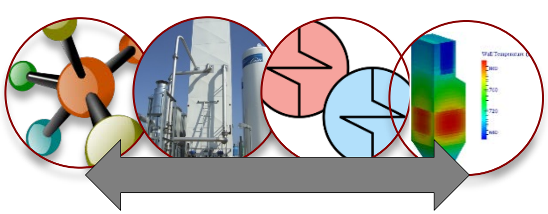
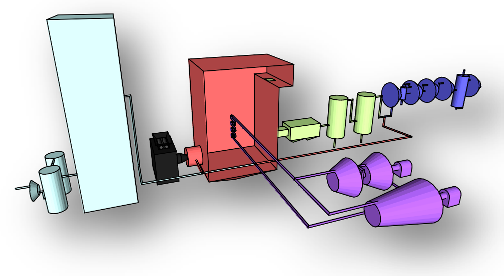
A Framework for Equation Based Optimization of Coal Oxycombustion Power Plants

Alex Dowling[1], **John Eason**[1], Jinliang Ma[2,3], David Miller[3] & Larry Biegler[1]

[1]Carnegie Mellon University
[2]URS Corporation
[3]National Energy Technology Laboratory



AIChE Annual Meeting
November 17th, 2014



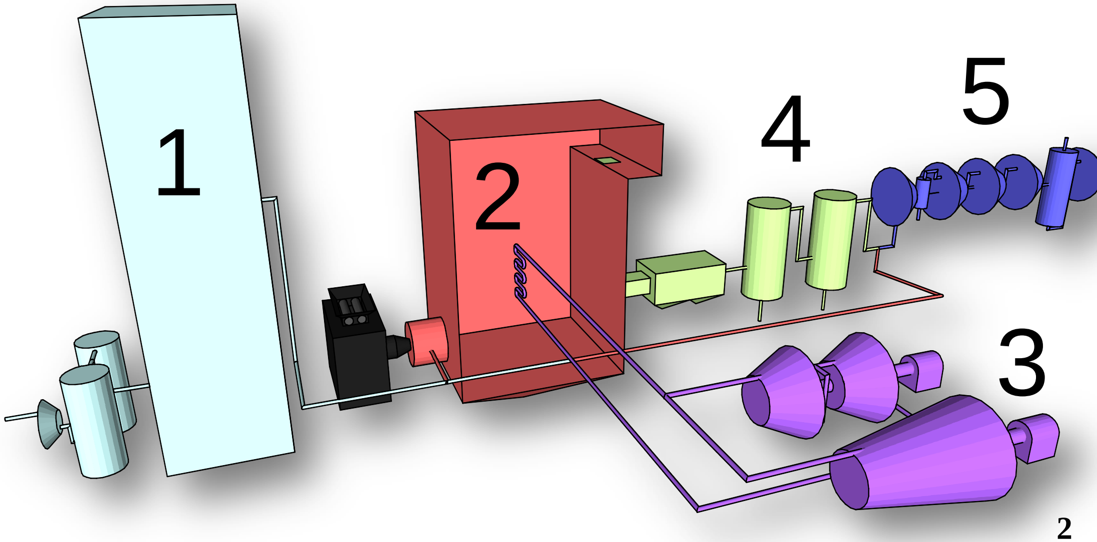
Motivation

Develop framework for full oxycombustion power plant optimization

- Minimize *cost of electricity* with carbon capture
- Comparison against mature technologies

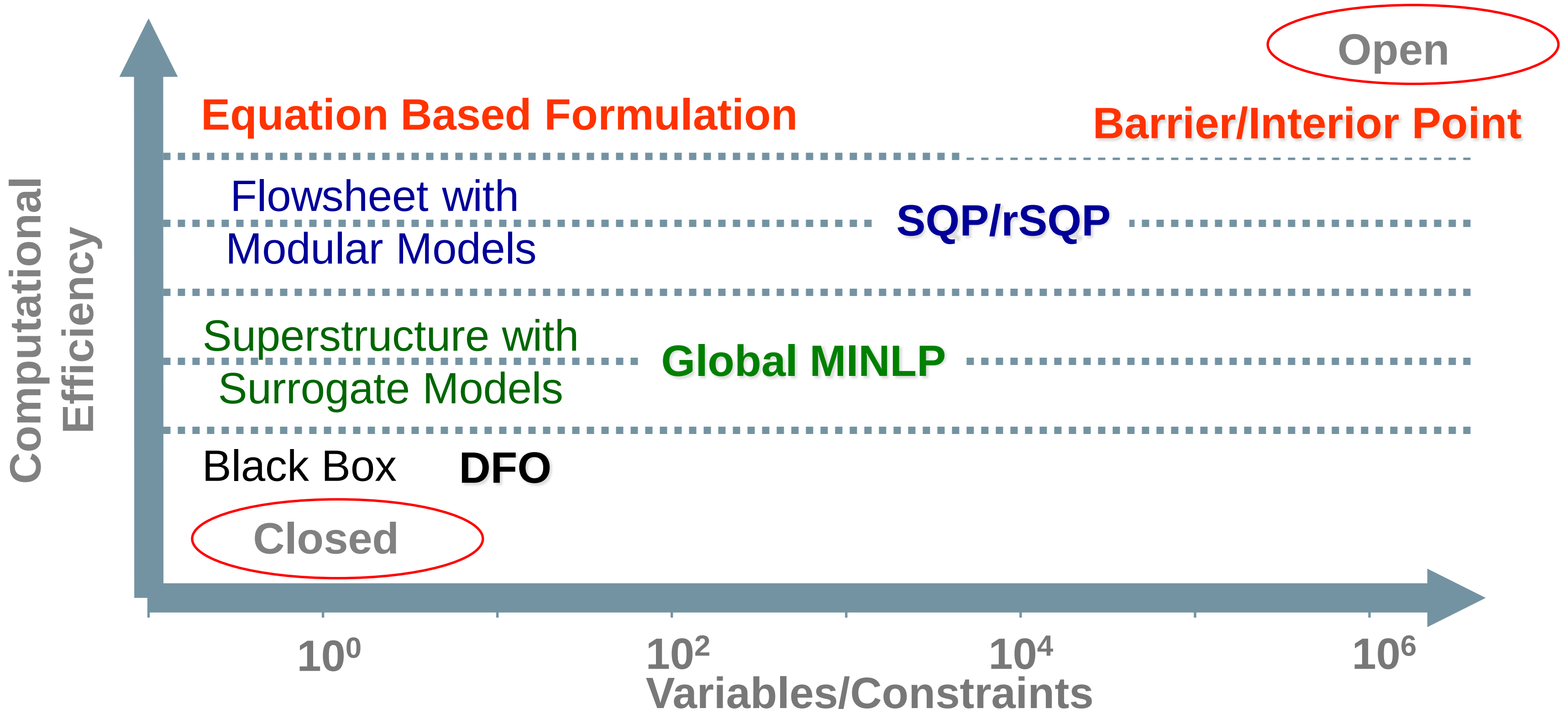
Oxycombustion Power Plant

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



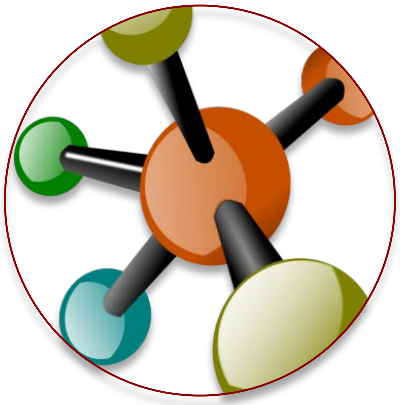
Methodology: Equation Oriented

Tightly coupled subsystems → Optimize using detailed models



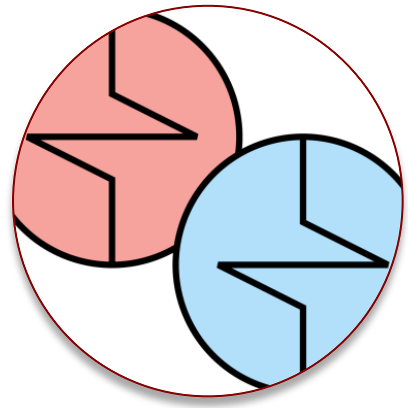
EO Benefit: Free linear sensitivity information at optimal solution

Framework for EO Flowsheet Optimization

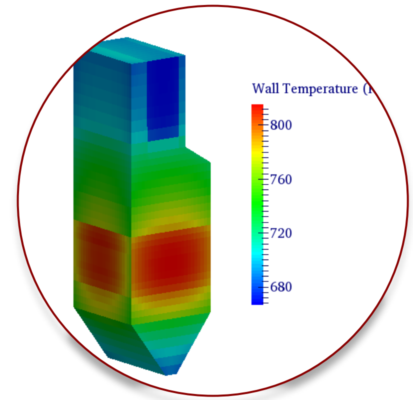


Thermodynamics
&
Flash Calculations

Distillation Cascades



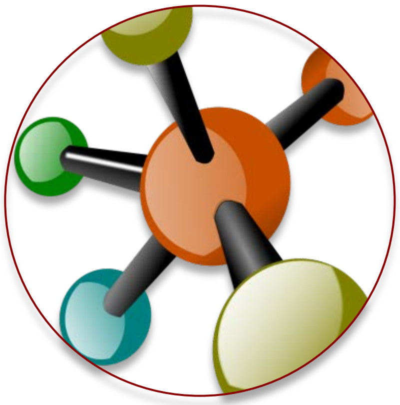
Heat Integration



Complex Reactors

Trust Region Optimization with Filter

Framework for EO Flowsheet Optimization



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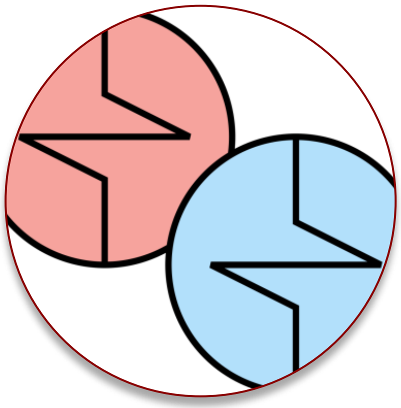

