# Design of Air Separation Units
## for Advanced Combustion via Equation Based Optimization

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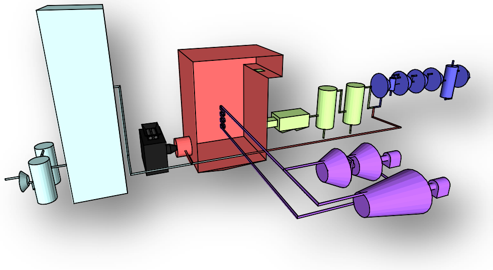


# Motivation

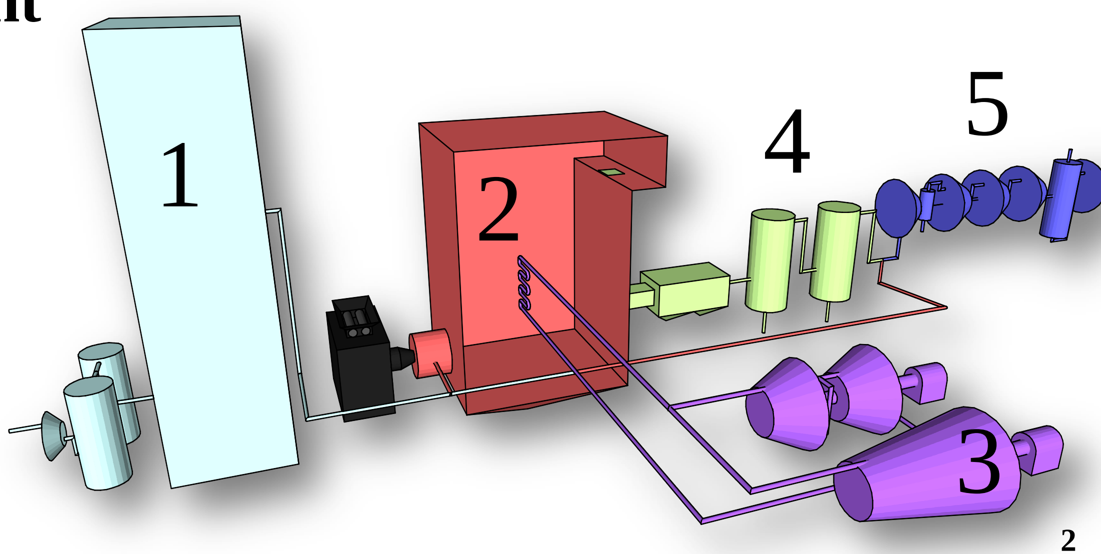
Develop framework for full oxycombustion power plant optimization

– 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



# Methodology: Equation Oriented

- High fidelity models (approaching first principles)
- Accurate derivative information → efficient large scale optimization algorithms (100,000+ variables)
- Consider integer decisions (MINLP)
- Low cost sensitivity information
- Optimality guarantees

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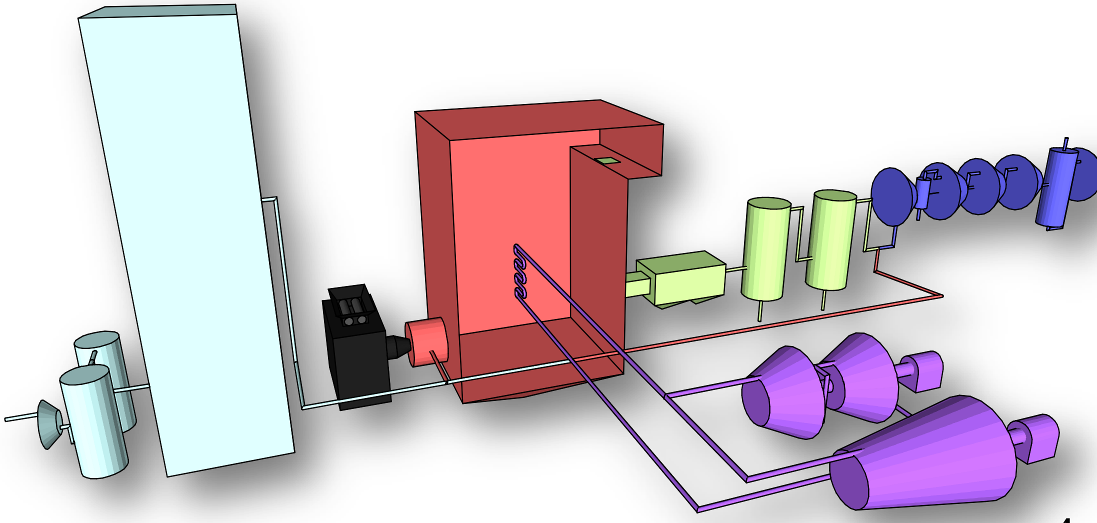
Start with cryogenic ASU



# Cryogenic Air Separation

Low pressure section

Boiling Points @ 1 atm

| | |
|---|---|
| Oxygen: | -183 °C |
| Argon: | -185.7 °C |
| Nitrogen: | -195.8 °C |

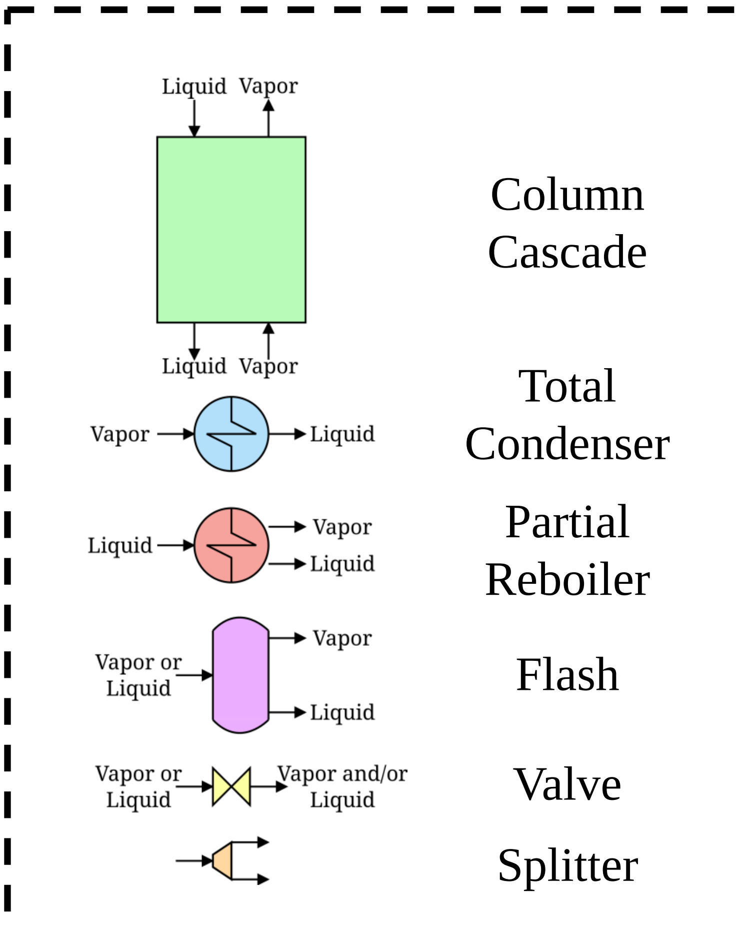
Multicomponent distillation with tight heat integration

