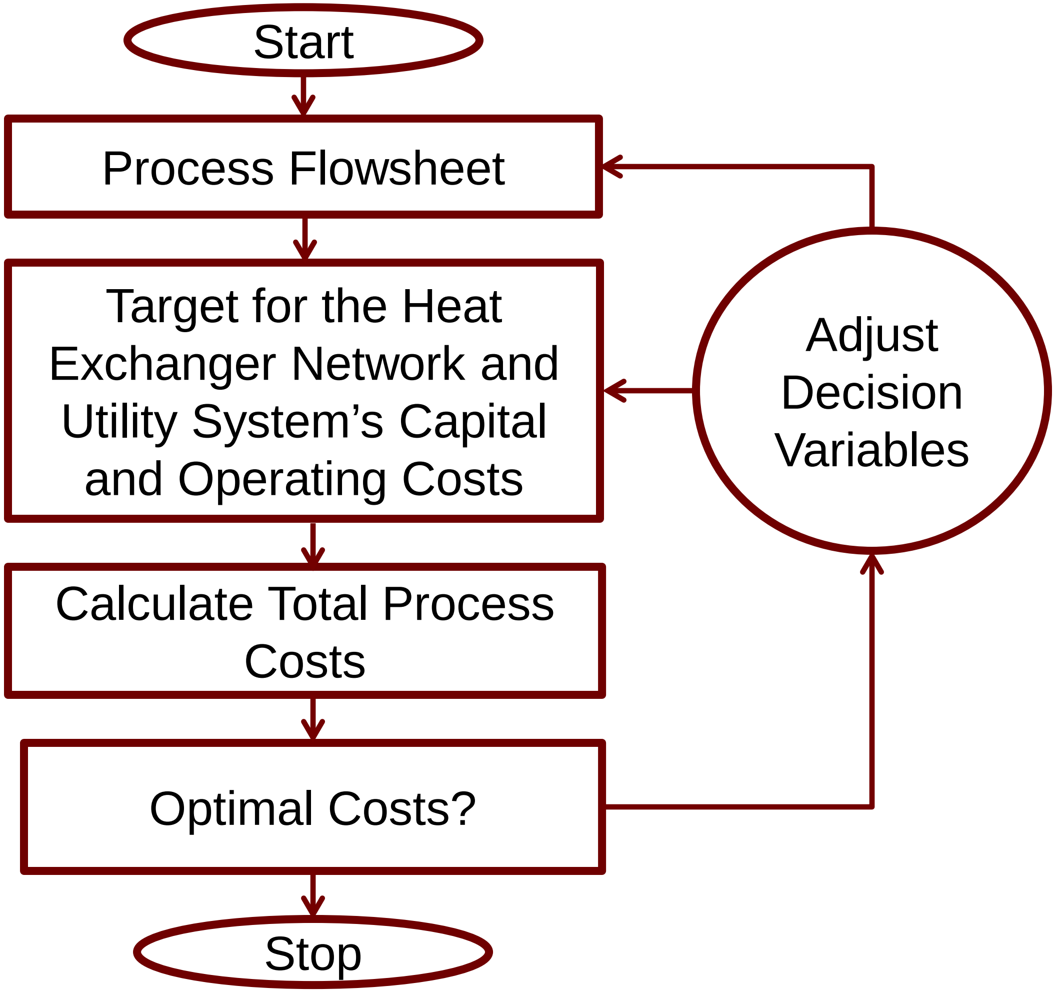
Goal: Add area costs to the Duran-Grossmann formulation.

Motivation

Same pinch point and utility loads but different driving forces and estimated areas



Previous Work: Gomez et al



Start

Process Flowsheet

Target for the Heat Exchanger Network and Utility System's Capital and Operating Costs

Calculate Total Process Costs

Optimal Costs?