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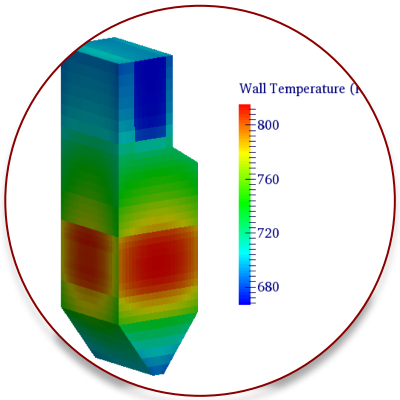
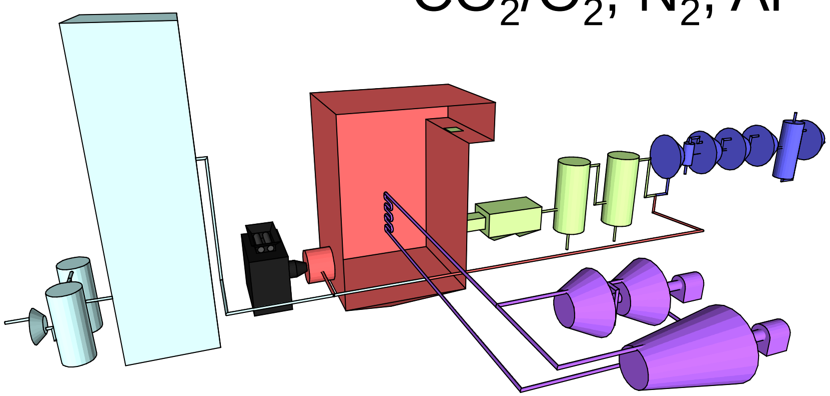


Complex Reactors

Trust Region Optimization with Filter

Cryogenic Separations

CO_2 Processing Unit
CO_2/O_2, N_2, Ar

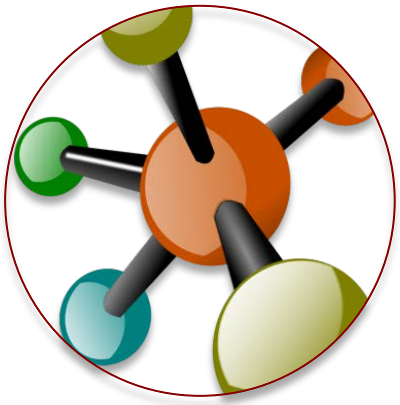


Air Separation Unit
O_2/N_2

- Minimized ASU specific energy
  - match industry designs, beats academic studies
- Investigated CPU energy/area tradeoffs
- Model structure will allow heat integration between subsystems

See companion presentations (627b) and (346a)

Framework for EO Flowsheet Optimization



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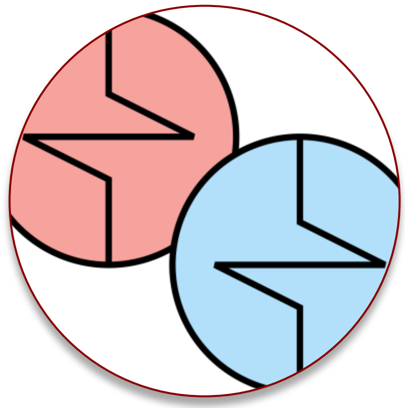
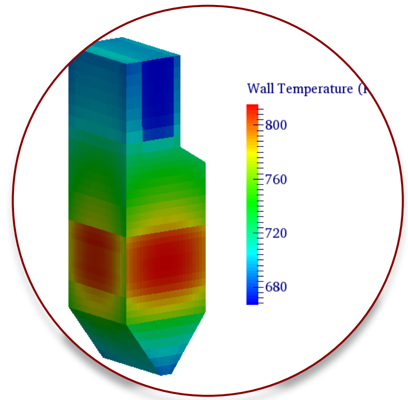


