Equation Oriented Coal Oxycombustion Flowsheet Optimization

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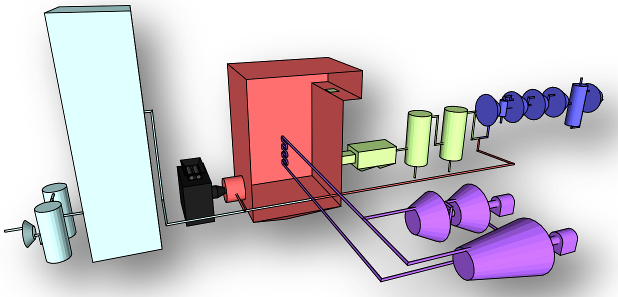
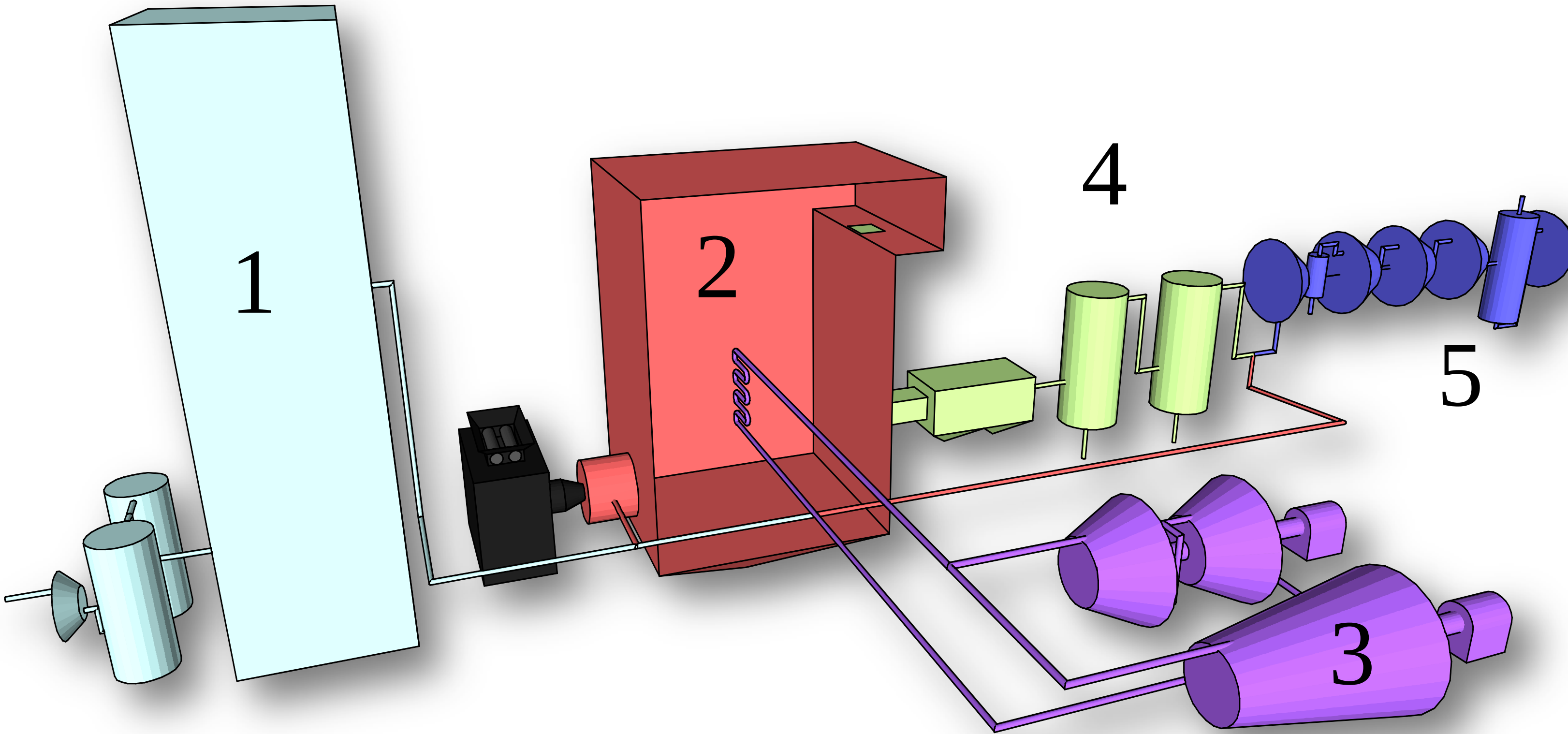