Stop

Adjust Decision Variables

Figure 5.4 of J. A. Gomez Giammattei (1994, PhD thesis)

Comments:

- Internally constructs grand composite curves
- Capital costs using Linnhoff and Ahmad's (1990) method

Properties:

- Implementation requires loops and logical statements
- **Non-differentiable optimization problem?**

Formulation Specifications

1. Express as algebraic equations
    - Enables calculation of exact derivatives

2. Temperature intervals and pinch temperature orderings not known *a priori*

3. Approximate area costs sufficiently for cost of electricity minimization

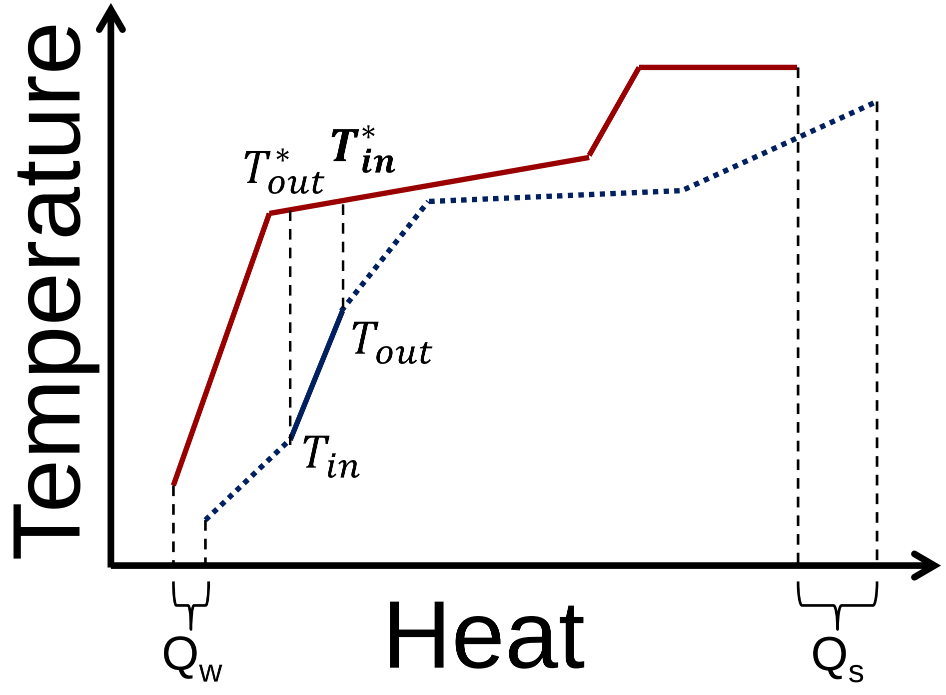
Driving Force Calculation

Consider a **cold stream**

Know T_{in} & T_{out}… calculate $\boldsymbol{T^*_{in}}$ & T^*_{out}

$Q^{Ah}(T^*_{in})$:= Heat exchanged above T^*_{in}

$Q^{Ac}(T_{out})$:= Cold exchanger above T_{out}



Energy Balance:

$$\underbrace{Q_s} + Q^{Ah}(\boldsymbol{T^*_{in}}) = \underbrace{Q^{Ac}(T_{out})}$$

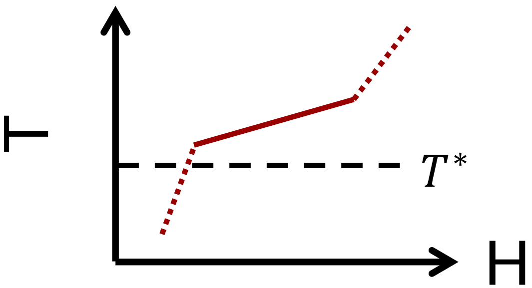
Calculated in Duran-Grossmann formulation

Q^{Ah} Calculation

$$\widetilde{\max}(x) \overset{\text{def}}{=} x + \sqrt{x^2 + \varepsilon^2} \approx \max(x, 0)$$

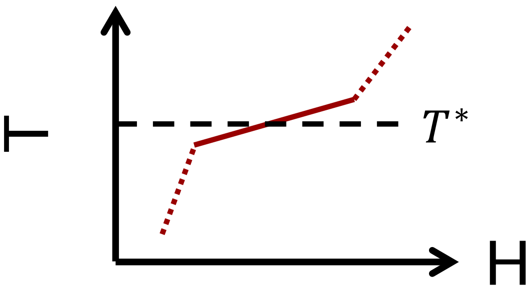
$$Q^{Ah}(T^*) = \sum_{i \in \{Hot\}} \underbrace{FCp_i[\widetilde{\max}(T_i^{in} - T^*) - \widetilde{\max}(T_i^{out} - T^*)]}_{Q_i^{Ah}(T^*)}$$