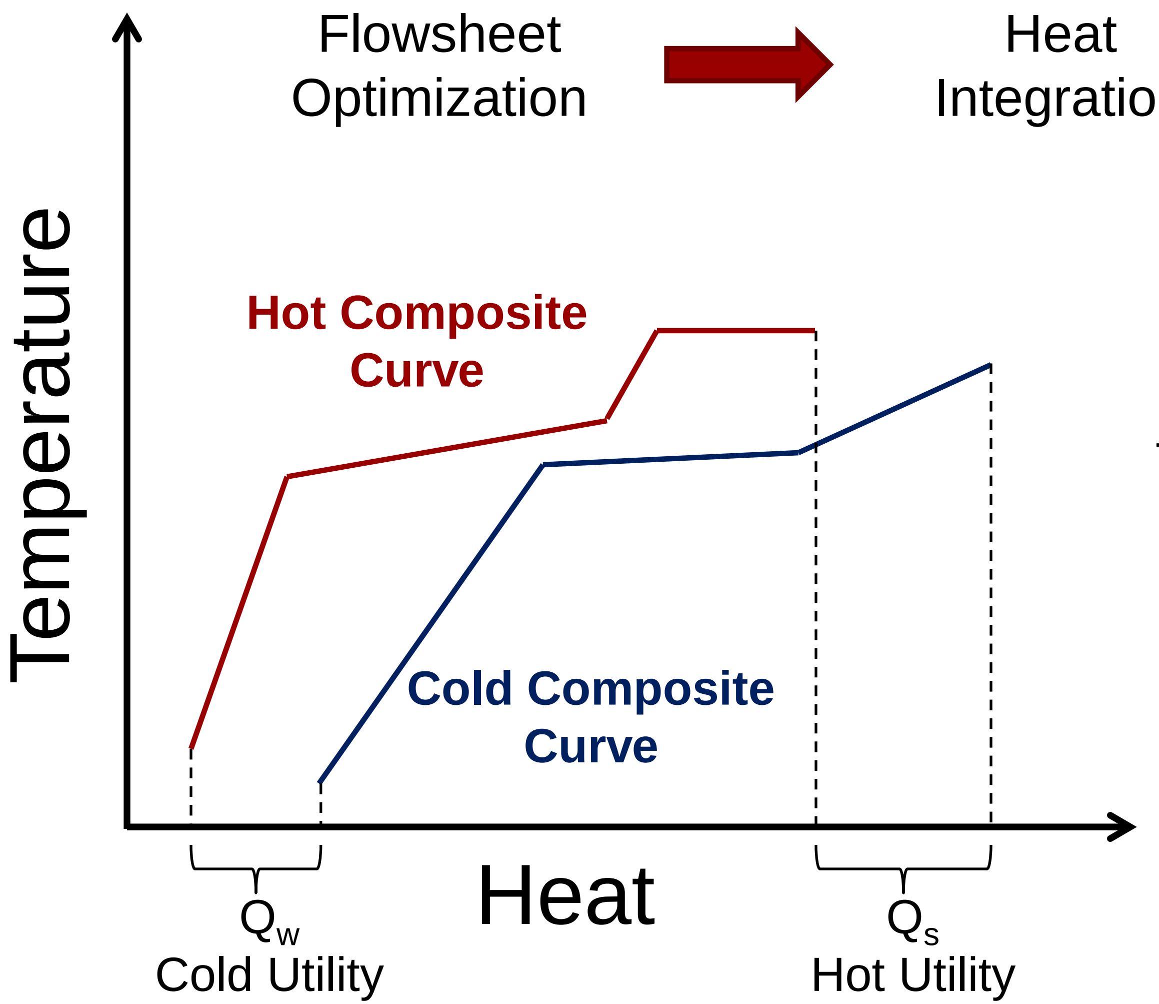
**Heat
Integration**



Complex
Reactors

Trust Region Optimization with Filter

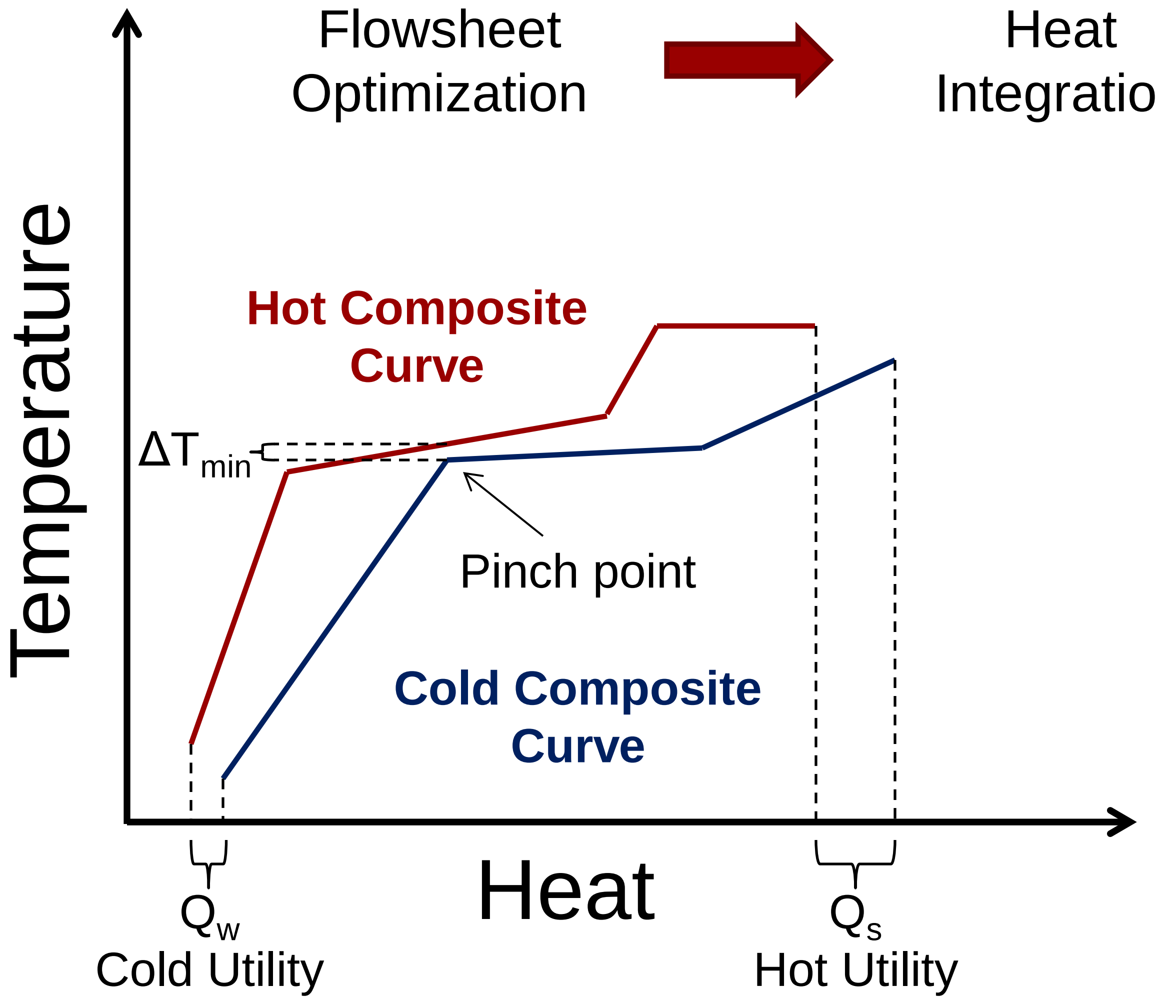
Pinch Based Heat Integration



Aggregate streams in temperature intervals where heating/cooling is required

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 ΔT_{min} is limiting → Minimum utilities

But composite curves depend on the stream data!

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.*

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

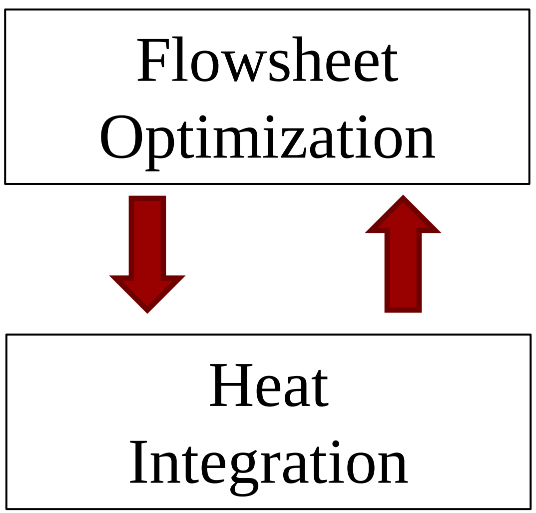
$$QA_H^p = \sum_{i \in \{Hot\}} FCp_i [\widetilde{\max}(T_i^{in} - T^p) - \widetilde{\max}(T_i^{out} - T^p)]$$

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

Utility calculations

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

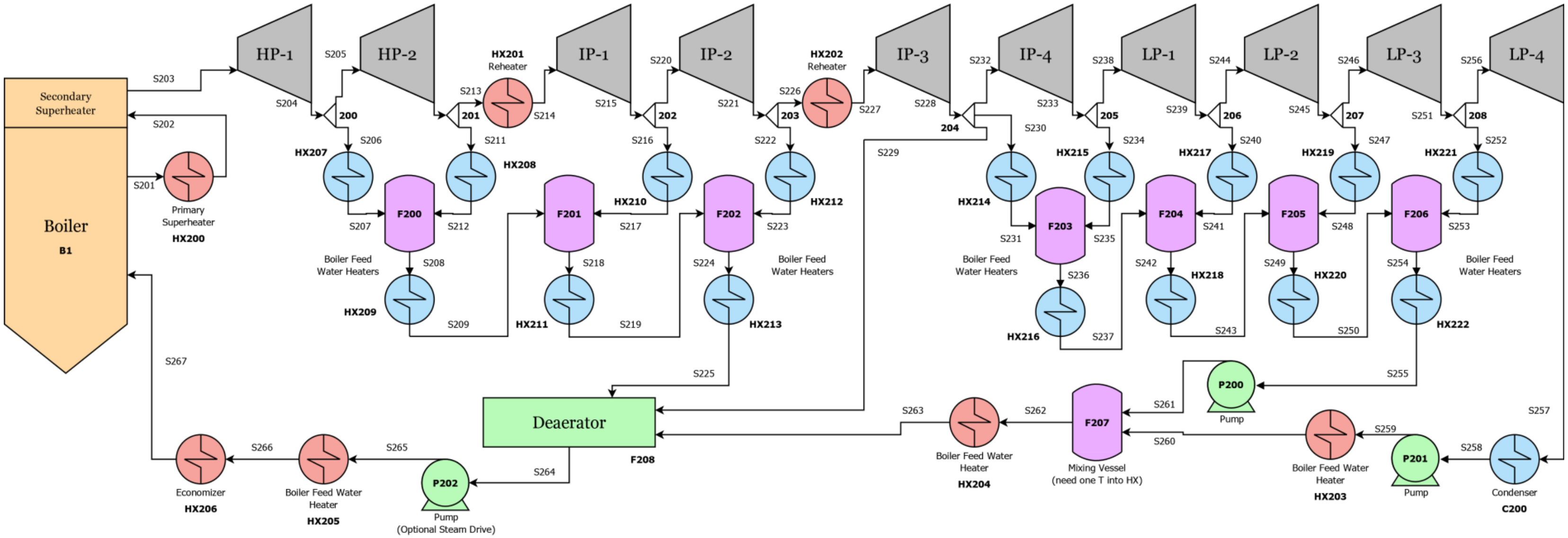
$$Q_w = Q_s + \sum_{j \in \{Cold\}} Q_j^{in} - \sum_{i \in \{Hot\}} Q_i^{out}$$



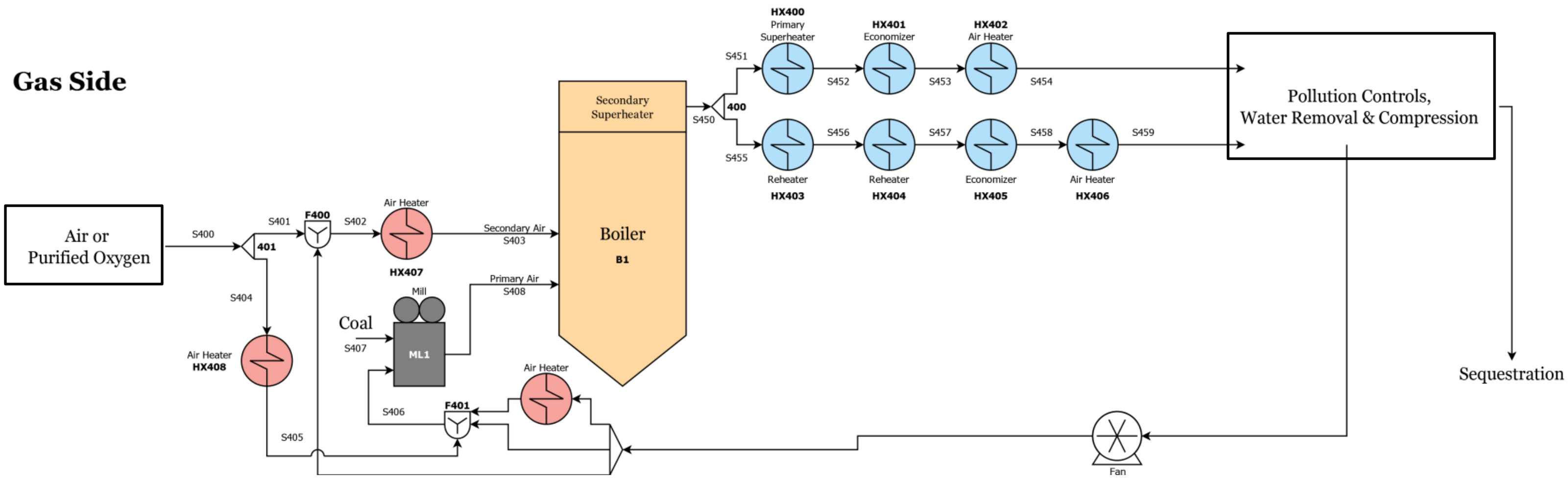
Duran, M. A., & Grossmann, I. E. (1986). Simultaneous optimization and heat integration of chemical processes. *AIChE Journal*, *32*(1), 123–138.