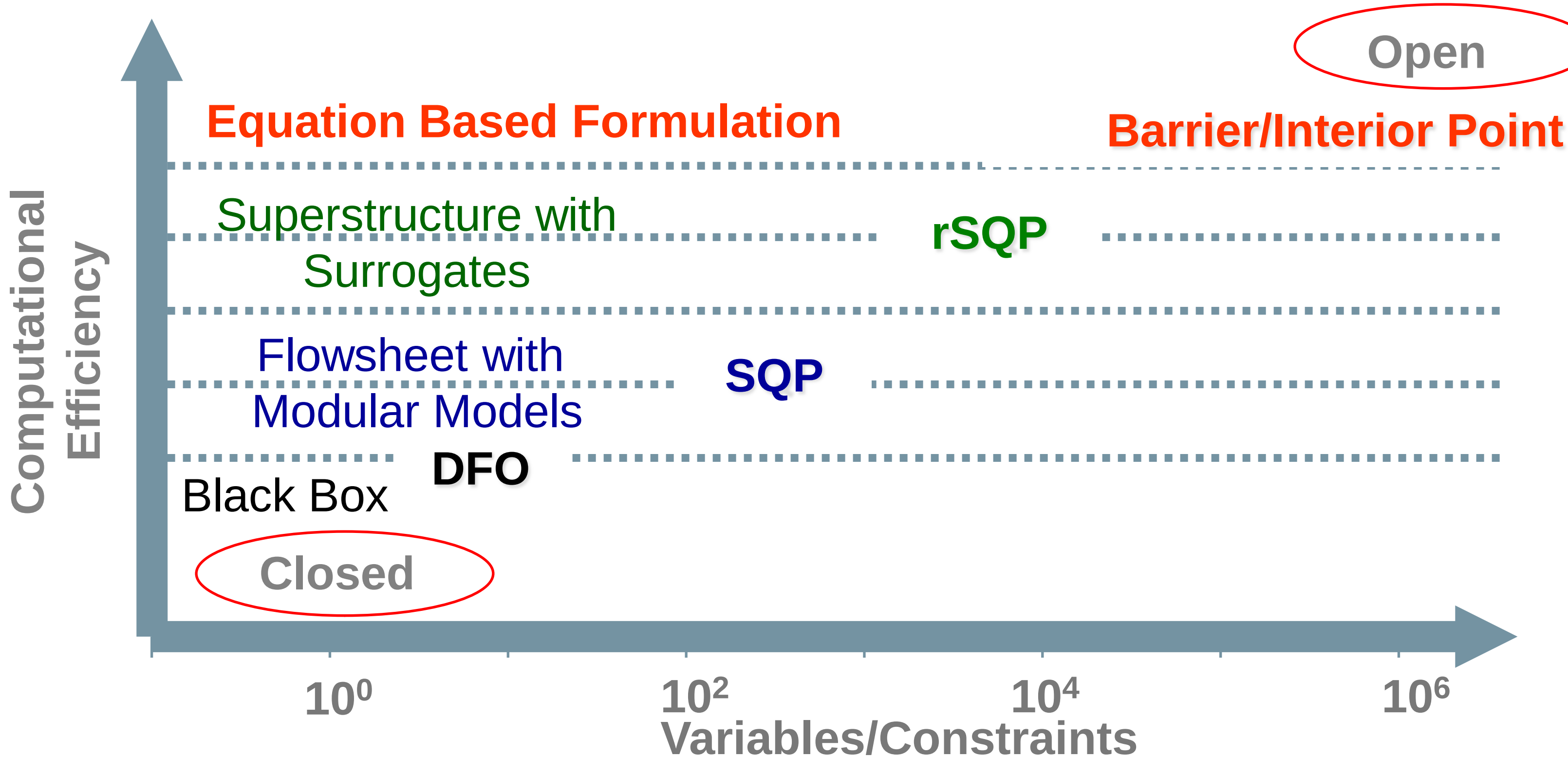
Oxycombustion Flowsheet



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

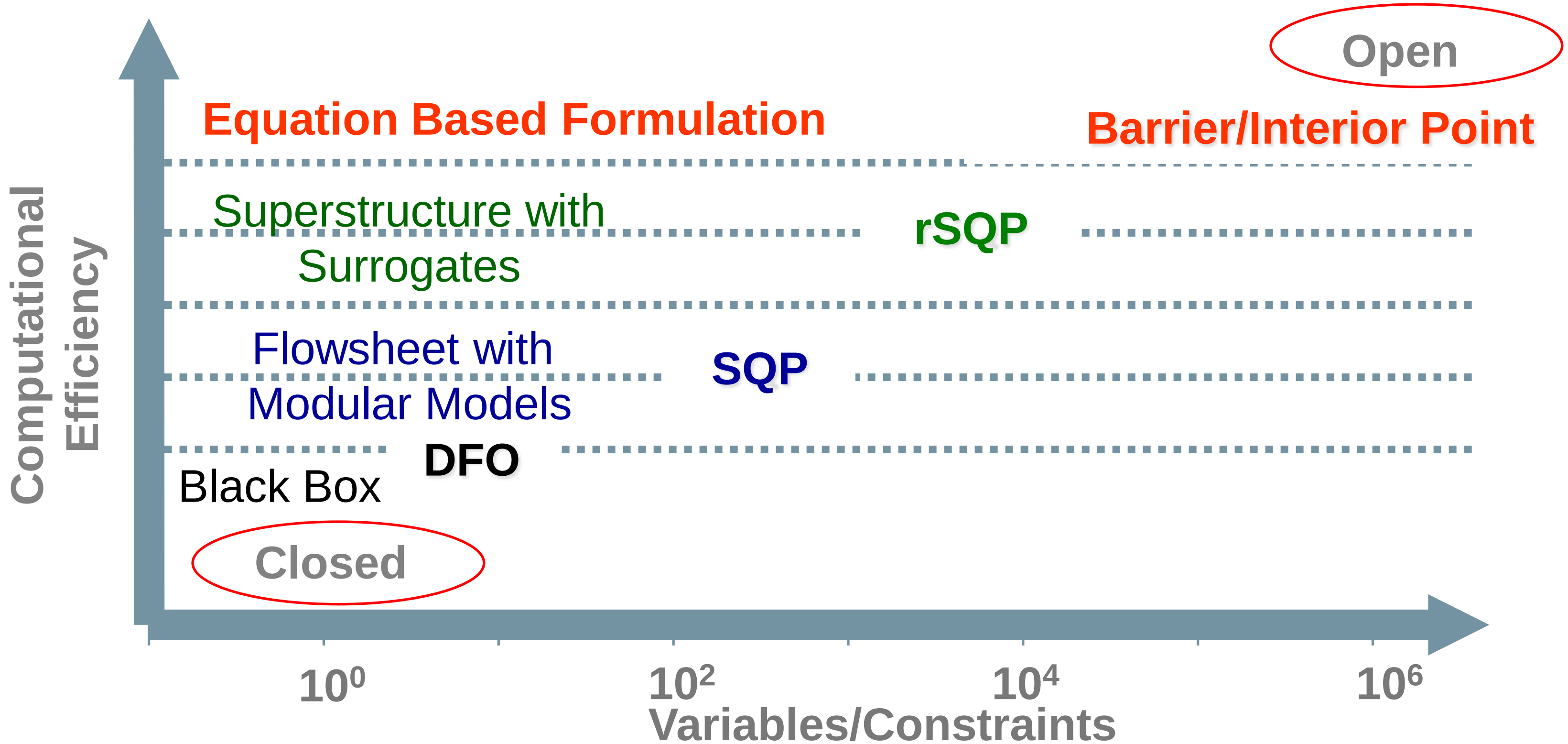
Project Objective

Tightly coupled subsystems → Optimize using detailed models



