CCSI

Carbon Capture Simulation Initiative

Advanced Heat Integration Tool for Simulation-based Optimization Framework

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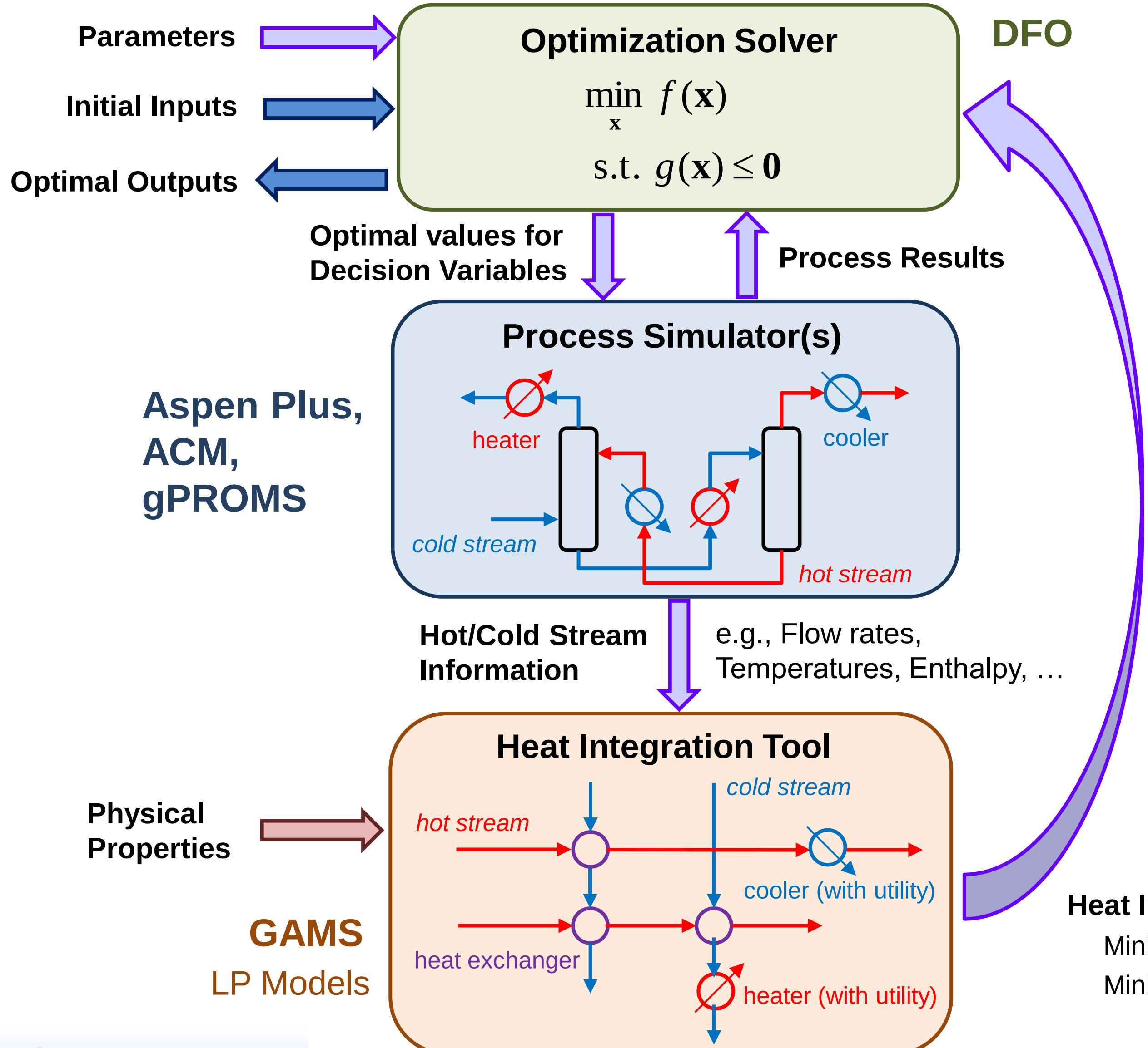
Simulation-Based Optimization