Steam Cycle Superstructure

Steam Side

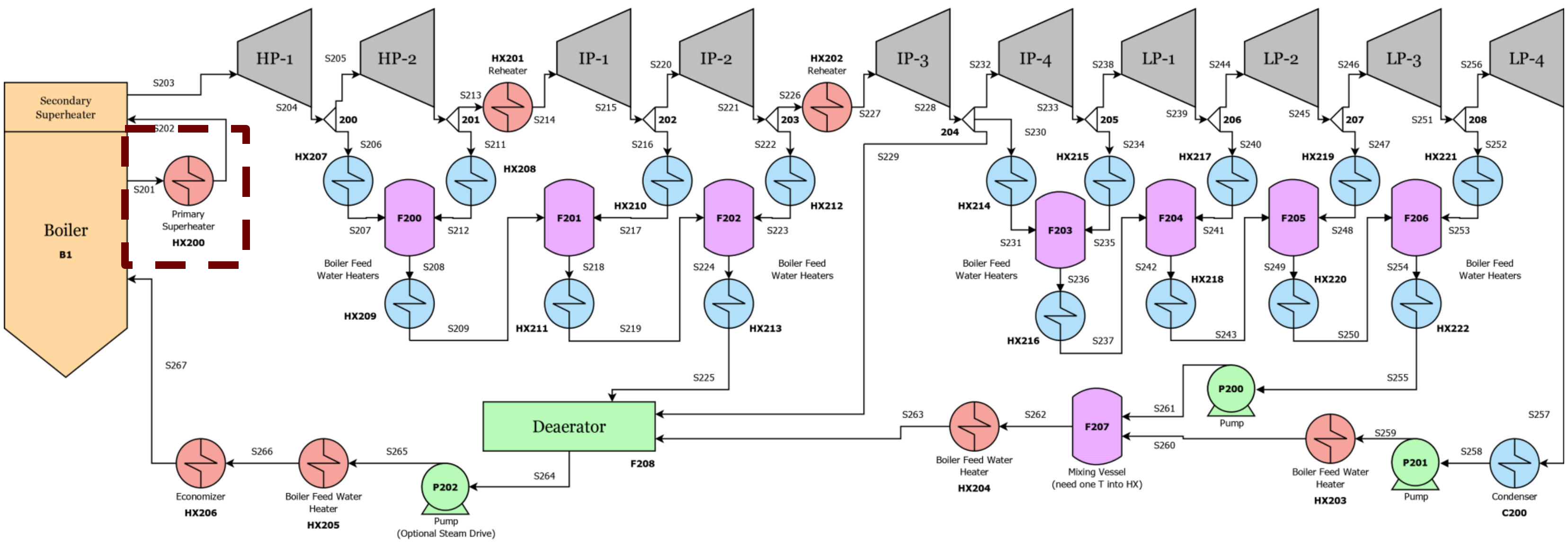


Gas Side

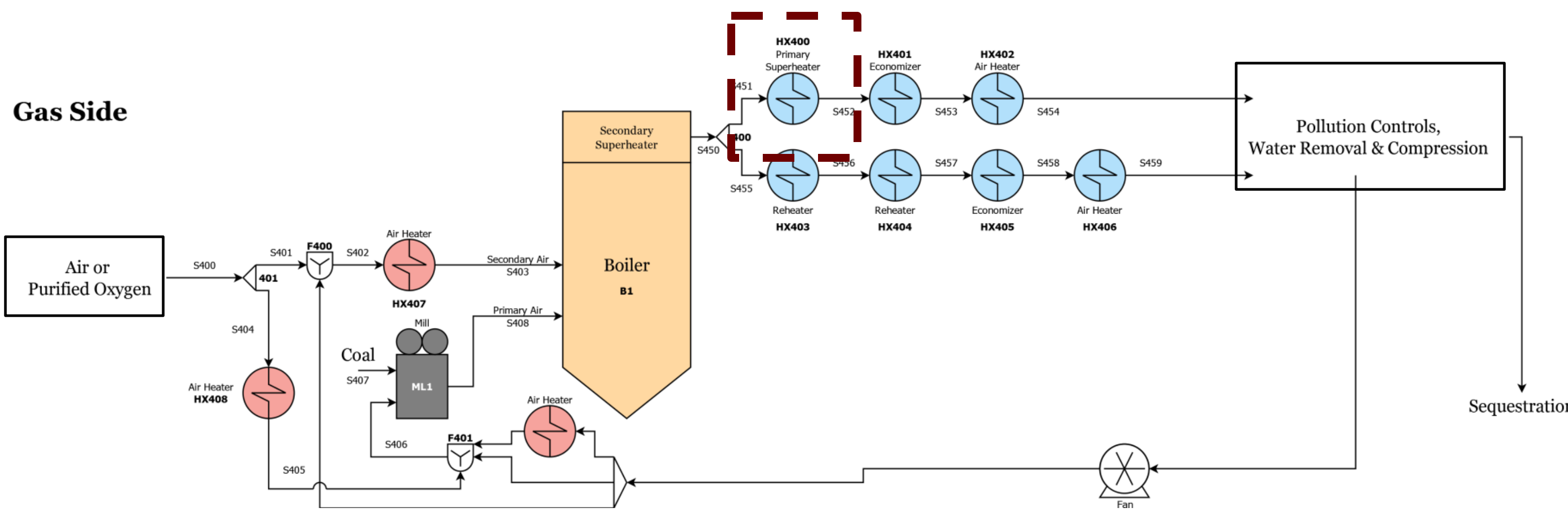


Steam Cycle & Heat Integration

Steam Side

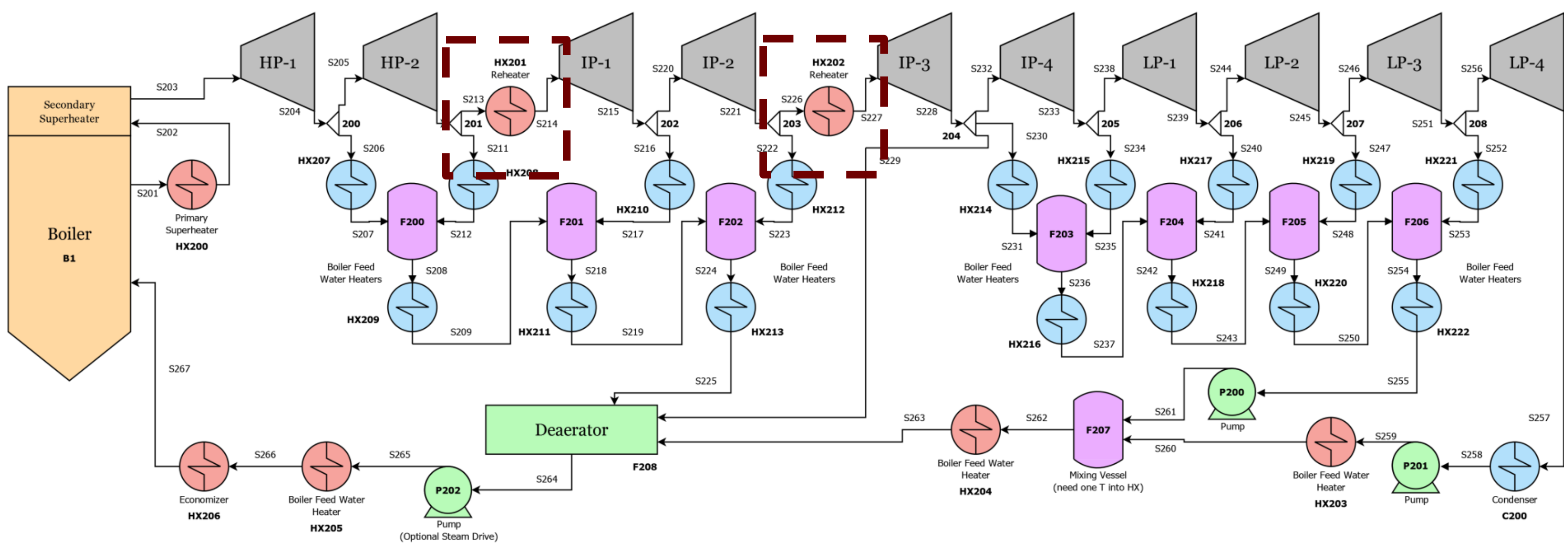


Gas Side

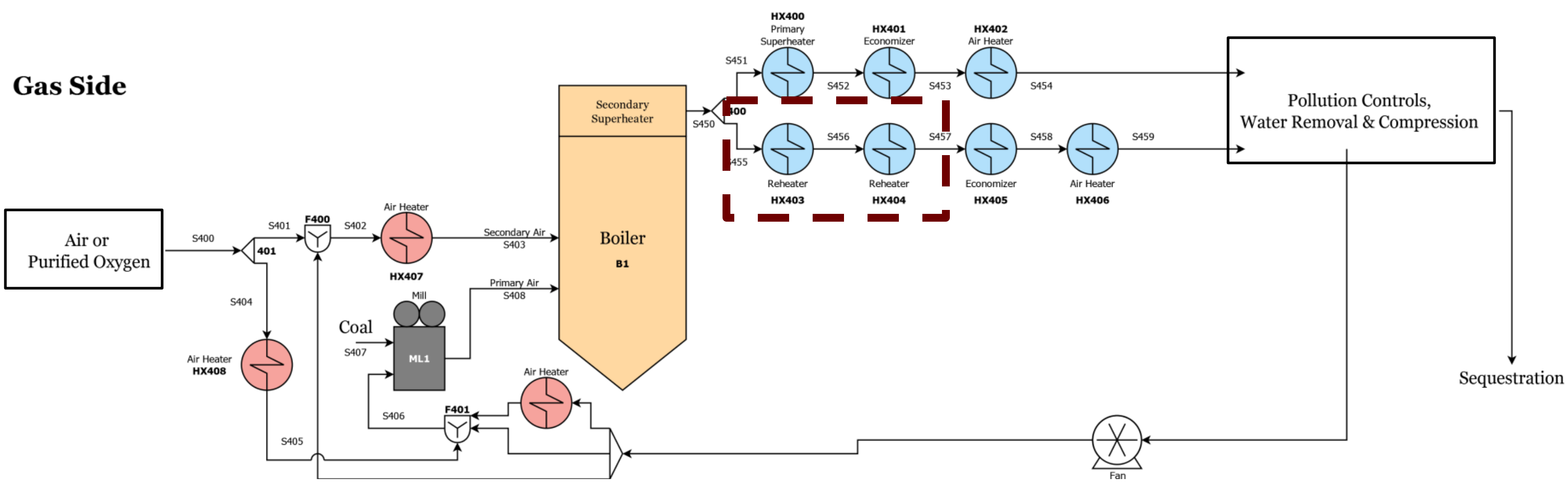


Steam Cycle & Heat Integration

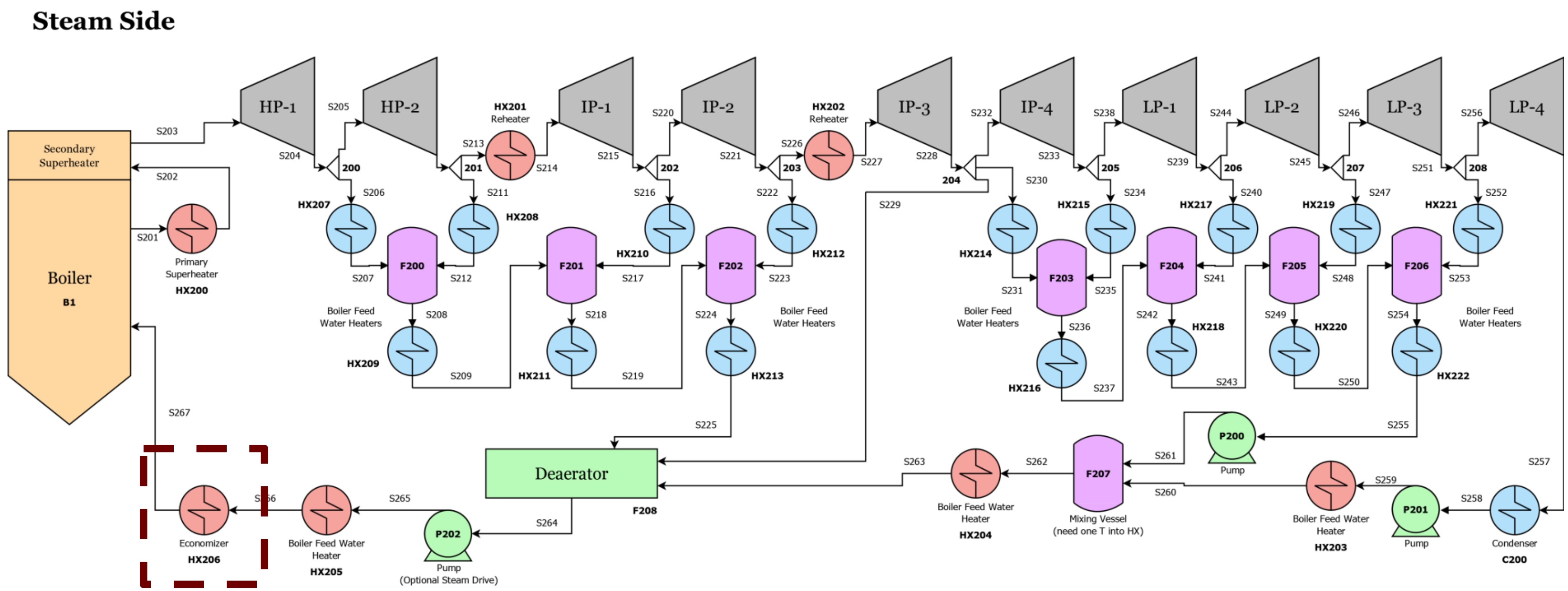
Steam Side

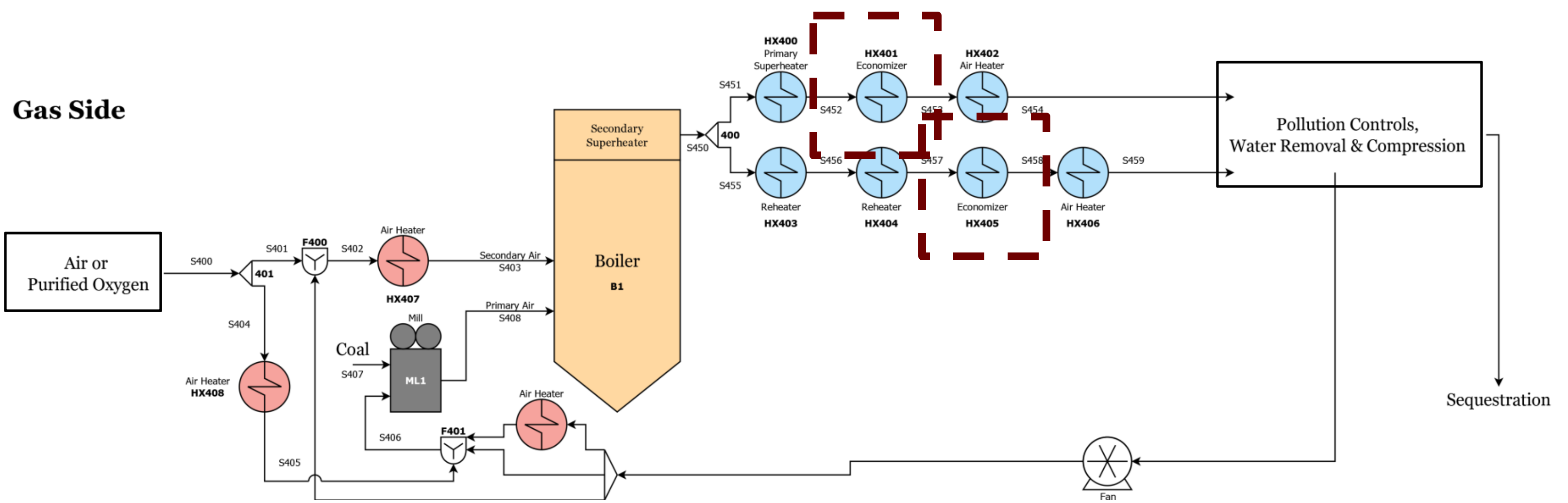


Gas Side



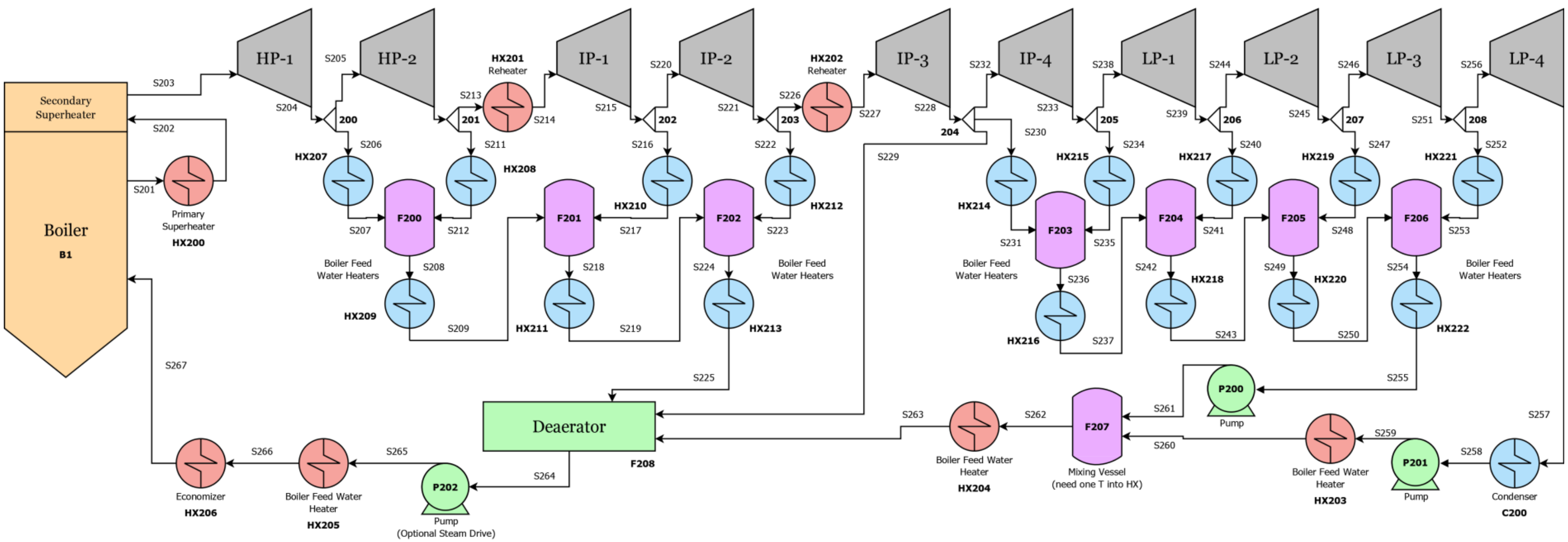
Steam Cycle & Heat Integration