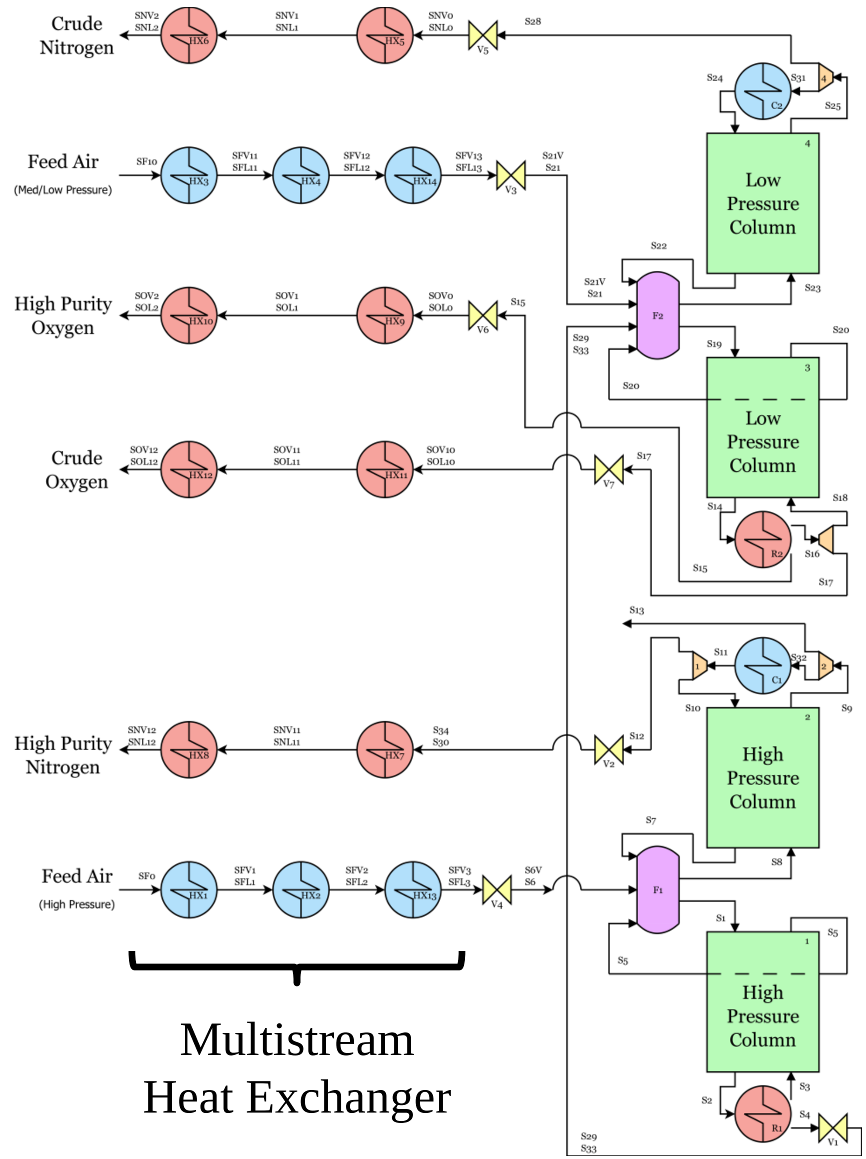

Photo from wikipedia.org

High pressure section

***Challenging to systematically optimize in AspenPlus.***

# Double Column Configuration

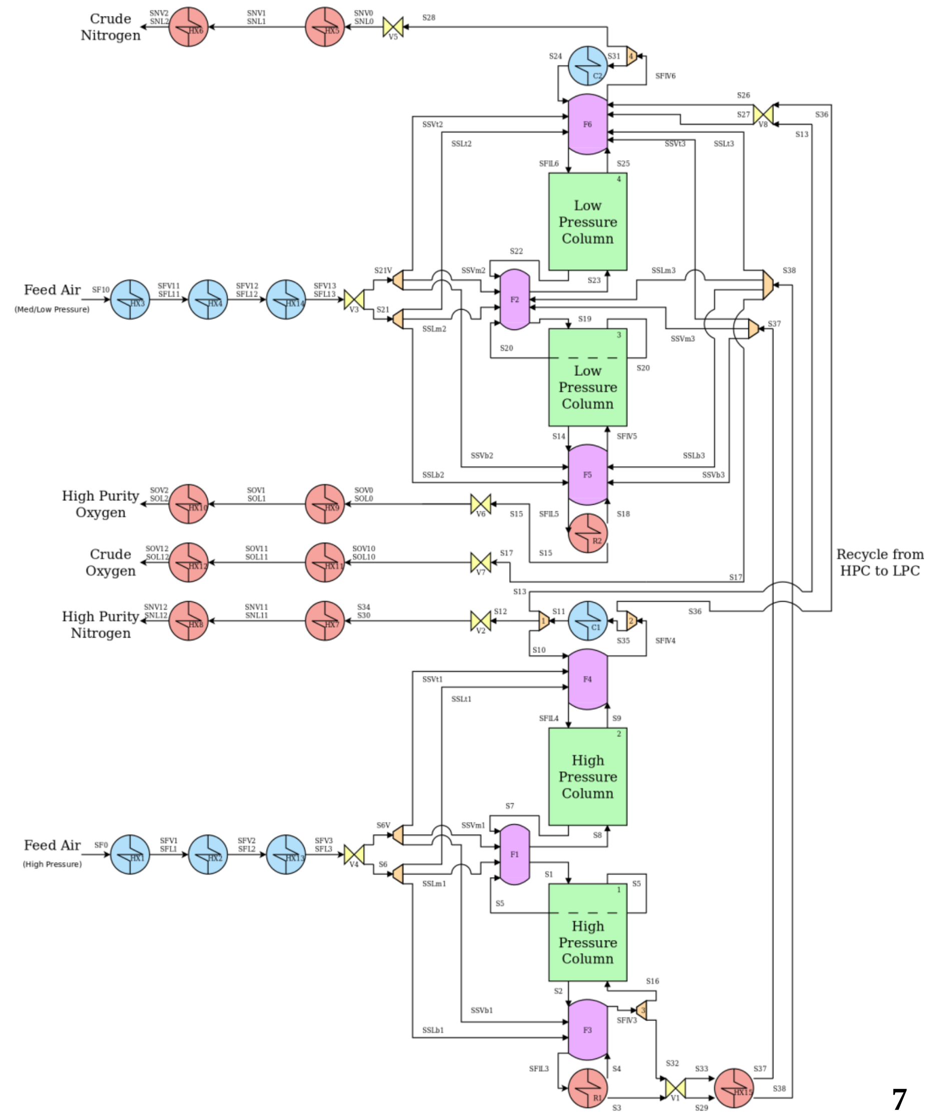


# ASU Superstructure

- *<u>Many</u>* different column configurations realizable

- NLP optimizer selects the best configuration



# Optimization Formulation

$$\min \quad \begin{array}{c}\text{ASU Compression Energy} \\ (\text{kWh / kg } O_2 \text{ product})\end{array}$$

$$\text{s.t.} \quad \begin{array}{c}\text{Flowsheet Superstructure} \\ \text{Thermodynamics Module} \\ \text{Unit Operation Models} \\ \text{Cascade Model} \\ \text{Heat Integration} \\ O_2 \text{ product purity} \geq 95 \text{ mol\%}\end{array}$$

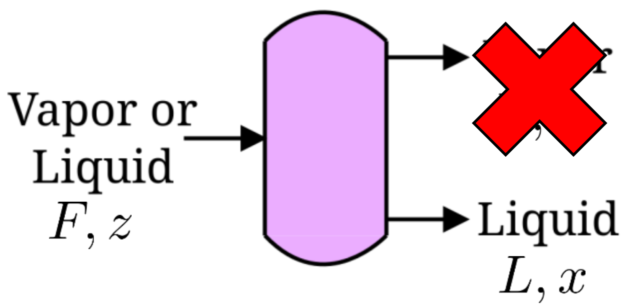
Note: **Upper and lower bounds not shown above** are considered for many variables including stream/equipment temperatures and pressures.

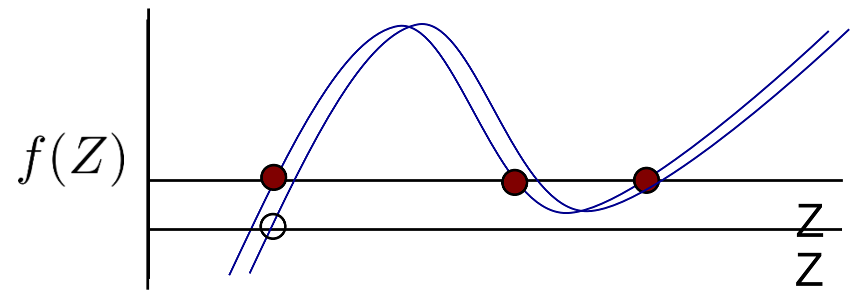
# Cubic Equation of State

Kamath, R. S., Biegler, L. T., & Grossmann, I. E. (2010). An equation-oriented approach for handling thermodynamics based on cubic equation of state in process optimization. *Computers & Chemical Engineering*, *34*(12), 2085–2096.