+ Treats simulation as black box (does not require mathematical details of model)
  → **Easy to implement**
+ Does not require simplification of the process model
  → **High-fidelity models applied**
+ Readily adapted for parallel computing
  → **Computational time reduced**
− Not well suited for problems with many variables such as heat integration, and superstructure optimization
  → **Heat integration is a separate module linked to simulation-based optimization algorithm**

Goal: Develop a simulation-based optimization framework with heat integration for large-scale high-fidelity process models.

Simulation-Based Optimization with Heat Integration



Simultaneous process optimization and heat integration based on **rigorous** process simulations are achieved in this framework

Heat Integration Results:

- Minimum utility cost (or consumption)
- Minimum heat exchanger area

Minimum Utility Cost (Consumption)

- LP Transshipment Model

$$\min \; Z = \sum_{m \in S} c_m Q_m^S + \sum_{n \in W} c_n Q_n^W$$

$$\text{s.t.} \; R_{ik} - R_{i,k-1} + \sum_{j \in C_k} Q_{ijk} + \sum_{n \in W_k} Q_{ink} = Q_{ik}^H \qquad i \in H_k'$$

$$R_{mk} - R_{m,k-1} + \sum_{j \in C_k} Q_{mjk} - Q_m^S = 0 \qquad m \in S_k'$$

$$\sum_{i \in H_k} Q_{ijk} + \sum_{m \in S_k} Q_{mjk} = Q_{jk}^C \qquad j \in C_k$$

$$\sum_{i \in H_k} Q_{ink} - Q_n^W = 0 \qquad n \in W_k \quad k = 1, \ldots, K$$

$$R_{ik},\; R_{mk},\; Q_{ijk},\; Q_{mjk},\; Q_{ink},\; Q_m^S,\; Q_n^W \geq 0 \qquad R_{i0} = R_{iK} = 0$$