Project Objective

Develop an **equation oriented** framework to optimize an entire coal oxycombustion flowsheet.



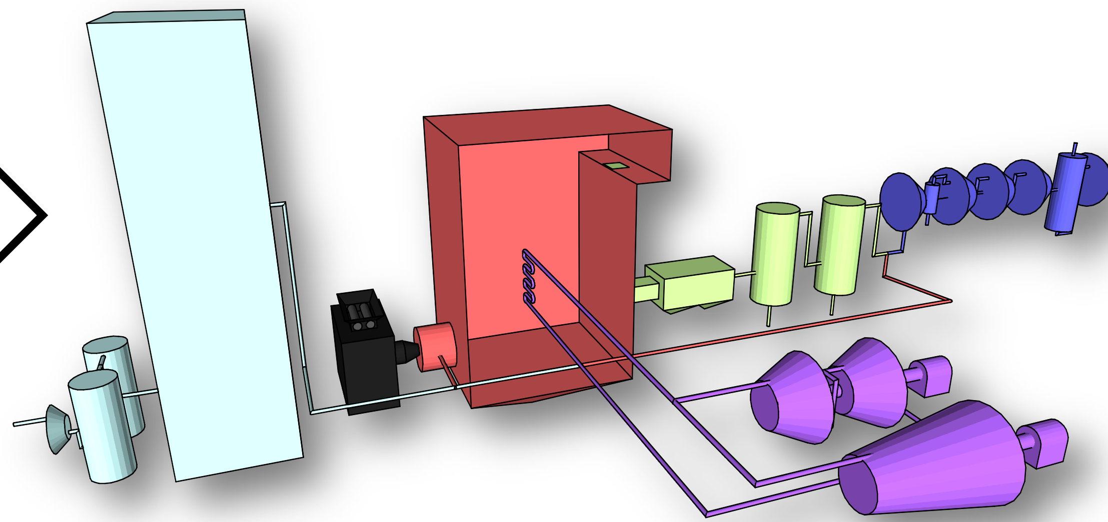
Project Objective

Goal: Consider complex trade-offs in flowsheet.