Ex: Peng-Robinson

$$Z^3 - (1 + B - uB)Z^2 + (A + wB^2 - uB - uB^2)Z - AB - wB^2 - wB^3 = 0$$




$$F = L + V$$
$$Fz_c = Lx_c + Vy_c, \quad \forall c \in \{Comps\}$$
$$FH^F + Q = LH^L + VH^V$$
$$y_c = \beta \ K_c(T, P, x, y)x_c$$
$$0 \leq x_c, y_c \leq 1$$
$$0 \leq L, V \leq F$$

**Mole balance**

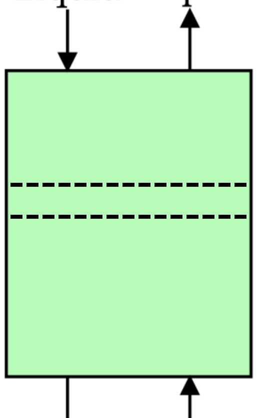
**Energy Balance**

**Equilibrium**

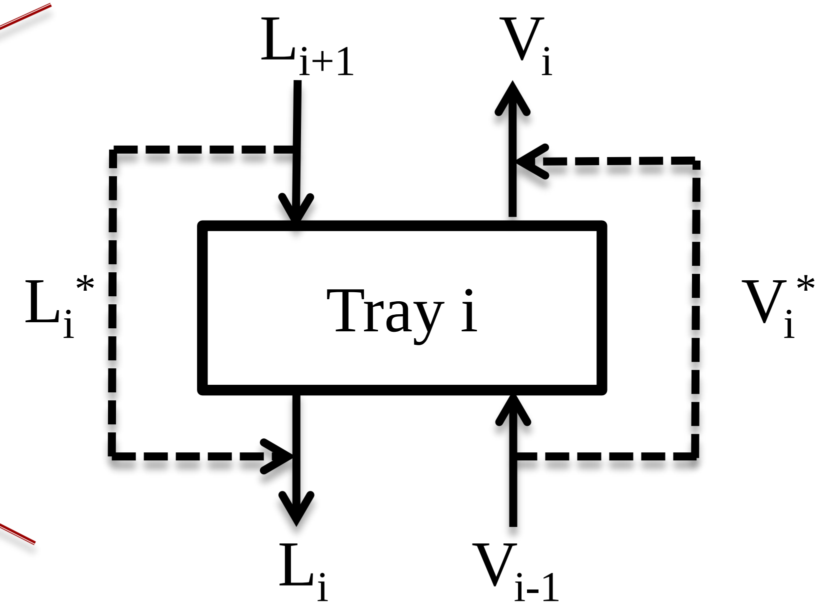
$$0 \leq s_V \perp V \geq 0 \qquad 0 \leq s_L \perp L \geq 0$$
$$-s_L \leq \beta - 1 \leq s_V$$
$$K_c = \phi_c^L / \phi_c^V, \quad \forall c \in \{Comps\}$$
$$f(z_V) = 0 \qquad f(z_L) = 0$$
$$f'(z_V) \geq 0 \qquad f'(z_L) \geq 0$$
$$f''(z_V) \geq -Ms_V \qquad f''(z_L) \leq Ms_L$$

# Cascade Models

Group Method | MESH Model with Bypass




**Simpler approximation**




$$\varepsilon = \frac{V_i^*}{V_{i-1}} = \frac{L_i^*}{L_{i+1}}$$

**Complex & rigorous**

# Cascade Models

**Group Method**

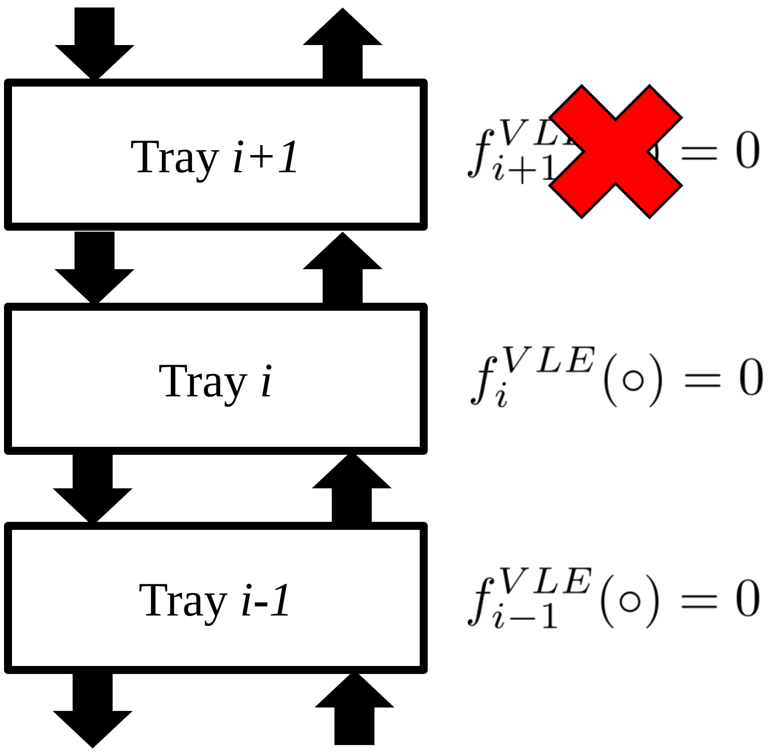
- **Continuous number** of ideal stages
- Based on the work of Kremser and Edmister
- Modified for general distillation by Kamath

**MESH Model with Bypass**

- *New distillation model*
- **M**ass, **E**quilibrium, **S**ummation and **H**eat equations
- Model discrete trays
- Bypass allows for tray (de)activation with **only continuous variables**

Kamath, Grossmann & Biegler (2010). Aggregate models based on improved group methods for simulation and optimization of distillation systems. *Computers & Chemical Engineering*.

# MESH with Bypass

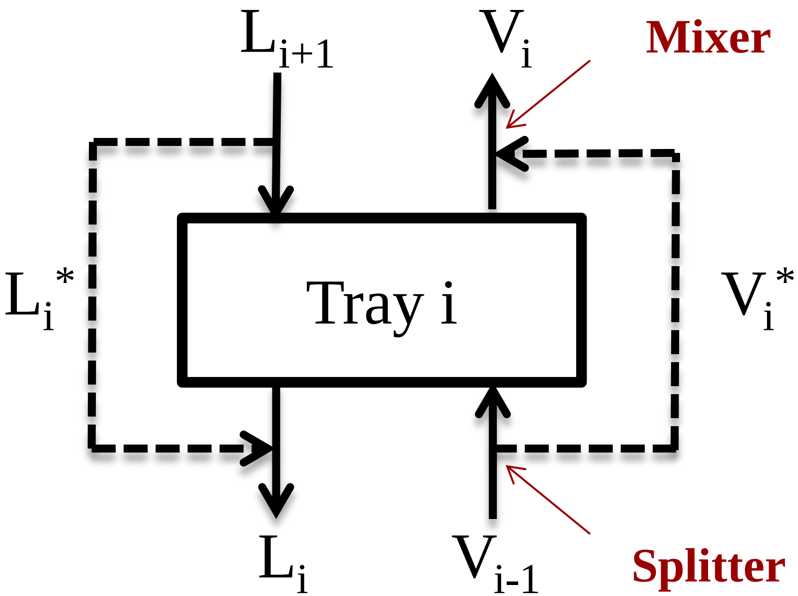



Yeomans & Grossmann (2000)

- Disjunctive model to (de)activate trays
- Logic based solution algorithm

Yeomans, H., & Grossmann, I. E. (2000). Disjunctive Programming Models for the Optimal Design of Distillation Columns and Separation Sequences. *Industrial & Engineering Chemistry Research*, 39(6), 1637–1648.