Steam Cycle & Heat Integration

Steam Side



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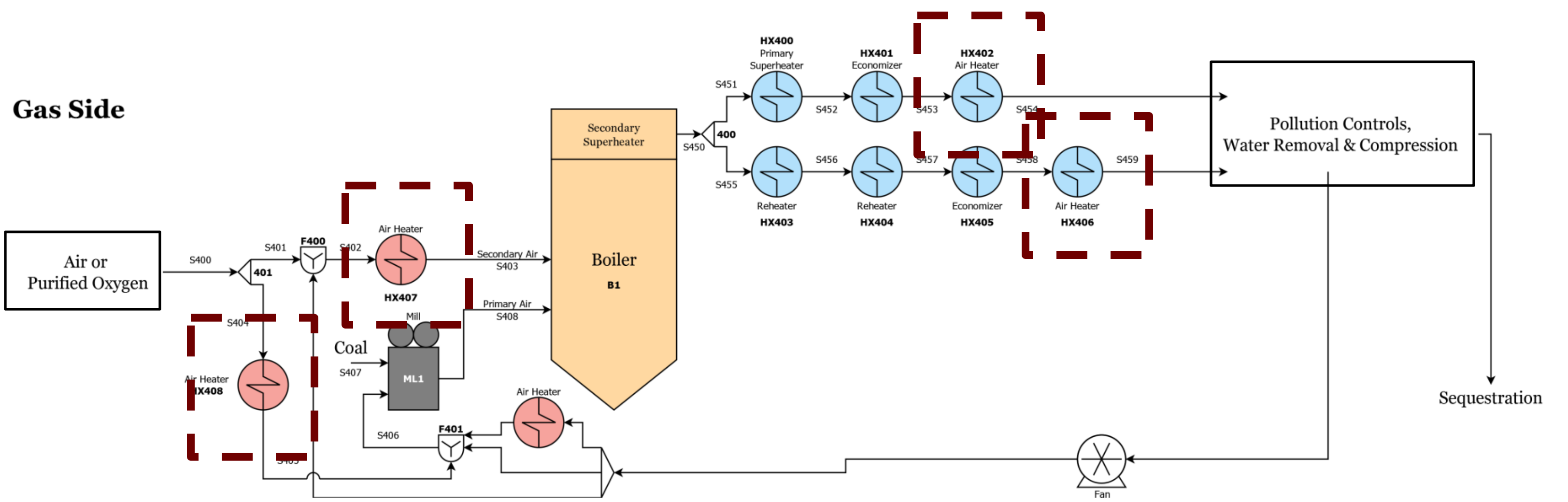
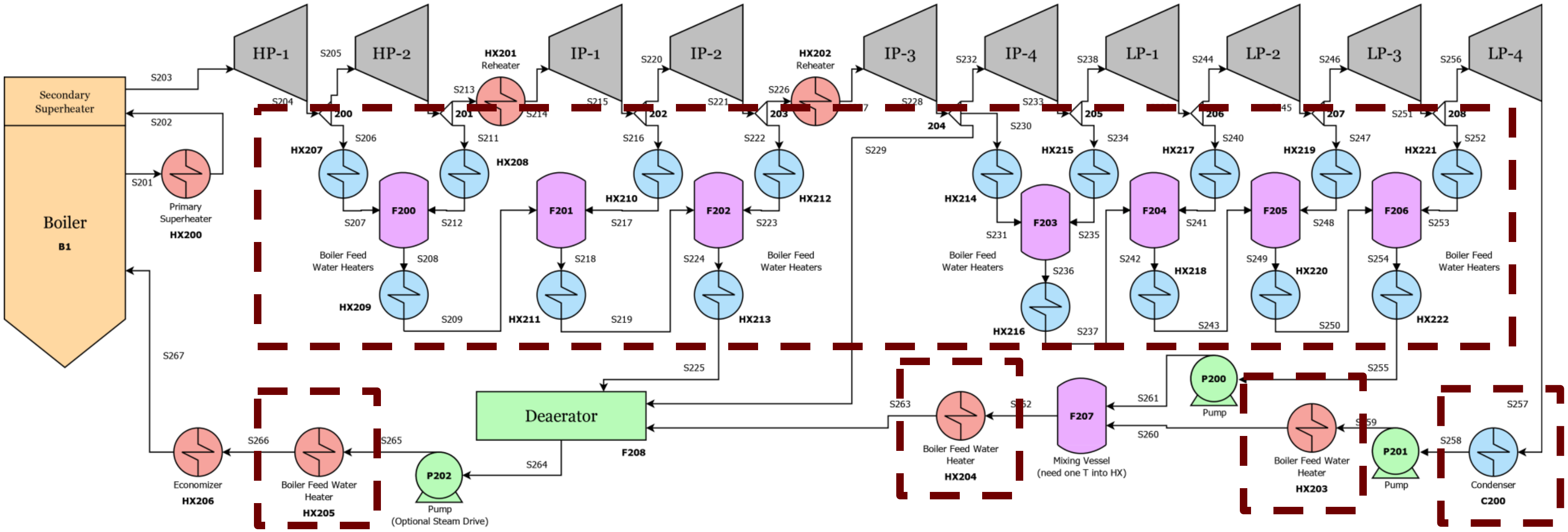


Steam Cycle & Heat Integration

Steam Side



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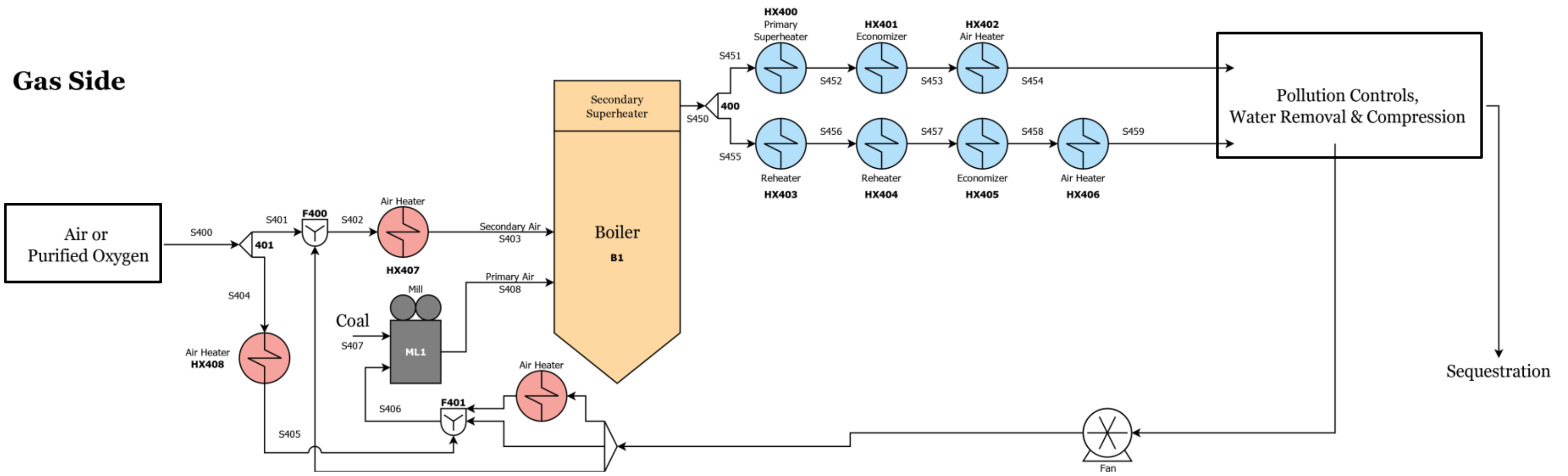
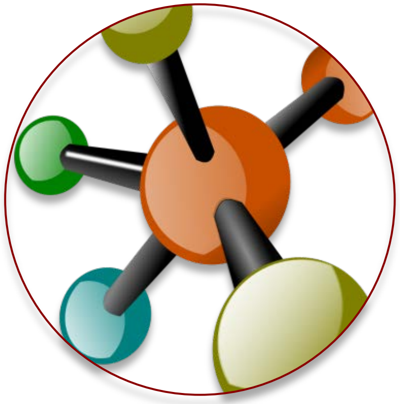


Framework for EO Flowsheet Optimization



Thermodynamics
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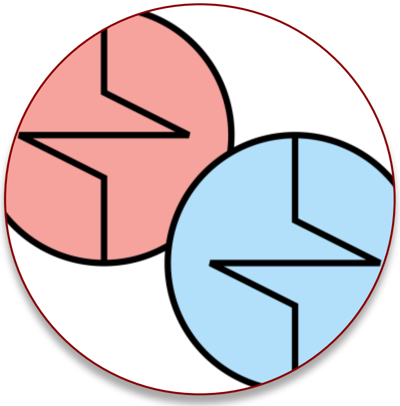