For hot streams i, $T_i^{in} > T_i^{out}$



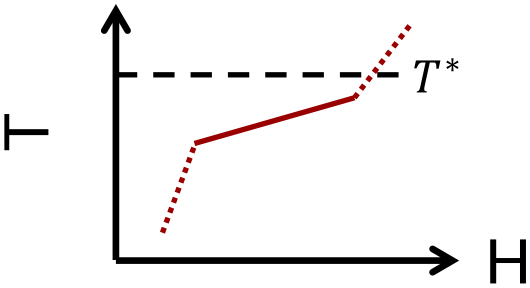
If $T_i^{out} \geq T^*$
then $Q_i^{Ah}(T^*) = Q_i$

(stream i is completely **above** T^*)



If $T_i^{out} < T^* < T_i^{in}$
then
$0 < Q_i^{Ah}(T^*) < Q_i$

(stream i is **split** by T^*)



If $T_i^{in} \leq T^*$
then $Q_i^{Ah}(T^*) = 0$

(stream i is completely **below** T^*)

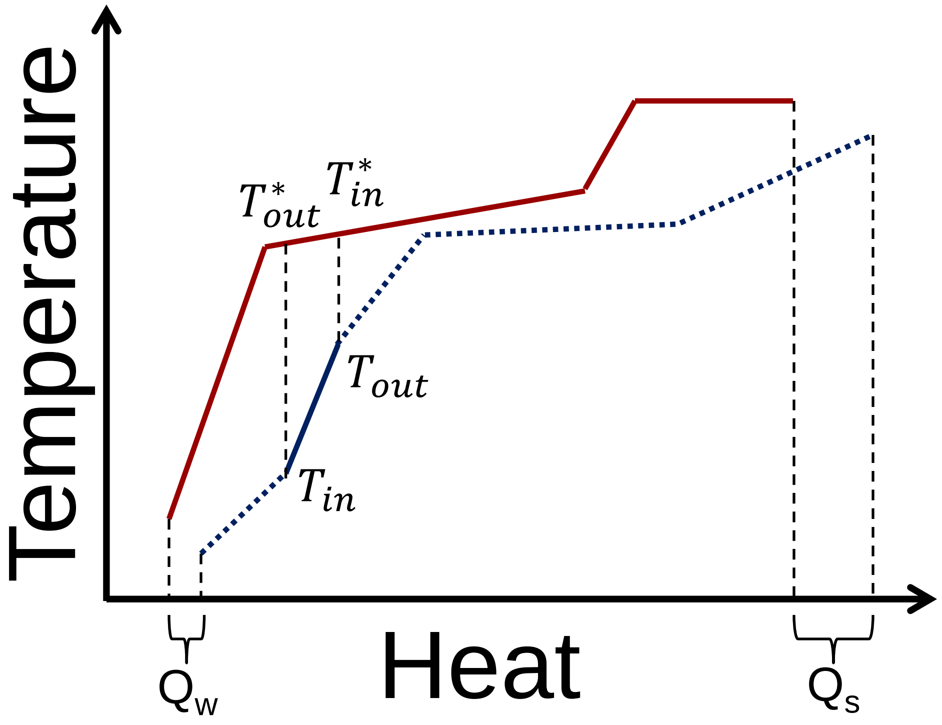
Driving Force Calculation

$$\Delta T_1, j = T^*_{out,j} - T_{in,j}$$

$$\Delta T_2, j = T^*_{in,j} - T_{out,j}$$

$$\Delta T_{LM,j} = \left(\frac{(\Delta T_{1,j})^{0.3275} + (\Delta T_{2,j})^{0.3275}}{2} \right)^{1/0.3275}$$

$$A_j \approx \frac{Q_j}{U_j \Delta T_{LM,j}}$$



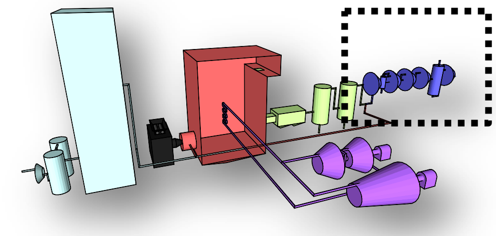
$$\text{Total Area} = \sum_{i \in \{Hot\}} A_i + \sum_{j \in \{Cold\}} A_j$$