# MESH with Bypass




$$\varepsilon = \frac{V_i^*}{V_{i-1}} = \frac{L_i^*}{L_{i+1}}$$

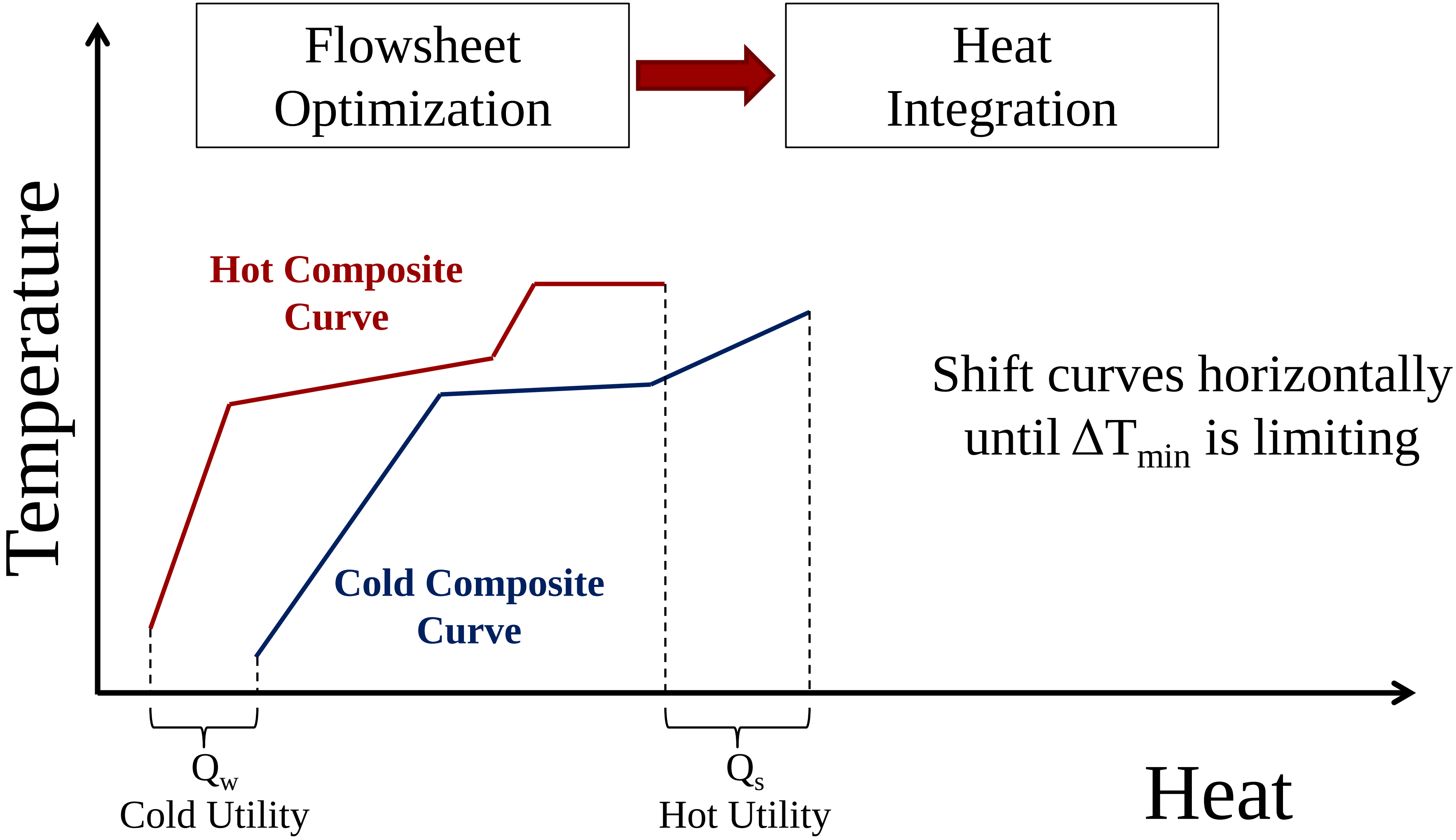
Yeomans & Grossmann (2000)

- Disjunctive model to (de)activate trays
- Logic based solution algorithm

New model

- Use generic NLP solver
- Equilibrium calculated with $V_{i\text{-}1}$ and $L_{i+1}$ to avoid degeneracies

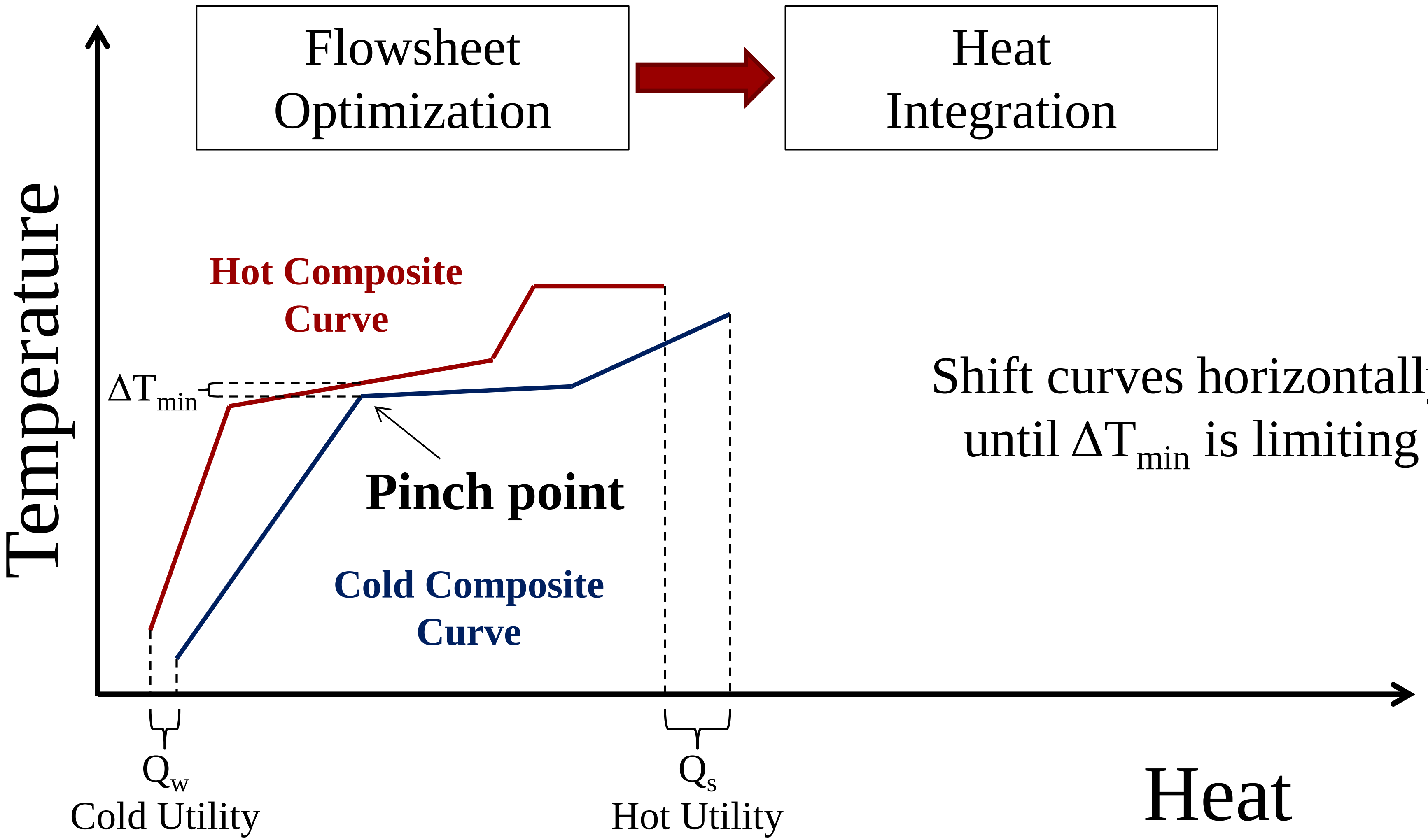
# Pinch Based Heat Integration





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




Shift curves horizontally until $\Delta T_{min}$ is limiting


Hohmann, E.C. (1971). *Optimum Networks for Heat Exchangers*. PhD Thesis, University of So. Cal.
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# Heat Integration Model

**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**

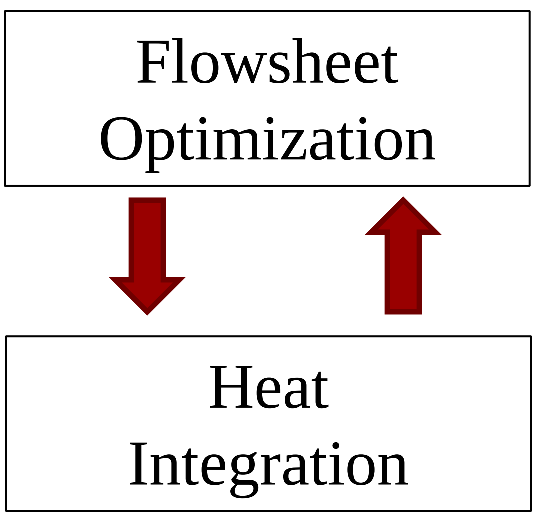
$$QA_H^p = \sum_{i \in \{Hot\}} FCp_i [\tilde{\max}(T_i^{in} - T^p) - \tilde{\max}(T_i^{out} - T^p)]$$