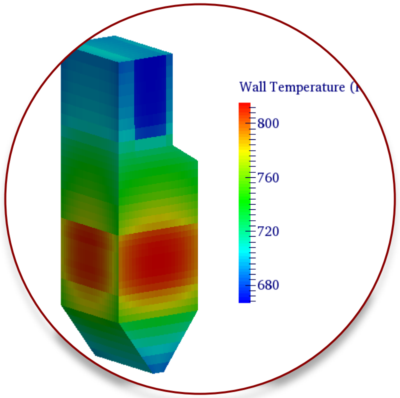


Heat Integration



Complex
Reactors

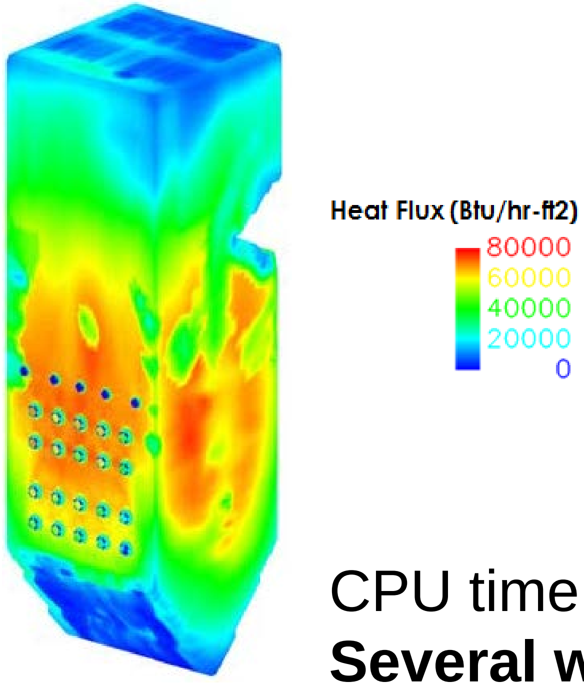
Trust Region Optimization with Filter

Detailed Boiler Models

Oxycombustion boilers are drastically different than air-fired boilers.

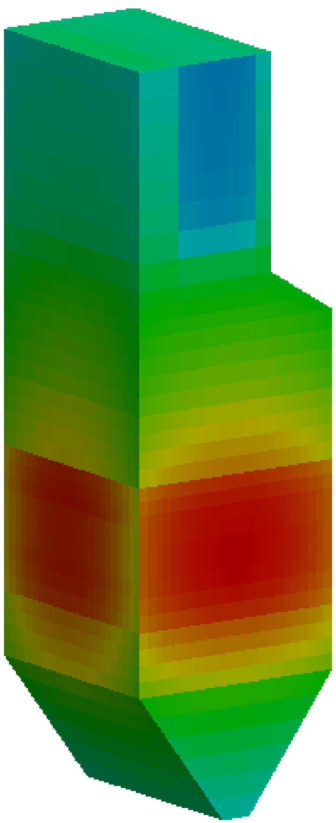
- Economics of the power generation process depend strongly on optimized boiler performance
- Radiative heat transfer dominates
  - O_2 and CO_2 different properties than air
- Need detailed first principles model