Future Refinements:

- Calculate heat exchanger area <u>costs</u>
- Subdivide each heat exchanger into subunits for more accurate area calculations

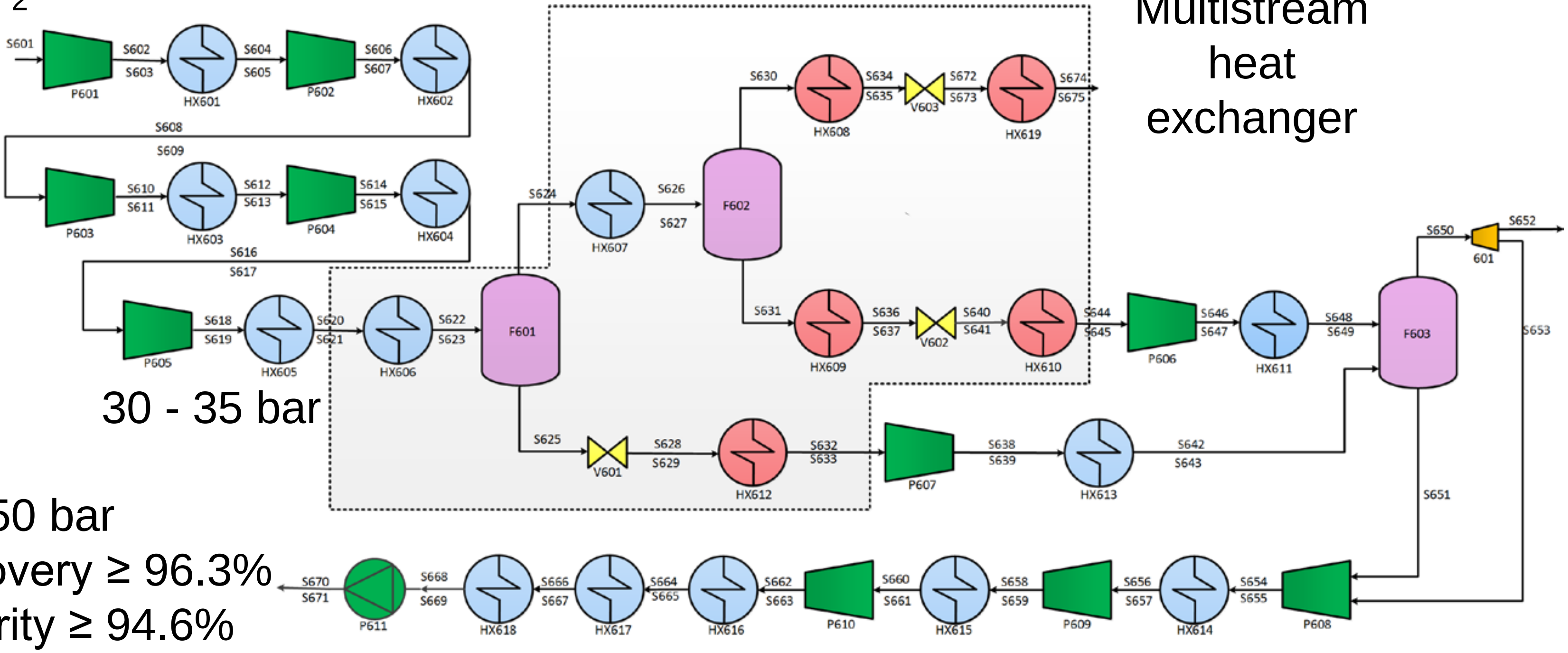
Chen, J. J. J. (1987). Comments on improvements on a replacement for the logarithmic mean. *Chem. Eng. Sci.*, 42(10) 2488 – 2489.