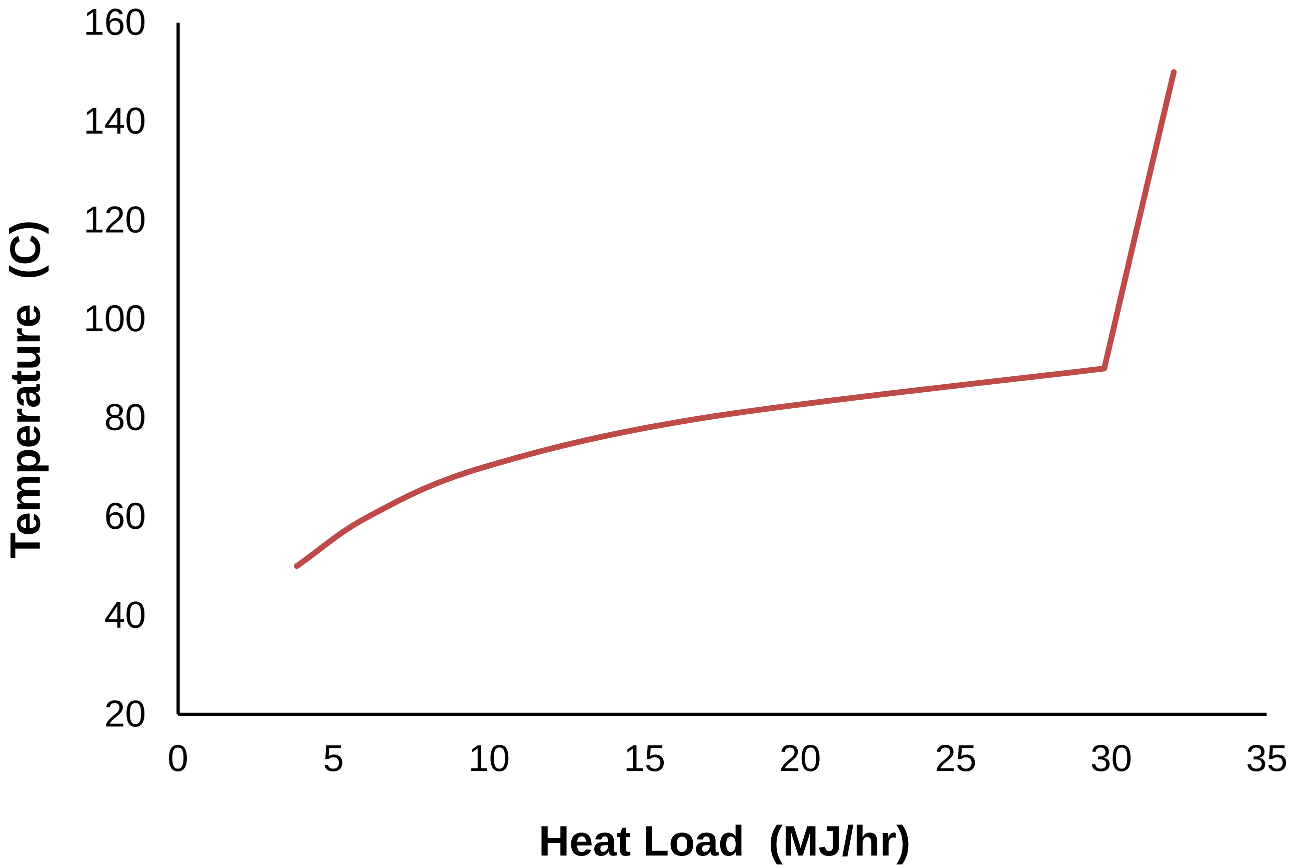
Q^S	heat load of hot utility
Q^W	heat load of cold utility
Q^H	heat load of hot process stream
Q^C	heat load of cold process stream
Q	exchange of heat
R	heat residual
c	unit cost of utility
k	temperature interval
i	hot process stream
j	cold process stream
m	hot utility
n	cold utility

- Heat loads of the streams are calculated directly from the total change of enthalpy from the simulation results.
- Assumption: **Constant** heat capacity flowrates (FCps) for streams.

Papoulias SA, Grossmann IE. *Comput. & Chem. Eng*. 1983;7(6):707-721.