What is the optimal flue gas recycle ratio?

Are there heat integration synergies with the ASU & CPU?

Start with cryogenic ASU



Cryogenic Air Separation

Low pressure section

<u>Boiling Points @ 1 atm</u>

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

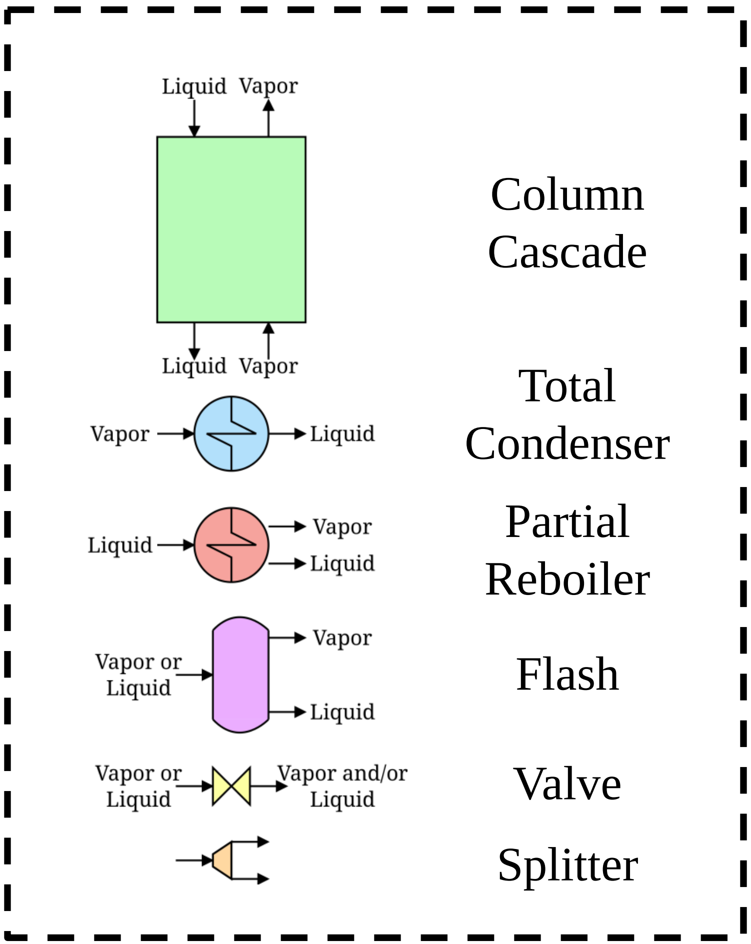
Photo from wikipedia.org

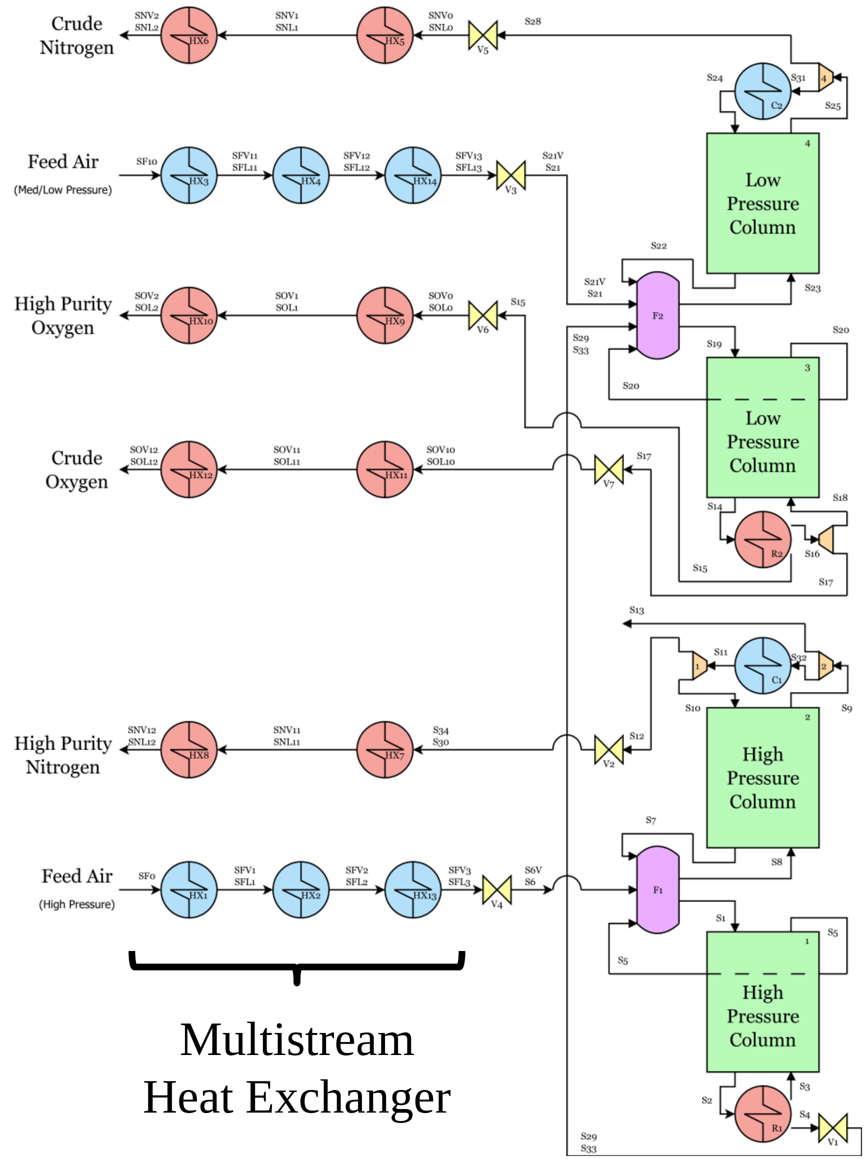
High pressure section

Multicomponent distillation with tight heat integration

Challenging to systematically optimize in AspenPlus.

Double Column Configuration





ASU: Optimization Formulation