Case Study: CO_2 Processing Unit



Minimize Shaft Work + 0.01 $Q_{\text{cooling water}}$ + α_A Total Area

using Peng-Robison thermodynamics



83.5% CO_2
330 K
1.03 bar

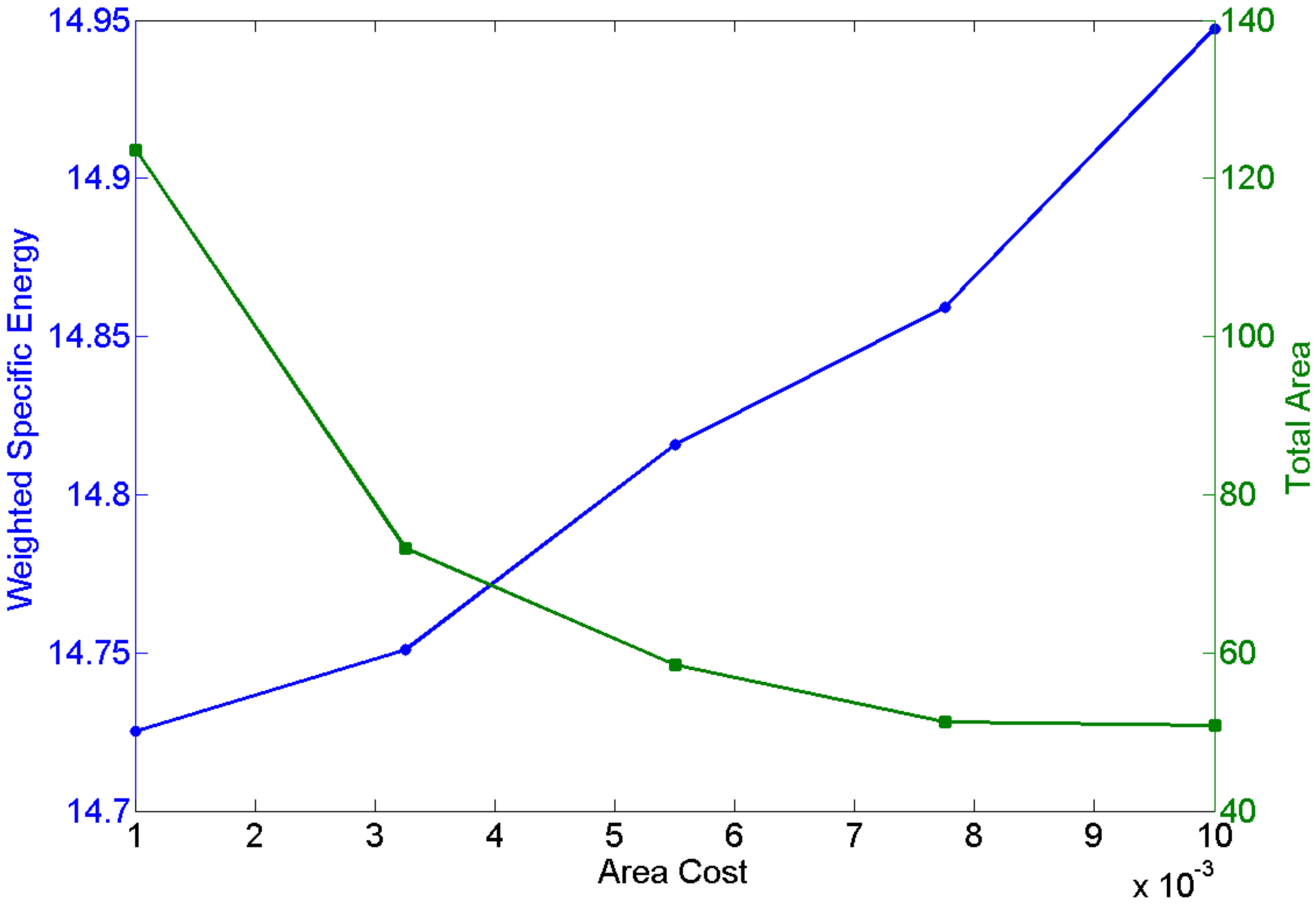
Multistream
heat
exchanger

30 - 35 bar

150 bar
CO_2 Recovery ≥ 96.3%
CO_2 Purity ≥ 94.6%

Based on two-flash system from Fu, C. & Gundersen, T. (2012). *Int. J. of Green. Gas Control*, 9, 419-727.