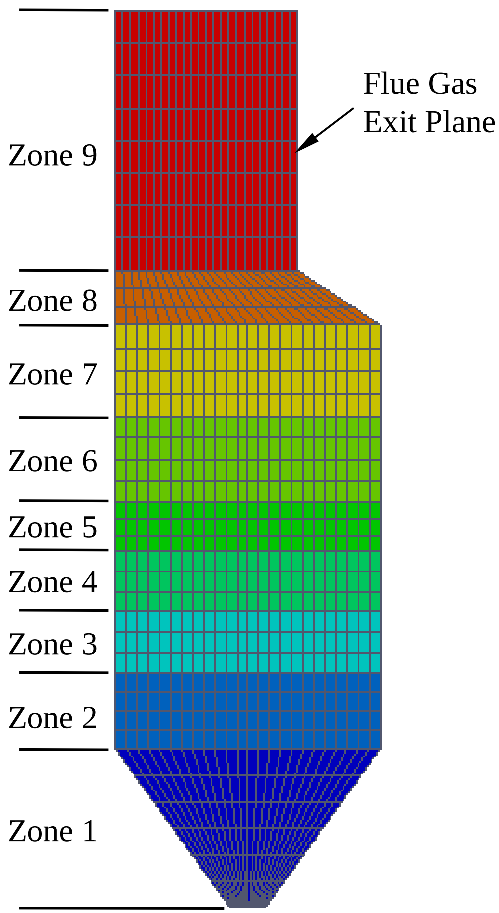
Traditional CFD (3D)



CPU time:
Several weeks

Hybrid 1D/3D Model



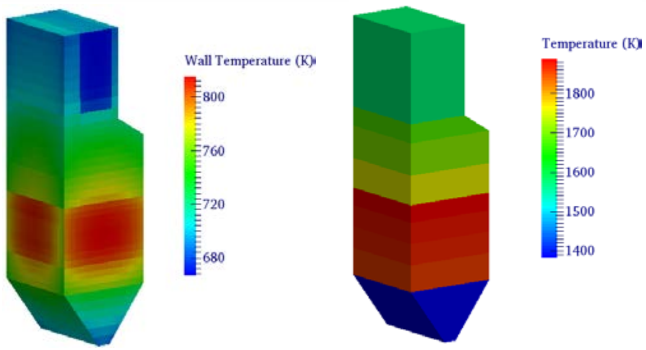


- 1D gas phases **zonal model**
  - Flow properties
  - Char reaction kinetics
  - Particle tracking
- 3D radiative heat transfer calculations
  - Solved using discrete ordinate method
  - Absorption efficiency based on Mie theory
- Run time: **72 CPU-seconds**

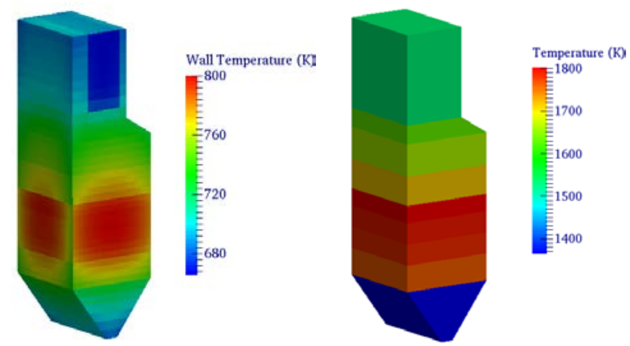
Ma, J., Dowling, A., Eason, J., Biegler, L., & Miller, D. (2014). Development of First Principle Boiler Model and Its Reduced Order Model for the Optimization of Oxy-combustion Power Generation System. In 39th International Technical Conference on Clean Coal & Fuel Systems.

Model Validation

Air-Firing



Oxy-Firing



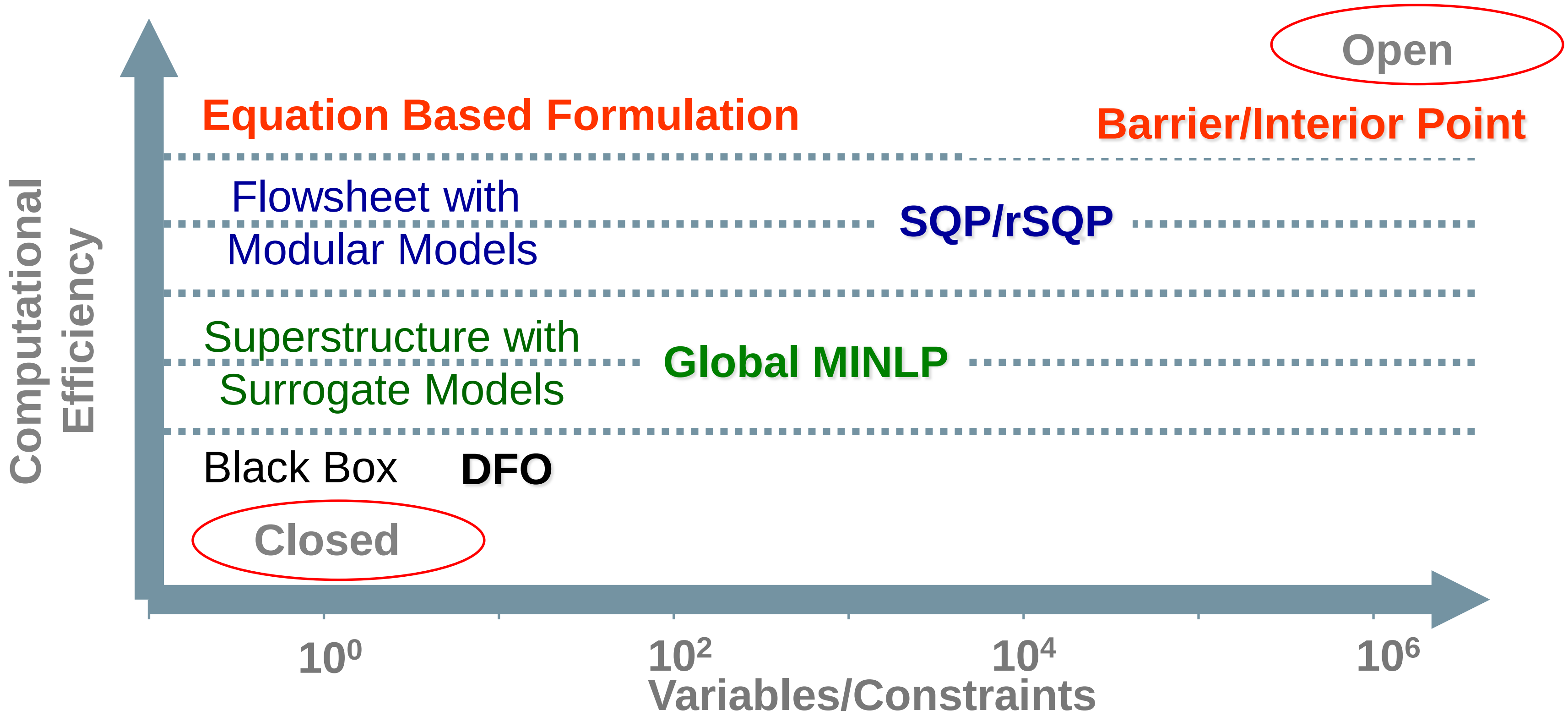
		Air-Firing			Oxy-Firing		
	Unit	**Hybrid Model**	**CFD Model**	**Error %**	**Hybrid Model**	**CFD Model**	**Error %**
Flue Gas Temp. at Horizontal Nose	K	1679	1674	**0.3%**	1628	1656	**1.7%**
Unburned Carbon	wt %	0.80	1.70		0.53	1.10	
Carbon Burnout	wt %	99.86	99.70	0.2%	99.90	99.80	0.1%
Heat Loss to Enclosure Wall *	W	4.108×10^8	4.36×10^8	5.8%	3.93×10^8	4.03×10^8	2.5%
Heat Loss to Platen SH Wall	W	1.018×10^8	1.02×10^8	0.2%	9.89×10^7	1.09×10^8	9.2%

*** CFD models include a section of enclosure wall above nose**

CFD data from NETL/**Reaction Engineering International** study

Methodology: Equation Oriented

Tightly coupled subsystems → Optimize using detailed models



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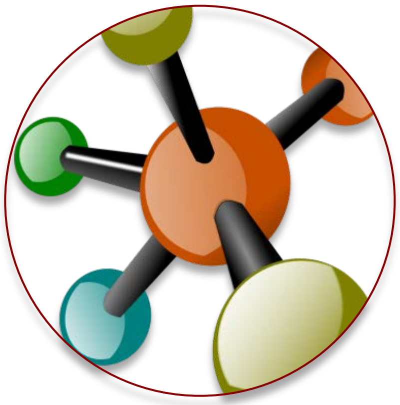
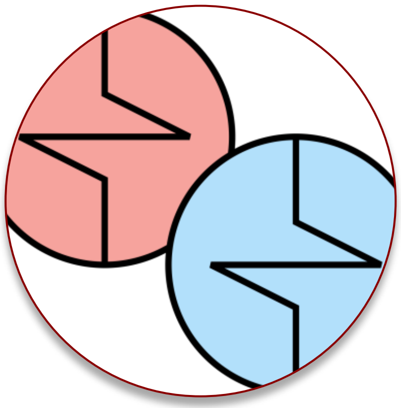
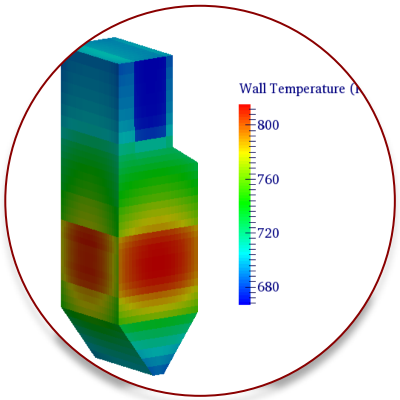


Thermodynamics & Flash Calculations

Distillation Cascades



Heat Integration

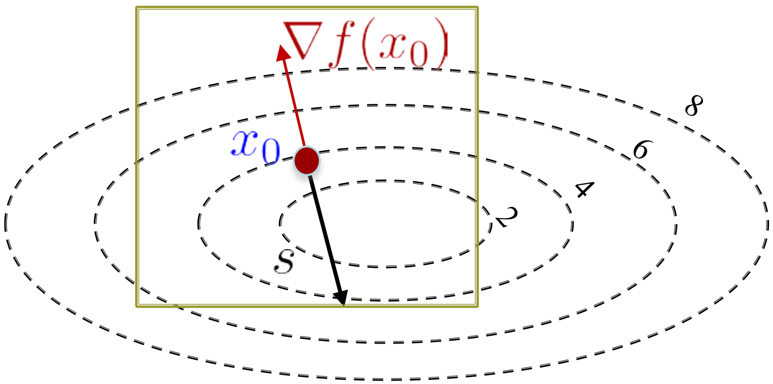


Complex Reactors

Trust Region Optimization with Filter

Trust region methods

- Build surrogate models that we "trust" in a local region
  - Satisfy certain conditions on accuracy
- Optimize within the trust region
- Adaptively adjust surrogate and trust region size
  - Guaranteed convergence
- Use filter method to extend to flowsheets with surrogates



$$\min_{s} \quad r(x_0 + s) = f(x_0) + \nabla f(x_0)^T s$$
$$\text{s.t.} \quad \|s\| \leq \Delta_0$$