min ASU Compression Energy (kWh / kg O_2 product)

s.t. Thermodynamics Module

Unit Operation Models

Cascade Model

Flowsheet Connectivity

Heat Integration

O_2 product purity $\geq$ 90 mol%

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

Cubic Equations of State

$$f(Z_s) = Z_s^3 - Z_s^2 + (A_s - B_s - B_s^2)Z_s - A_sB_s = 0$$

Examples: Peng-Robinson, Soave-Redlich-Kwong

Up to 3 Roots?!?

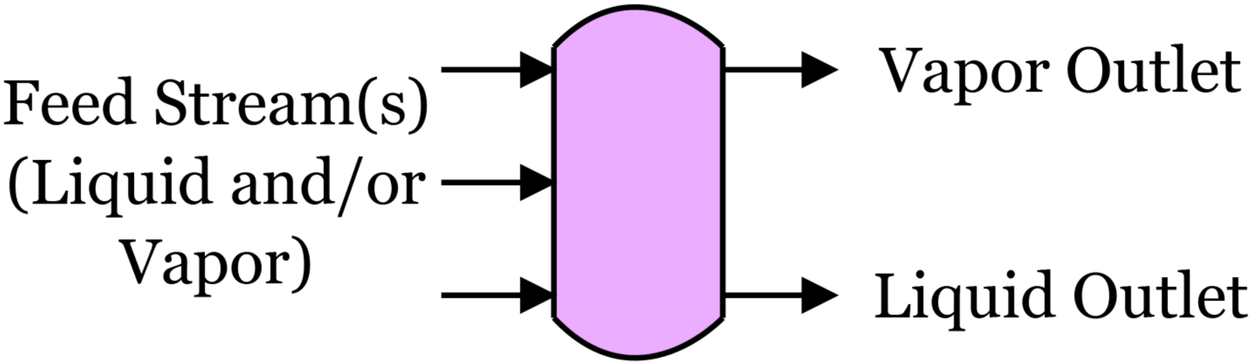
Phase	CEOS	1st Derivative	2nd Derivative
Liquid	$f(Z_s) = 0$	$f'(Z_s) \geq 0$	$f''(Z_s) \leq 0$
Vapor	$f(Z_s) = 0$	$f'(Z_s) \geq 0$	$f''(Z_s) \geq 0$