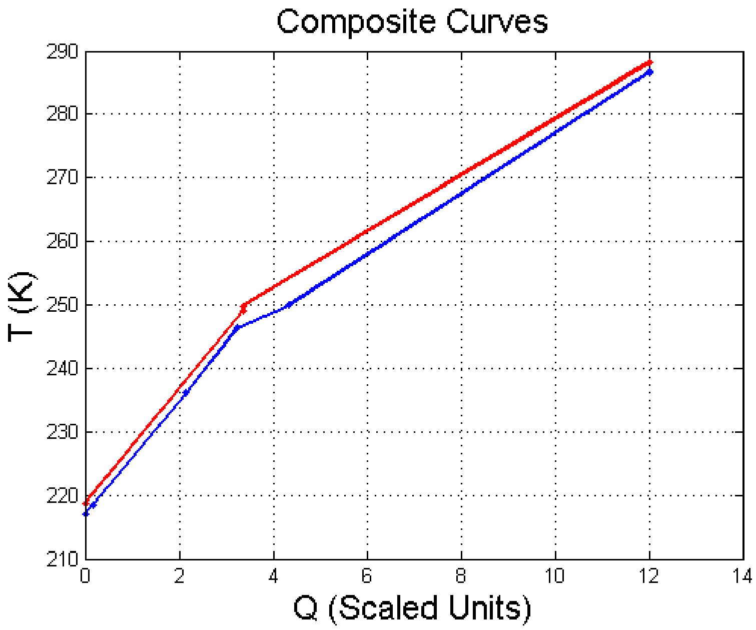
Sensitivity to Area Cost



Comparison of Extremes

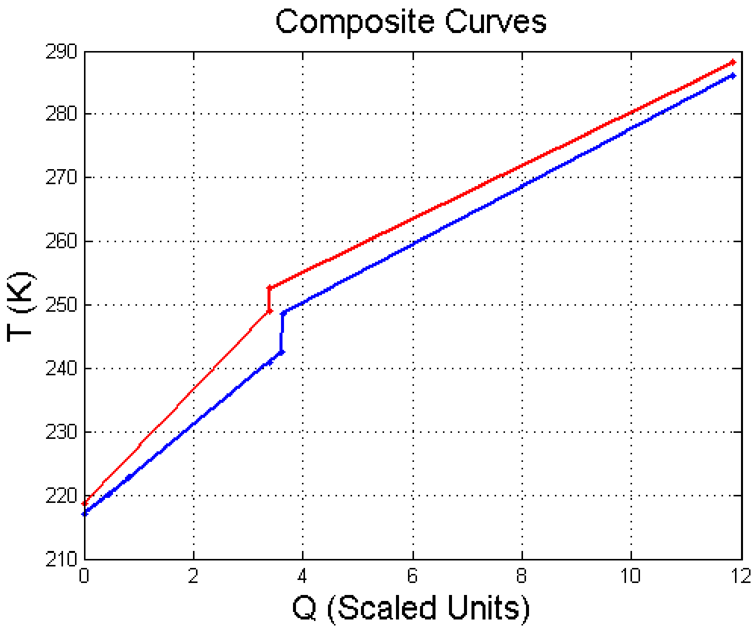
Cheap Area

$\alpha_A = 10^{-3}\ \mathrm{kW/m^2}$



Expensive Area

$\alpha_A = 10^{-2}\ \mathrm{kW/m^2}$



23.9	$Q^{cooling}_{water}$ $\left(\frac{kJ}{mole\ feed}\right)$	24.1
123.6	Total Area $\left(\frac{m^2}{mole\ feed}\right)$	**58.0**
14.73	Specific Energy $\left(\frac{kWh}{kg\ CO_2}\right)$	14.95