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

**Utility calculations**

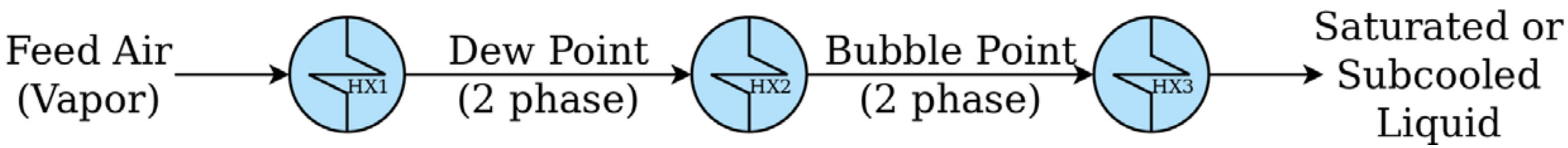
$$Q_s \geq QA_C^p - QA_H^p \quad \text{for all } p$$

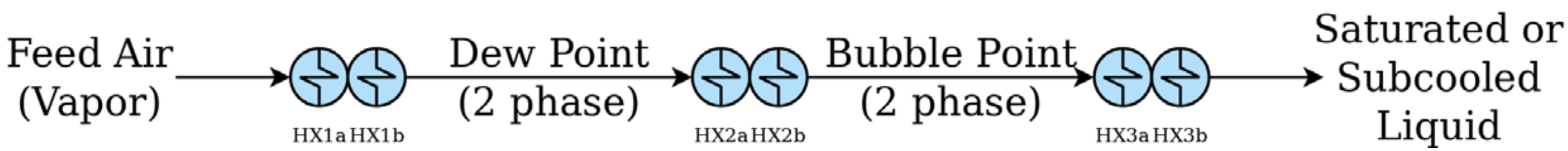
$$Q_w = Q_s + \sum_{j \in \{Cold\}} Q_j^{in} - \sum_{i \in \{Hot\}} Q_i^{out}$$

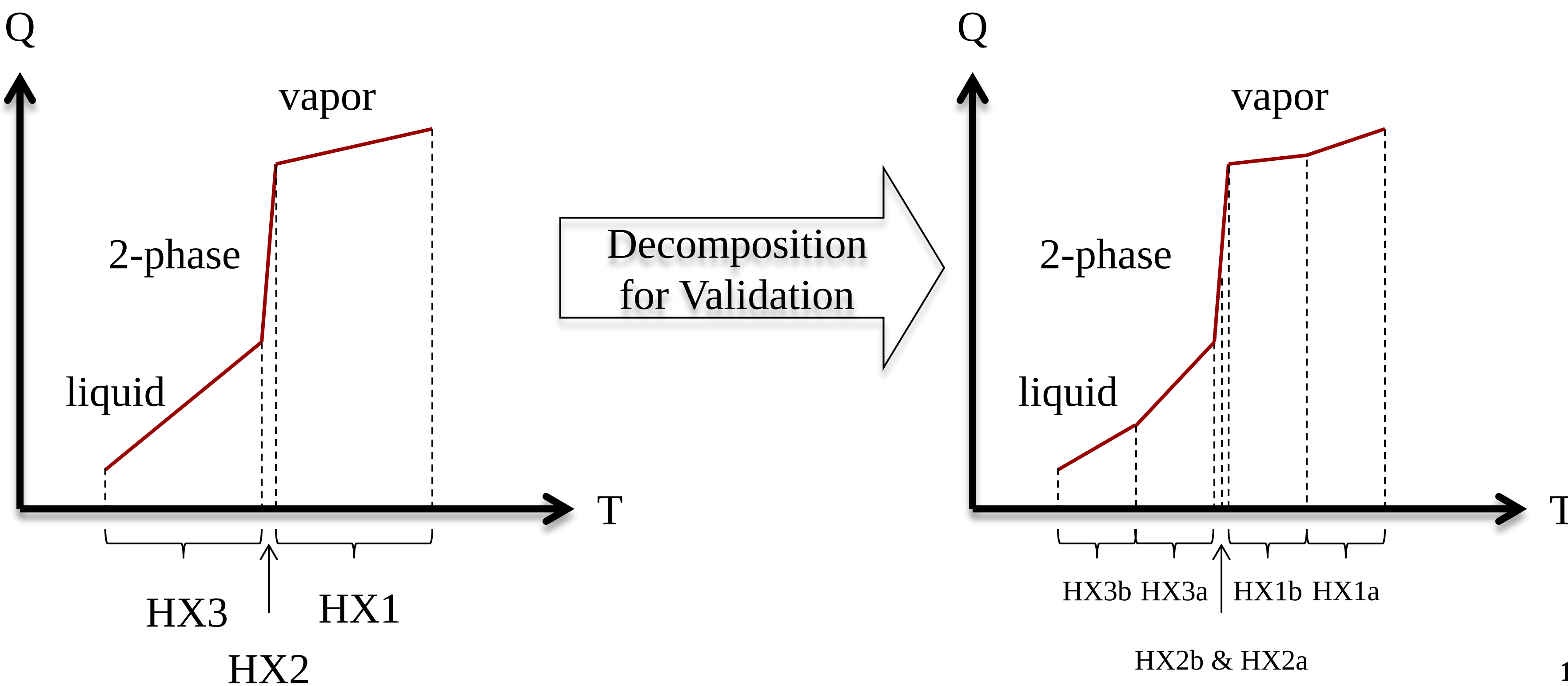



Duran, M. A., & Grossmann, I. E. (1986). Simultaneous optimization and heat integration of chemical processes. *AIChE Journal*, *32*(1), 123–138.

# Heat Exchanger Decomposition



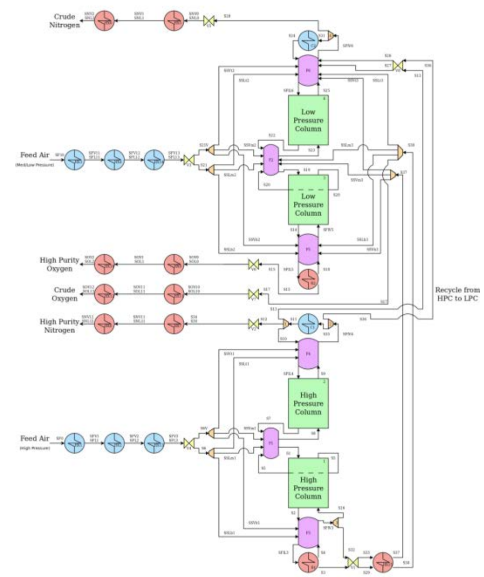



# Implementation Details

- Non-convex problem
  - 12,000 variables & constraints
- Automated initialization
  - Simple → complex models
  - Custom multistart procedure
- Solved using **CONOPT3** in GAMS
  - **12 CPU minutes** on Intel i7 desktop for one initial point

min ASU Compression Energy (kWh / kg $O_2$ product)

s.t.
Flowsheet Superstructure
Thermodynamics Module
Unit Operation Models
Cascade Model
Heat Integration
$O_2$ product purity $\geq$ 95 mol%