$$f'(Z_s) = 3(Z_s)^2 - 2Z_s + (A_s - B_s - (B_s)^2) \geq 0$$

$$f''(Z_s) = 6Z_s - 2 \geq 0, \quad s \in \{Vapor\ Streams\}$$

$$f''(Z_s) = 6Z_s - 2 \leq 0, \quad s \in \{Liquid\ Streams\}$$

Flash Example & Thermodynamics



Material Balance

$$\sum F_c^{in} = F_c^v + F_c^l$$

Energy Balance

$$\sum F^{in} H^{in} = F^v H^v + F^l H^l$$

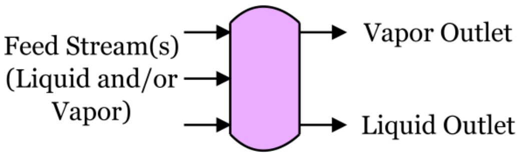
Phase Equilibrium

$$y_c^v = K_c x_c^l$$

$$K_c = \frac{\phi_c^l}{\phi_c^v}$$

Phase Disappearance

Thermodynamics must be relaxed when a phase disappears.



Thermodynamics Relaxation

$$f''(Z^l) \leq M \ \sigma^l$$
$$f''(Z^v) \geq -M \ \sigma^v$$

Complementarity Condition

$$0 \leq F^v \perp \sigma^v \geq 0$$
$$0 \leq F^l \perp \sigma^l \geq 0$$

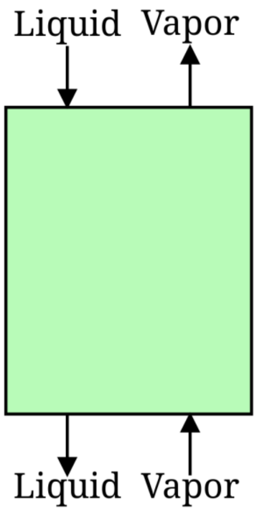
Phase Equilibrium

$$y_c^v = \beta K_c x_c^l$$
$$K_c = \frac{\phi_c^l}{\phi_c^v}$$

Equilibrium Relaxation

$$-\sigma^l \leq \beta - 1$$
$$\beta - 1 \leq \sigma^v$$

Cascade Model



- Group method
  - Continuous number of ideal stages
  - Based on work of Kremser and Edmister
  - Requires specification of stripping and absorbing section
- Modifications for distillation:
  - Exit streams at dew/bubble point
  - Decrease vapor at bottom = increase liquid at top

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

ASU: Heat Integration Model

Based on work of Duran & Grossmann (1986)

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

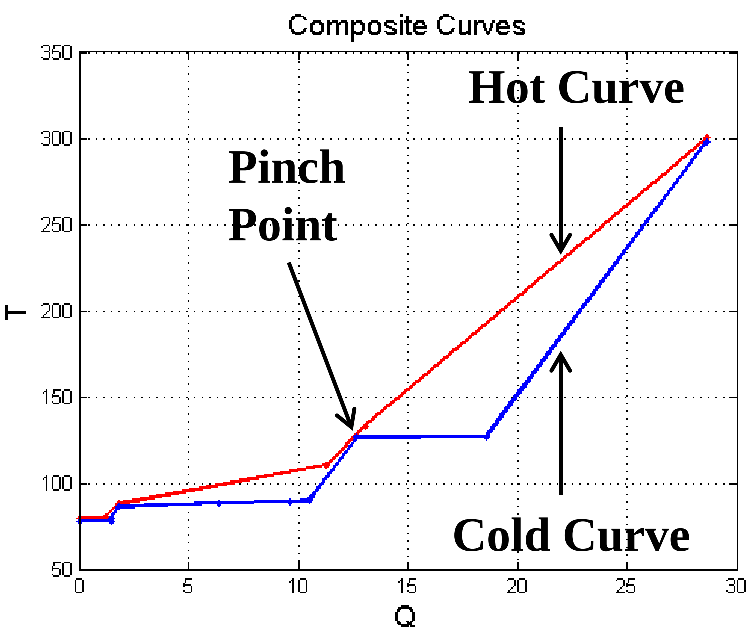
$$QA_H^p = \sum_{i \in \{Hot\}} FCp_i [\tilde{\max}(T_i^{in} - T^p) - \tilde{\max}(T_i^{out} - T^p)]$$