Evaluate $f(x_0 + s)$.

$$f(x_0 + s) - f(x_0) = 0$$

No improvement! Shrink trust region Δ_0

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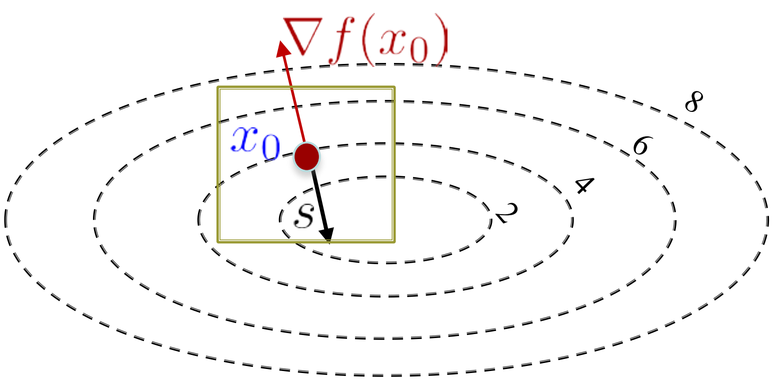


New step s within smaller trust region

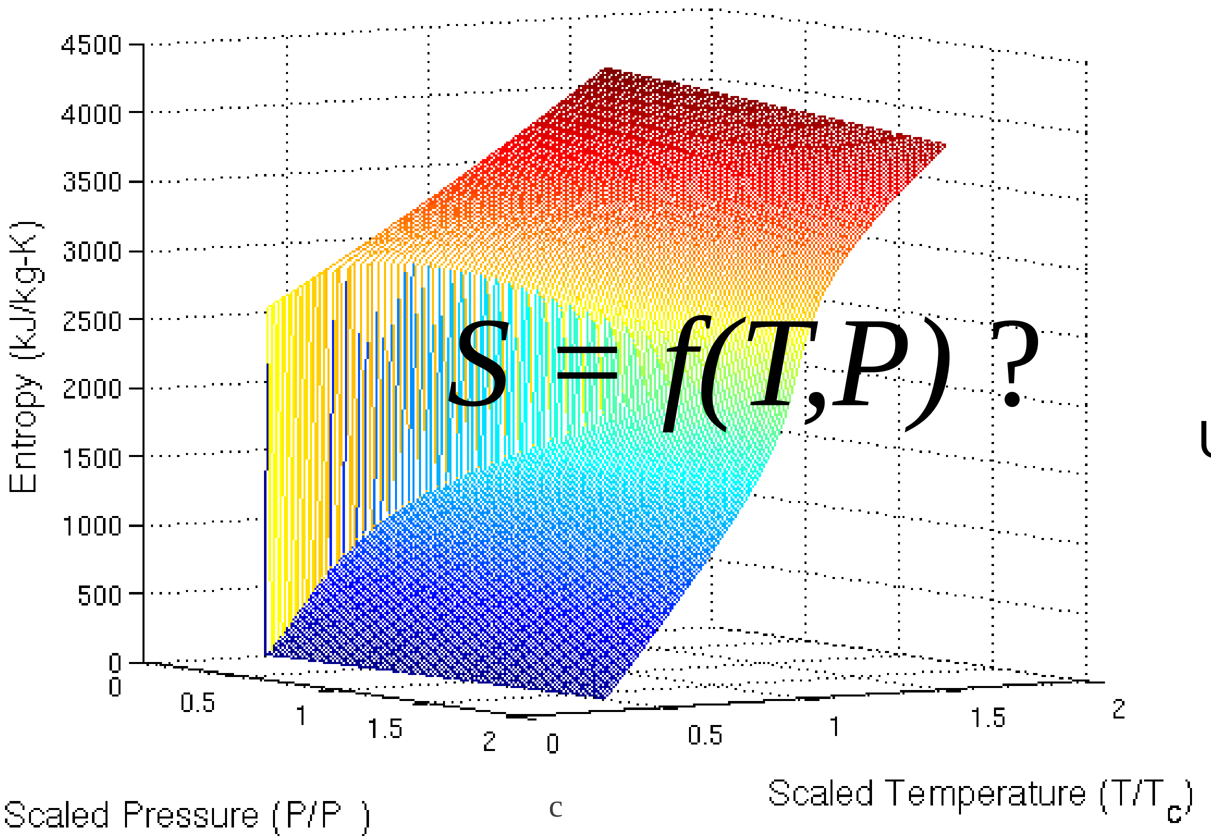
Evaluate $f(x_0 + s)$.

$$\frac{f(x_0+s) - f(x_0)}{r(x_0+s) - r(x_0)} = 0.75$$

Sufficiently decreased the objective

See companion poster (566b) for details

Steam Thermodynamics



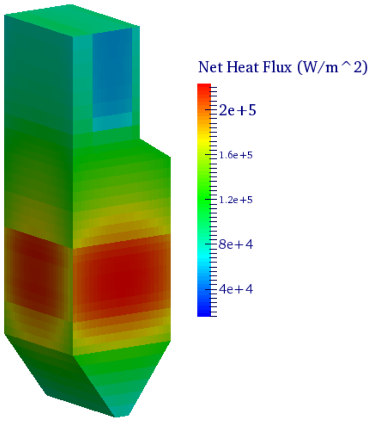
IAPWS IF-97 standard

Use linear surrogate models in trust region framework

$$S(T,P) \cong \tau(T - T_0) + \rho(P - P_0) + S_0$$

Case Studies: *Air-fired Steam Cycle*

- **Simultaneous steam cycle & boiler optimization**
- Boiler design variables
  - Fixed coal feed rate (match CFD case)
  - Primary air temperature & flowrate
  - Secondary/over-fired air temperature
  - Secondary air flowrate
  - Overfire air flowrate
  - Water wall temperature



- Future:
  - Boiler geometry
  - Gas composition (for oxycombustion)

Case Studies: *Air-fired Steam Cycle*

maximize **Thermal Efficiency**

s.t. Steam cycle connectivity

Heat exchanger model

Pump model

Fixed isentropic efficiency turbine model

Hybrid boiler model with fixed fuel rate

Heat integration model

Steam thermodynamics

Using trust region method

Solved in GAMS 24.2.1 with CONOPT 3

Trust region algorithm in MATLAB R2013a

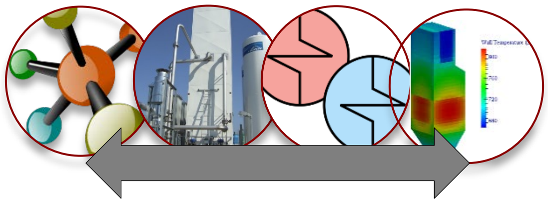
Case Studies: *Air-fired Steam Cycle*

- **Gross electrical efficiency: 46.04%** (HHV)
- Optimized steam extraction and feed water heating
- Ongoing work: assumption refinement

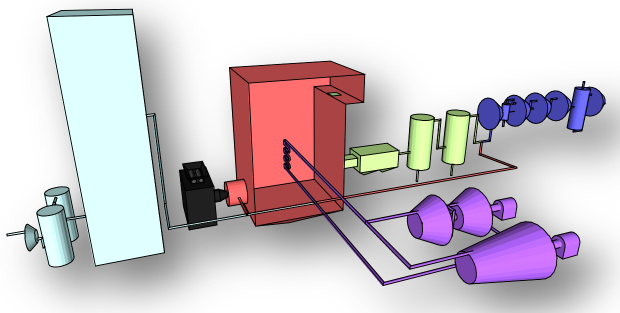
Solution time:	**167.1 minutes**
Total boiler simulations:	247 (run on 4 cores)
HP turbines work	126.1 MW
IP turbines work	309.7 MW
LP turbines work	347.4 MW
Fuel rate (HHV)	1325.5 MW
Steam exit temperature	863 K
Steam exit pressure	350 bar

Conclusions

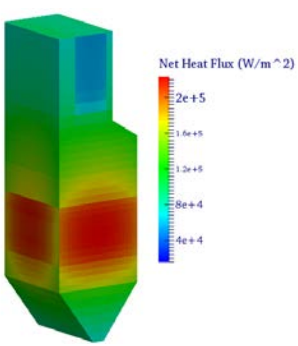
- Developing EO framework for full oxycombustion power plant optimization
  - General structure, extends easily to other emerging energy technologies



- Trust region framework embeds steam table thermodynamics and surrogate boiler model into equation-based optimization problems
  - Guaranteed accuracy



- Future work will include investigation of
  - Heat integration and sizing trade-offs
  - Optimization of firing conditions and CO_2 recycle strategy
  - Full optimization of oxycombustion process



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David Miller, DOE/NETL	CCSI Technical Team Lead
Jinliang Ma, NETL/URS	1D/3D hybrid boiler model
Cheshta Balwani, CMU	CPU optimization, CEOS refinement
Zixiang Gao, CMU	SO_x scrubber modeling

Trust Region Framework

- Desire mathematical guarantees regarding the optimal of the “full detail” model
- Restricts optimizer step size to within trust region
- Adjust trust region size based on local model accuracy
- Use **filter method** to simultaneously optimize objective function and converge equality constraints

Agarwal, A., & Biegler, L. T. (2013) A trust-region framework for constrained optimization using reduced order modeling. *Optimization and Engineering*, *14*(1), 3–35.