# Initialization Procedure

Ideal Thermo & Shortcut Cascade

↓

CEOS Thermo & Shortcut Cascade

↓

CEOS Thermo & MESH Cascade

↓

Decompose Heat Exchange Units & Reoptimize

Repeat with different combinations of initial values and bounds

Sort local solutions by final obj. function value

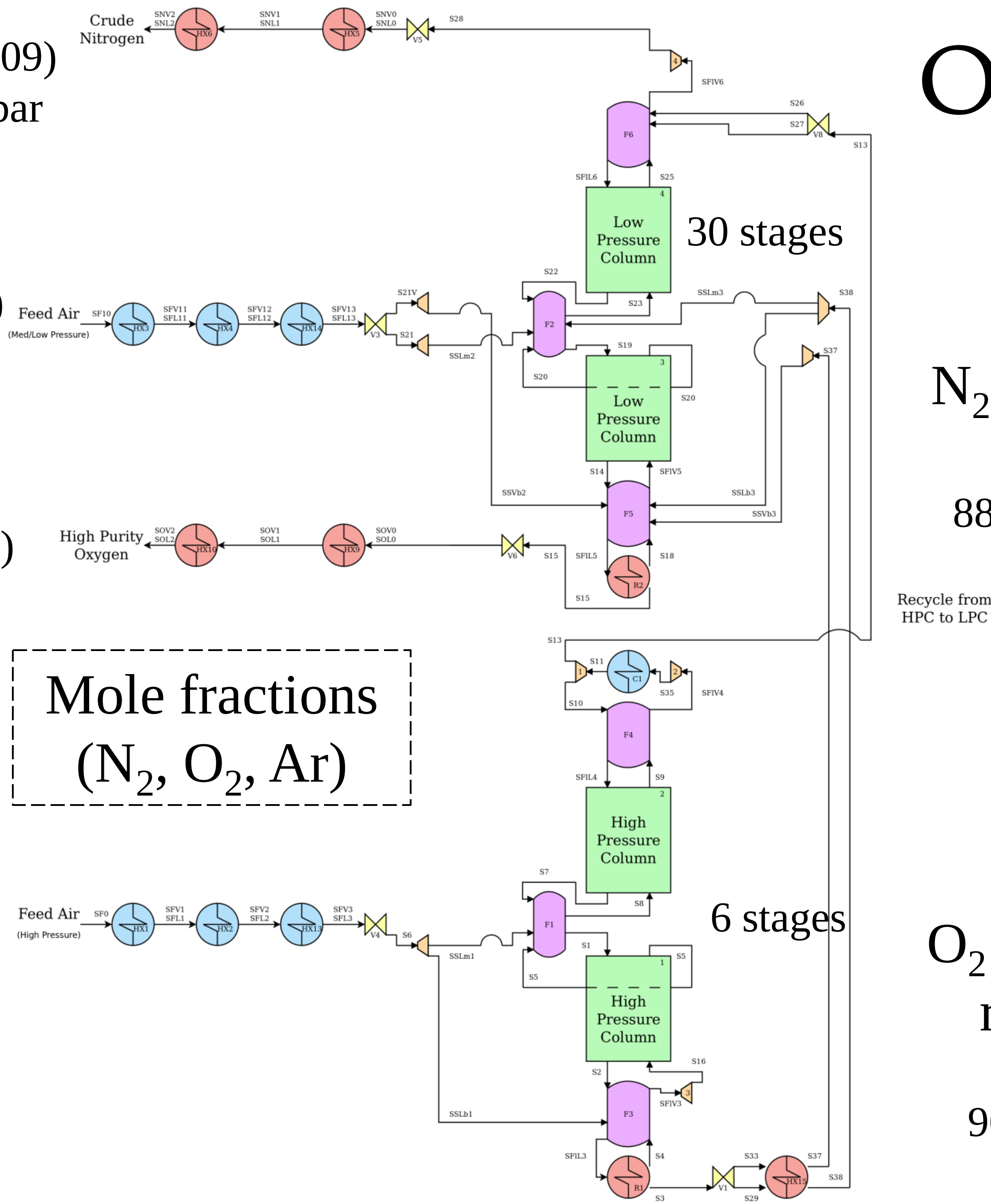
# Optimal ASU

1.58 mol/t
(**.978**, .013, .009)
298 K, 1.01 bar

0.20 mol/t
(.78, 0.21, 0.01)
333 K, 40 bar

0.42 mol/t
(.036, **.950,** .014)
315 K, 1.01 bar

1.80 mol/t
(.78, 0.21, 0.01)
300 K, 3 bar




30 stages

6 stages

Mole fractions
($N_2$, $O_2$, Ar)

$N_2$ enriched reflux
88.7 K liquid

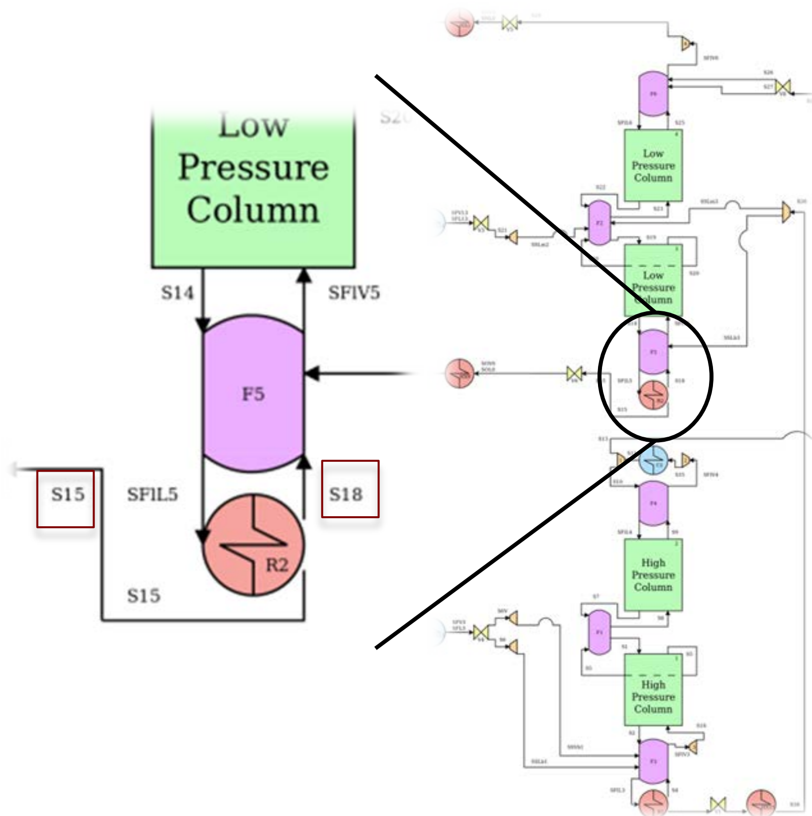
$O_2$ enriched recycle
81.4 K
90% liquid

# Validation with Aspen Plus®

Specifications:

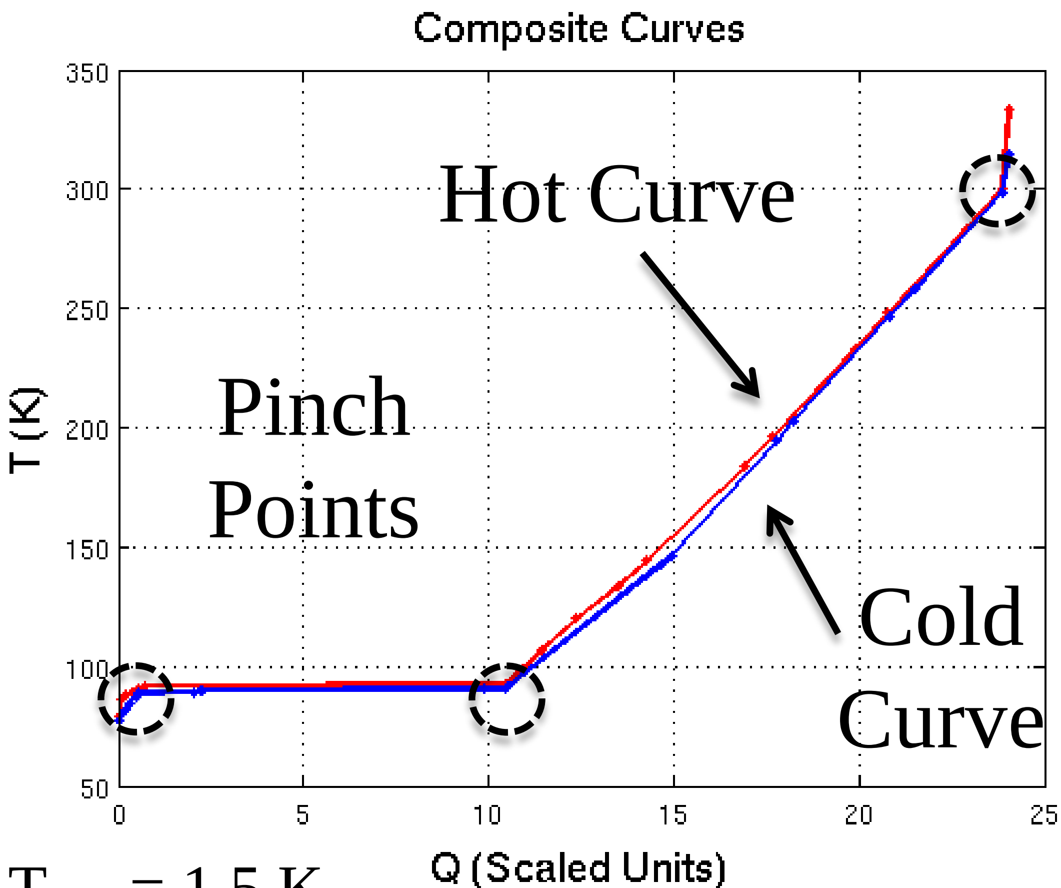
- Peng-Robinson thermodynamics model
- R2 feed conditions match GAMS results
- R2 outlet: 74.7% vapor
- Pressure: 1.053 bar

| Stream | Prop | GAMS | Aspen |
|---|---|---|---|
| S18 (vapor) | $N_2$ | 11.03% | 11.05% |
| | $O_2$ | 86.33% | 86.31% |
| | Ar | 2.64% | 2.64% |
| S15 (liquid) | $N_2$ | 3.07% | 3.09% |
| | **$O_2$** | **95.00%** | **94.96%** |
| | Ar | 1.93% | 1.95% |
| | Temp. | 89.42 K | 89.39 K |