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

Utility calculations

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

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



Implementation Details

- Medium-size non-convex problem
  - 4418 variables
  - 4586 constraints

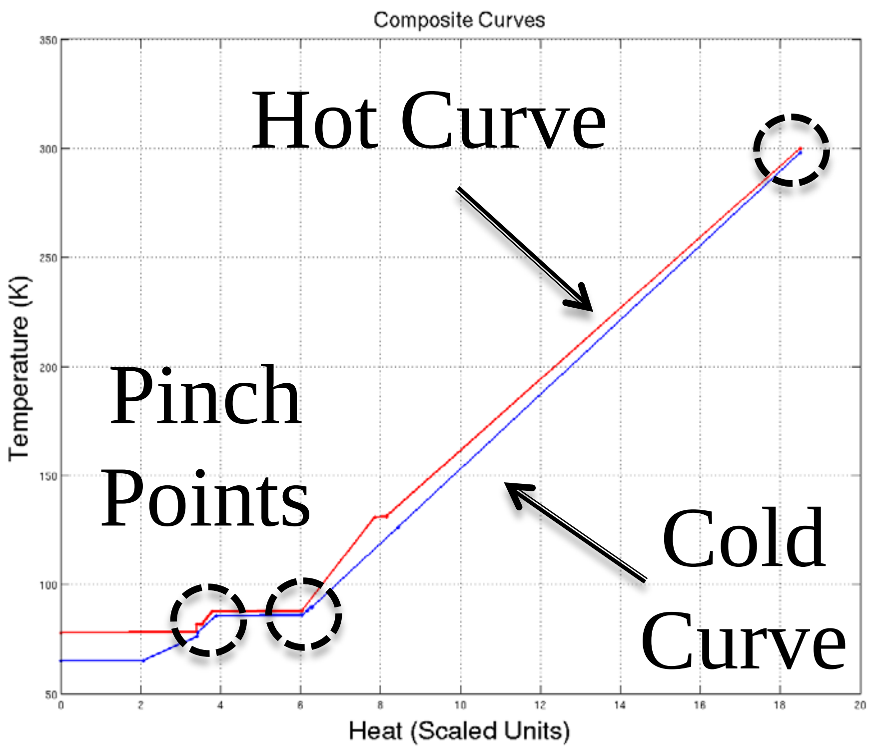
- Automated initialization procedure

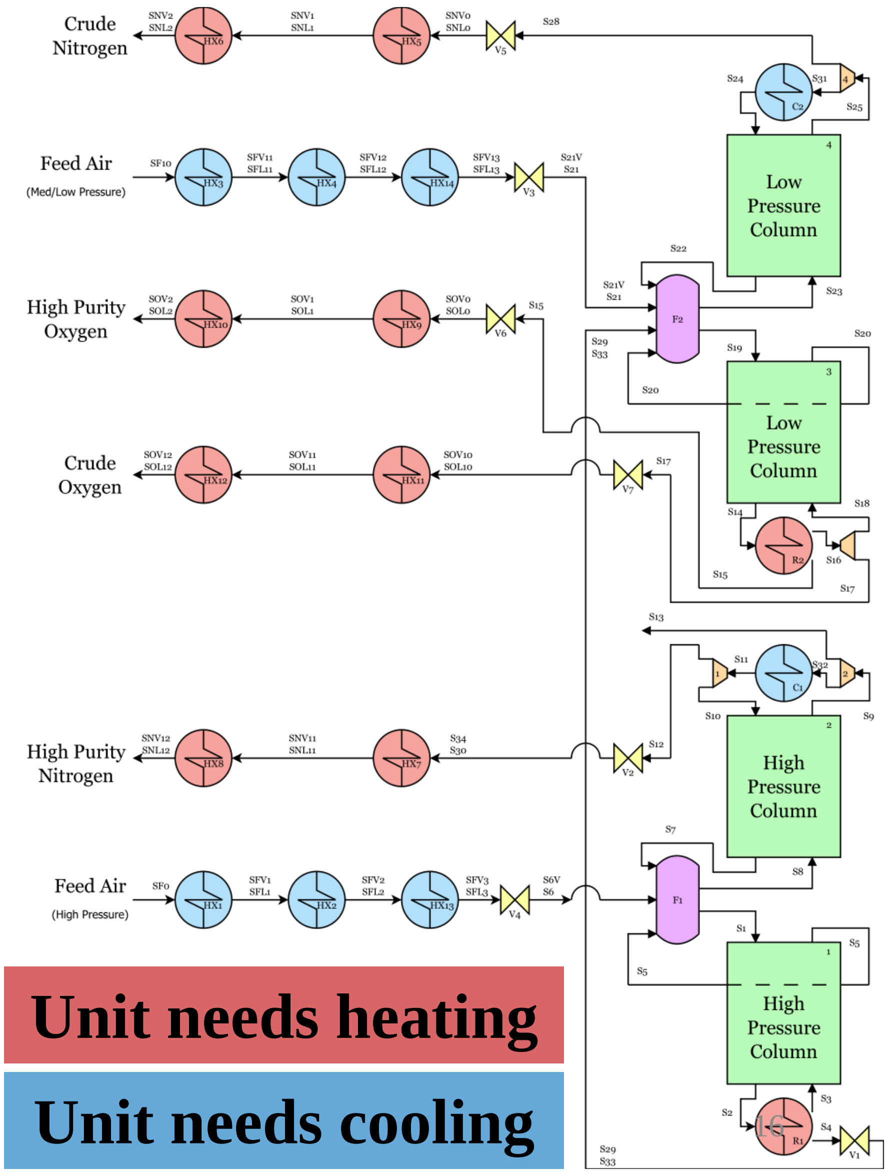
- Solved using **CONOPT3** in GAMS (General Algebraic Modeling System)
  - **3 minutes** with an Intel i7 processor