Preliminary CPU Timings

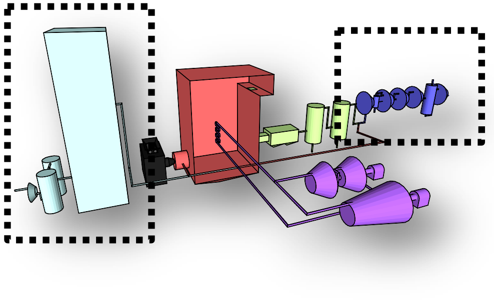
Considered 256 runs using multi-start procedure, Area Cost = 10^{-3}

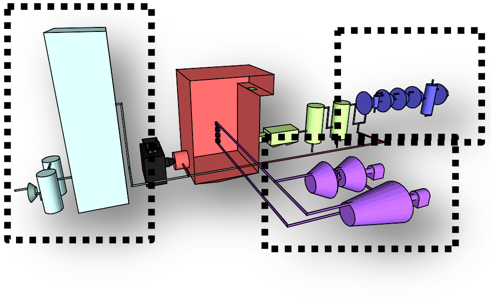
	Average CPU Time	**Frequency of "Good" Solutions**
Without Area Calculation	105.0 s	99
With Area Calculation	185.7 s	75

Future Work

- Refine initialization procedure – especially early NLPs
- Additional model refinements
  - Heat exchanger decompositions
  - Incorporate correlations for *U* and ΔP

Integration Opportunities





ASU & CPU

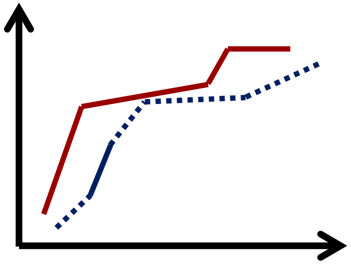
- Use refrigeration from the ASU to liquefy CO_2
- Less energy required to pump CO_2
- Feasibility depends on capital costs

Waste Heat from Compression

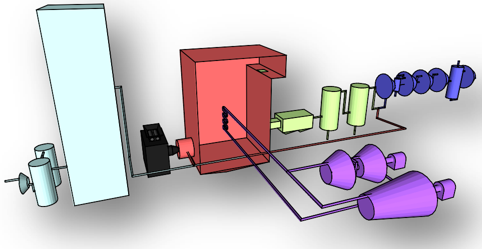
- Integrate waste heat from compressors into steam cycle
- Solution strongly sensitive to **capital costs**

Conclusions

- Embedded area estimates in **simultaneous heat integration** and **flowsheet optimization** problems
  - Variable stream data = add'n degrees of freedom
  - Does not require order of pinch candidates *a priori*



- Considered two cases studies with multistream heat exchangers
  - Air Separation Unit
  - CO_2 Processing Unit



Funding: CCSI Carbon Capture Simulation Initiative NETL NATIONAL ENERGY TECHNOLOGY LABORATORY