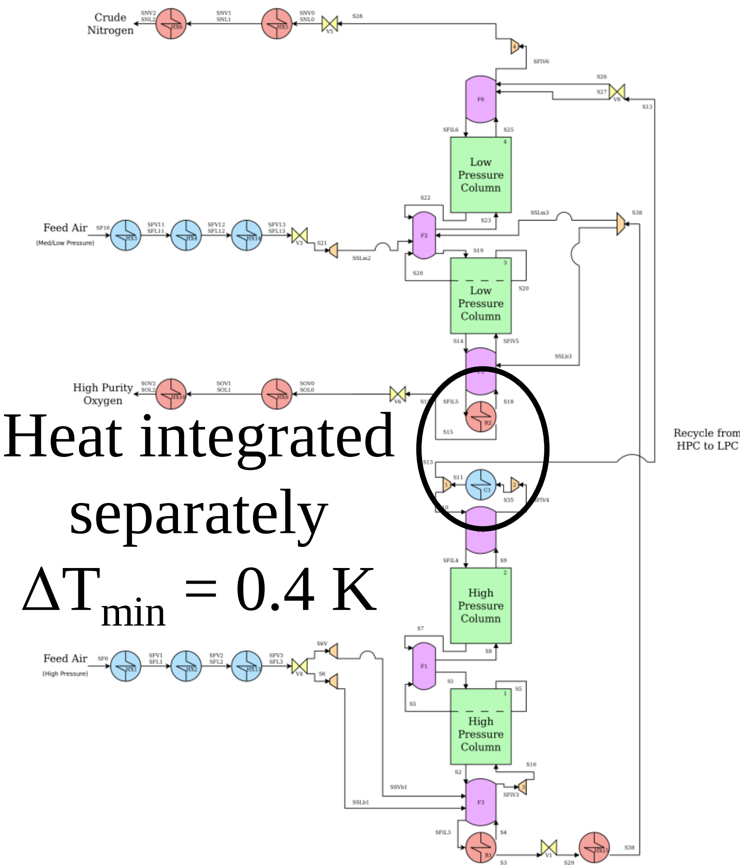



Discrepancy likely due to mismatch with input data for thermodynamic models

# Heat Integration Results




$\Delta T_{min} = 1.5$ K




Heat integrated separately

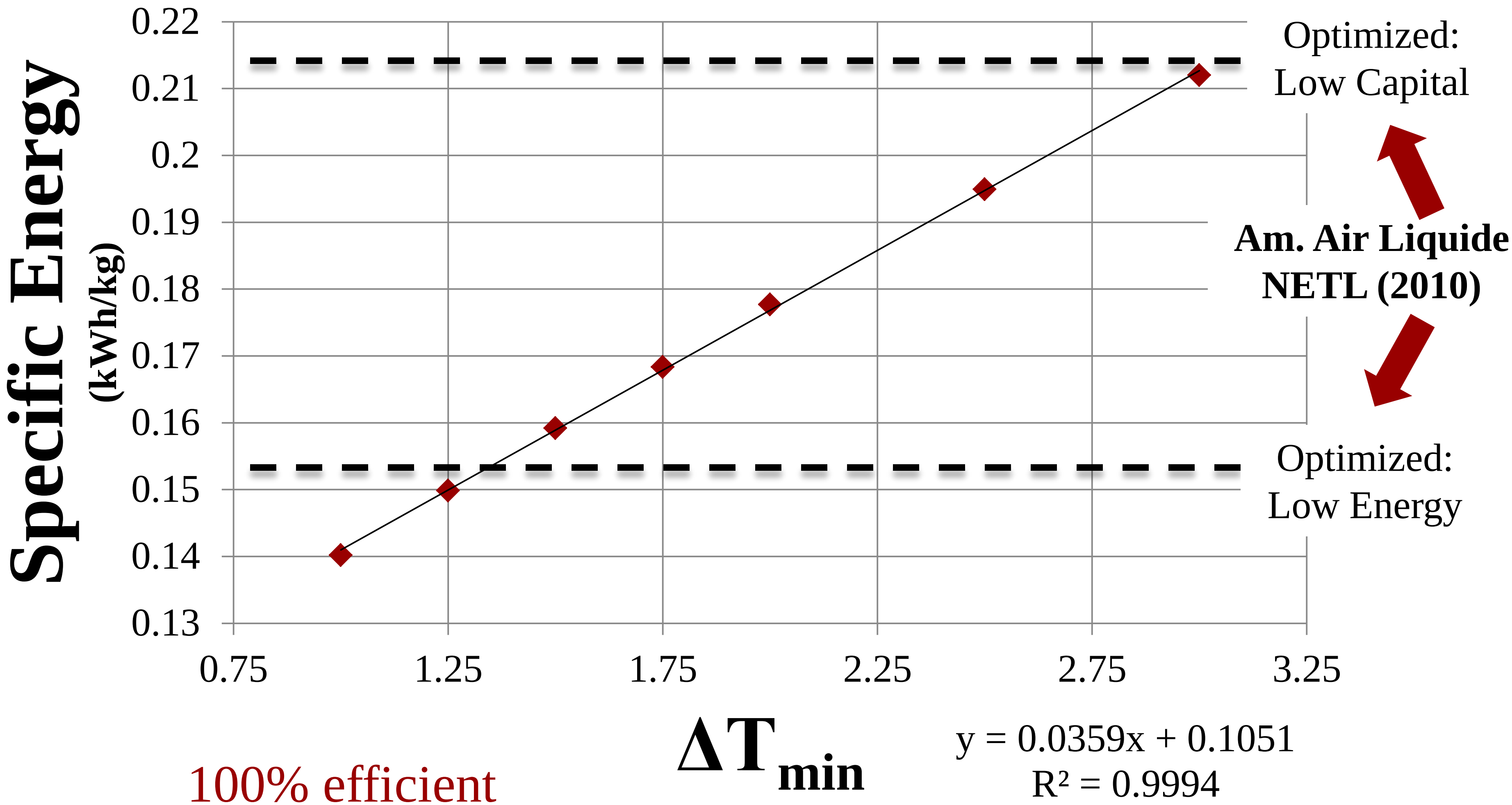
$\Delta T_{min} = 0.4$ K

**0.185 kWh/kg** $O_2$ product (86% eff. compressors)

Industrial Optimized Design (NETL, 2010)