Results Summary for 90 mol% O_2

- Energy usage: **0.17** kWh/kg O_2
  typical designs: ~**0.22** kWh/kg O_2
- Low pressure column (LPC): **19 stages**
  High pressure column (HPC): **11 stages**
- LPC: **1.0 bar** literature: **1.7 – 4.3 atm**
  HPC: **2.5 bar** literature: **6.8 – 13.5 atm**
- Only ¼ of feed air sent to HPC
  typical designs: **all**

Heat Integration Results



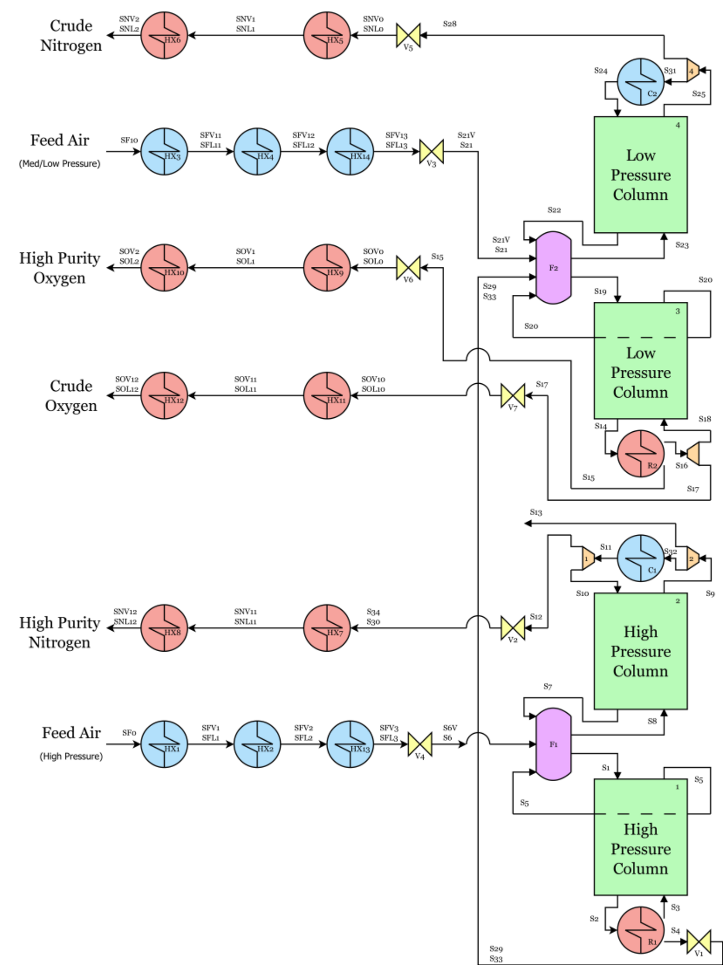


No external cooling or heating required

Future ASU Work

- Explore alternate ASU configurations and applications
  - Elevated pressure ASU?
  - Side draws?

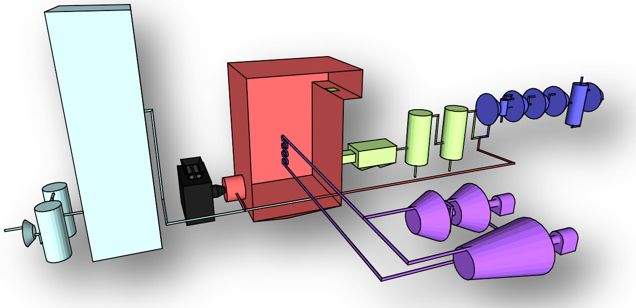
- Model capital costs and re-optimize



Future Flowsheet Work

- Integrate ASU model with remaining flowsheet sections

- Explore potential heat integration synergies
  - ASU with post combustion cryogenics
  - ASU with compression train
  - Compression train with boiler
  - Feed water heater train design



Conclusions

Optimized ASU with equation-based model:

- Cubic equation of state with accurate derivatives
- Pinch location heat integration
- Pure nonlinear program – no discrete variables

Acknowledgements:

CCSI Carbon Capture Simulation Initiative

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