Initialization Procedure

Ideal Thermo & Shortcut Cascade

CEOS Thermo & Shortcut Cascade

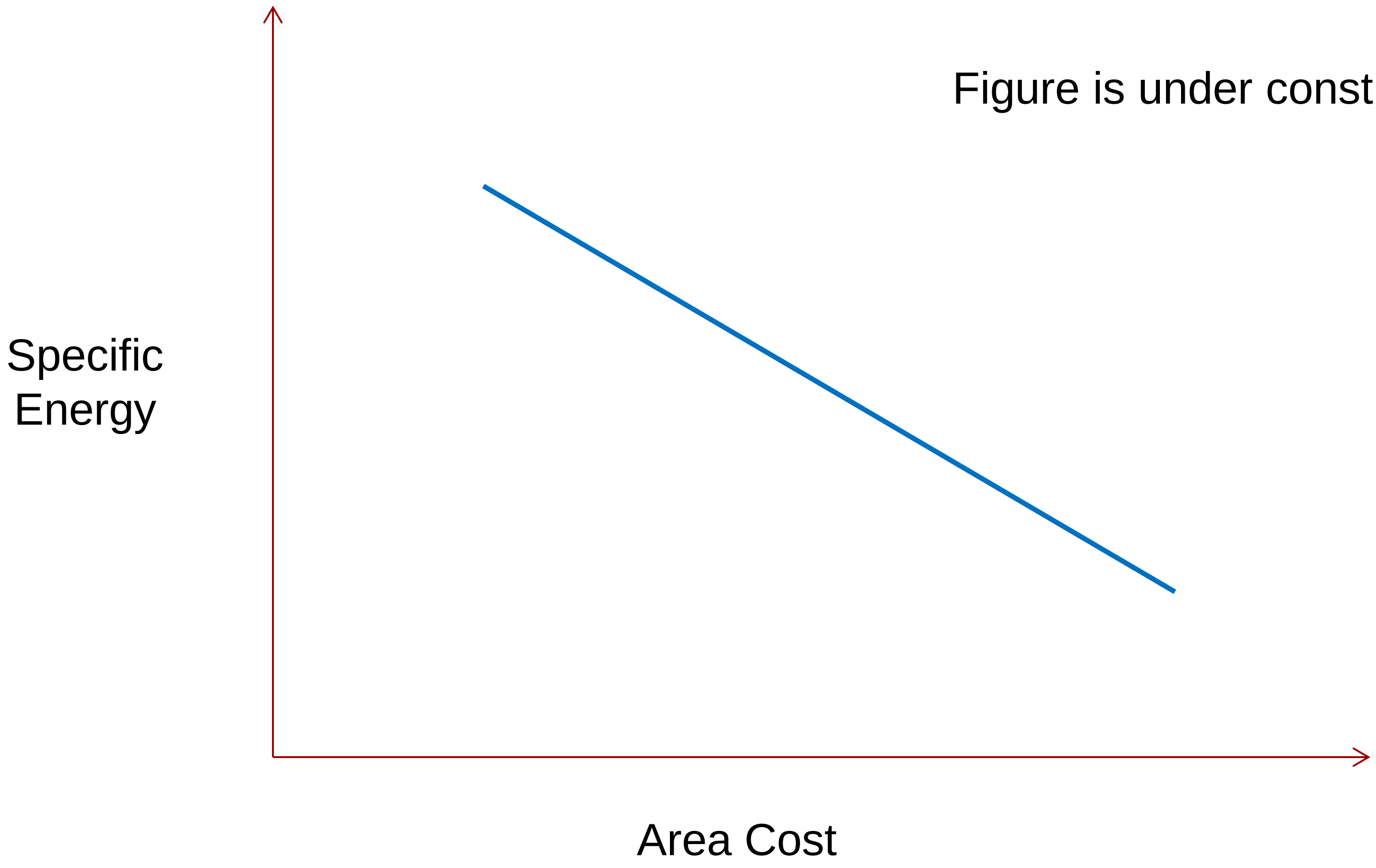
CEOS Thermo & MESH Cascade

Decompose Heat Exchange Units & Reoptimize

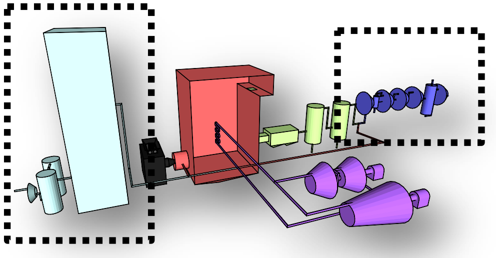
Repeat with different combinations (<u>factorial design</u>) of initial values and bounds

Sort local solutions by final obj. function value

Sensitivity to Area Cost



Future Work: ASU Integration



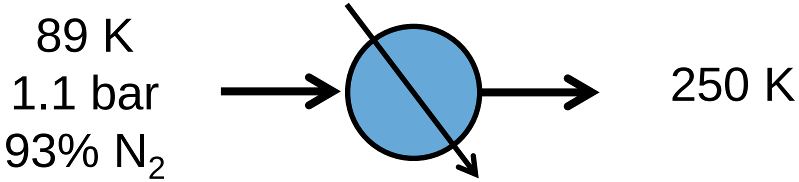


Figure is under construction