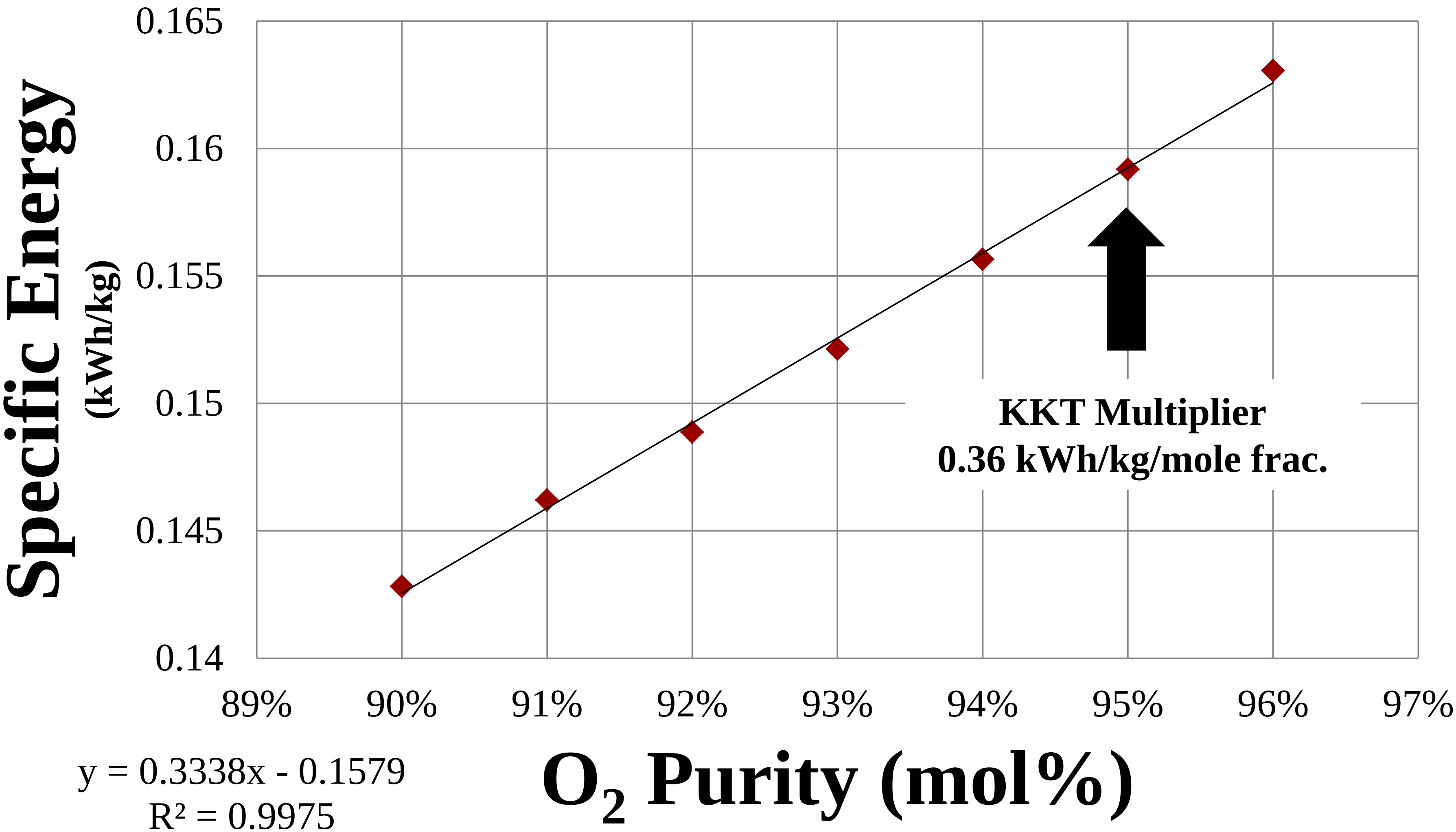
0.179 kWh/kg $O_2$ product (possible 86% eff.)

# Heat Integration Sensitivity




100% efficient compressors

# $O_2$ Purity Sensitivity




100% efficient compressors

# Future Work

**Oxycombustion Power Plant**

1. Air Separation Unit
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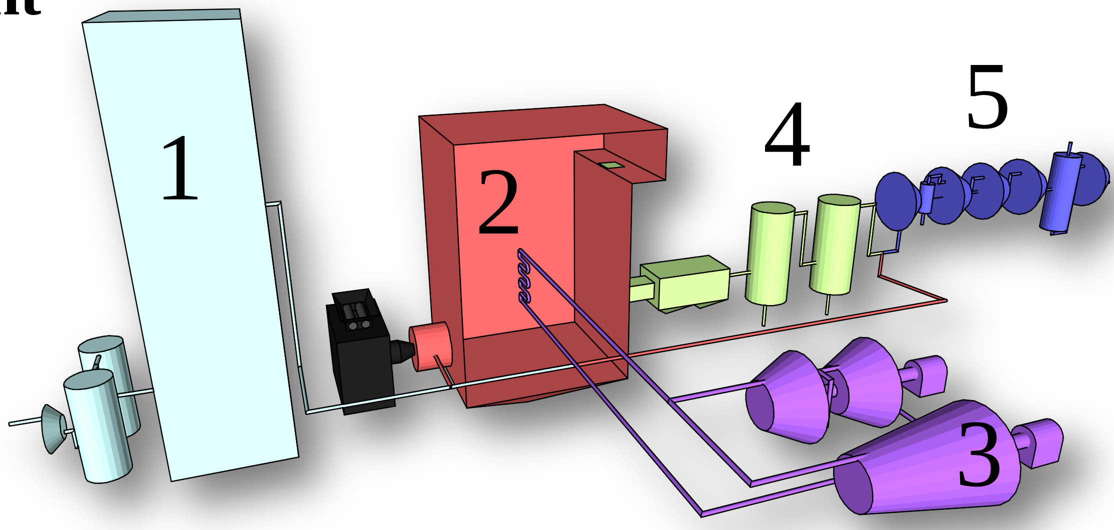
5. $CO_2$ Compression Train




Optimize trade-offs across systems in oxycombustion power plant

# Conclusions

## Optimized ASU with equation-based model:

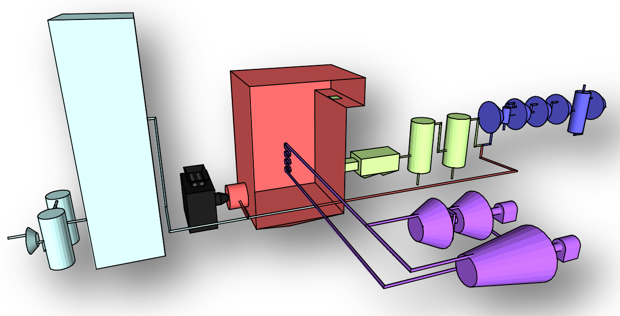
– Cubic equation of state & simultaneous heat integration

– *New distillation model*: MESH with bypass

– Pure nonlinear program – no discrete variables

– Comparison with NETL/industry report


## Acknowledgements:

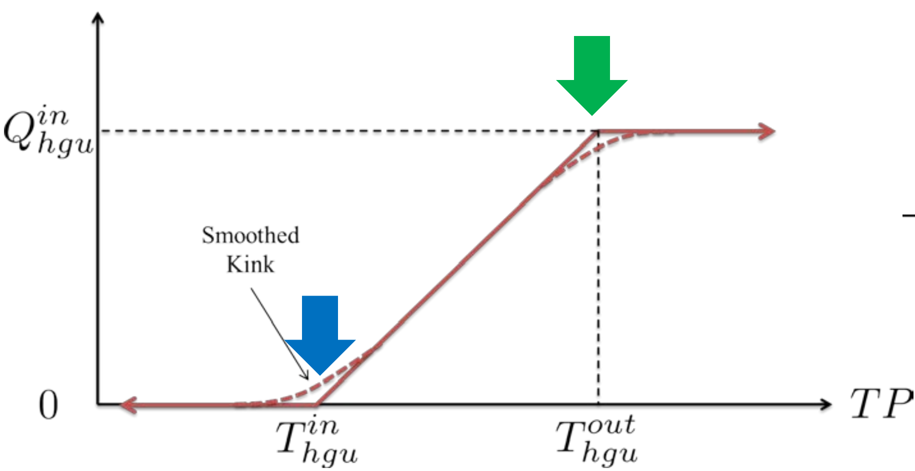



# Heat Integration Reformulation

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

**Consider contribution of single unit *hgu***

Integrated Heat from Heating Unit $hgu$




| | Heating Unit ($T^{in} \leq T^{out}$) | Cooling Unit ($T^{in} \geq T^{out}$) |
|---|---|---|
| $T_{cgu}^{in} = TP_{s^P}$ | 0 | $Q_{cgu}^{out}$ |
| $T_{hgu}^{out} = TP_{s^P}$ | $Q_{hgu}^{in}$ | 0 |

$$Q_{s^p}^{Ac} = \sum_{hgu^1} FCp_{hgu^1}[\tilde{\max}(T_{hgu^1}^{out} - TP_{s^p} + \Delta T_{min}) - \tilde{\max}(T_{hgu^1}^{in} - TP_{s^p} + \Delta T_{min})]$$

$$+ \sum_{hgu^2} Q_{cgu^2}^{in} + \sum_{hgu^3} 0$$