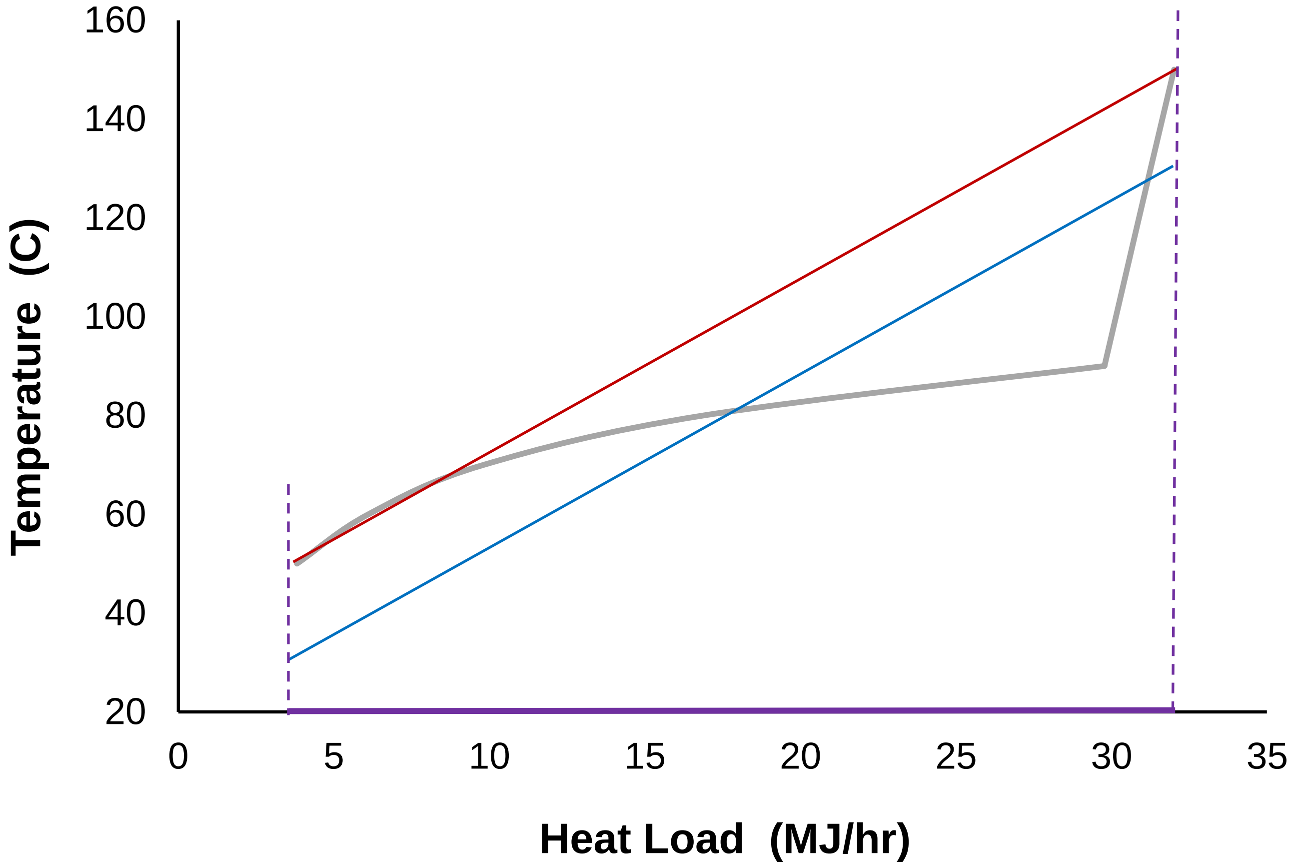
Stream with Variable FCp

- A process stream with phase change



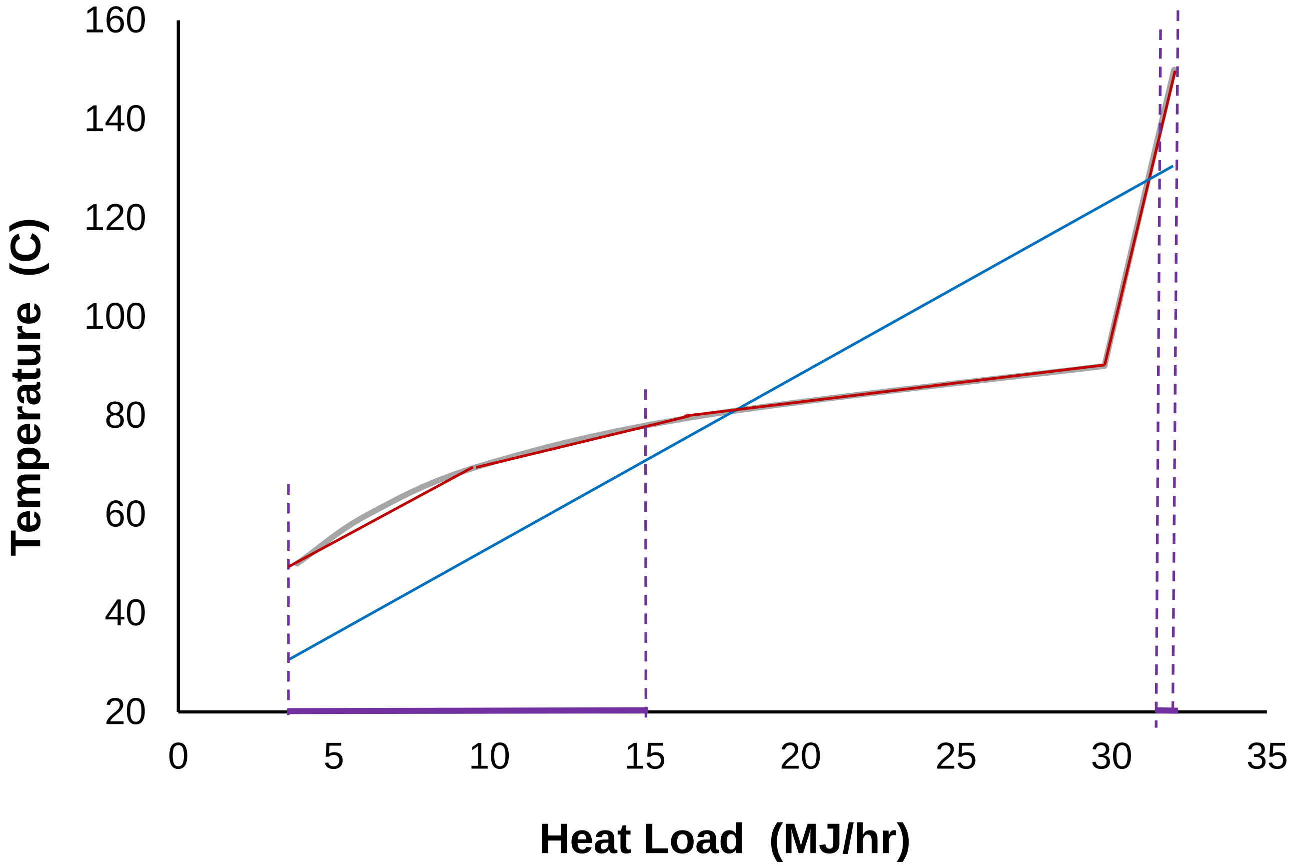
A mixture stream of CO_2 and H_2O (CO_2: 40%, H_2O: 60%; 1kmol/hr; 1 bar)

Problems with Constant FCps



- Overestimate the heat recovery
- Infeasible heat exchanger network design

Piecewise Linear Approximation



- More accurate heat integration results
- Assume constant FCps in each small temperature interval
- Build a series of sub-streams with identical temperature change or heat load in process models

Minimum Heat Exchanger Area

- LP Area Targeting Model (Modified from LP Transportation Model)

$$\min \frac{1}{Ft}\sum_{k=1}^{K}\sum_{l=1}^{K}\frac{1}{LMTD_{k,l}}\sum_{i\in H_k}\sum_{j\in C_l}\frac{q_{ik,jl}}{h_i+h_j}$$

$$\text{s.t.} \quad \sum_{l=k}^{K}\sum_{j\in C_l} q_{ik,jl} = Q_{ik}^{H} \qquad i\in H_k \quad k=1,\dots,K$$

$$\sum_{k=1}^{l}\sum_{i\in H_k} q_{ik,jl} = Q_{jl}^{C} \qquad j\in C_l \quad l=1,\dots,K$$

Q^H	heat load of hot stream
Q^C	heat load of cold stream
q	exchange of heat
Ft	correction factor for a non-countercurrent flow
h	stream film heat transfer coefficient
LMTD	logarithmic-mean temperature difference
k	temperature interval
l	temperature interval
i	hot stream
j	cold stream

  - Temperature interval should be smaller than the minimum utility problem for accurate area targets.
  - Number of temperature intervals: accurate results vs. CPU times.
  - Double-temperature approach: HRAT & EMAT.

Jezowski JM, Shethna HK, Castillo FJL. *Ind. Eng. Chem. Res*. 2003;42(8):1723-1730.

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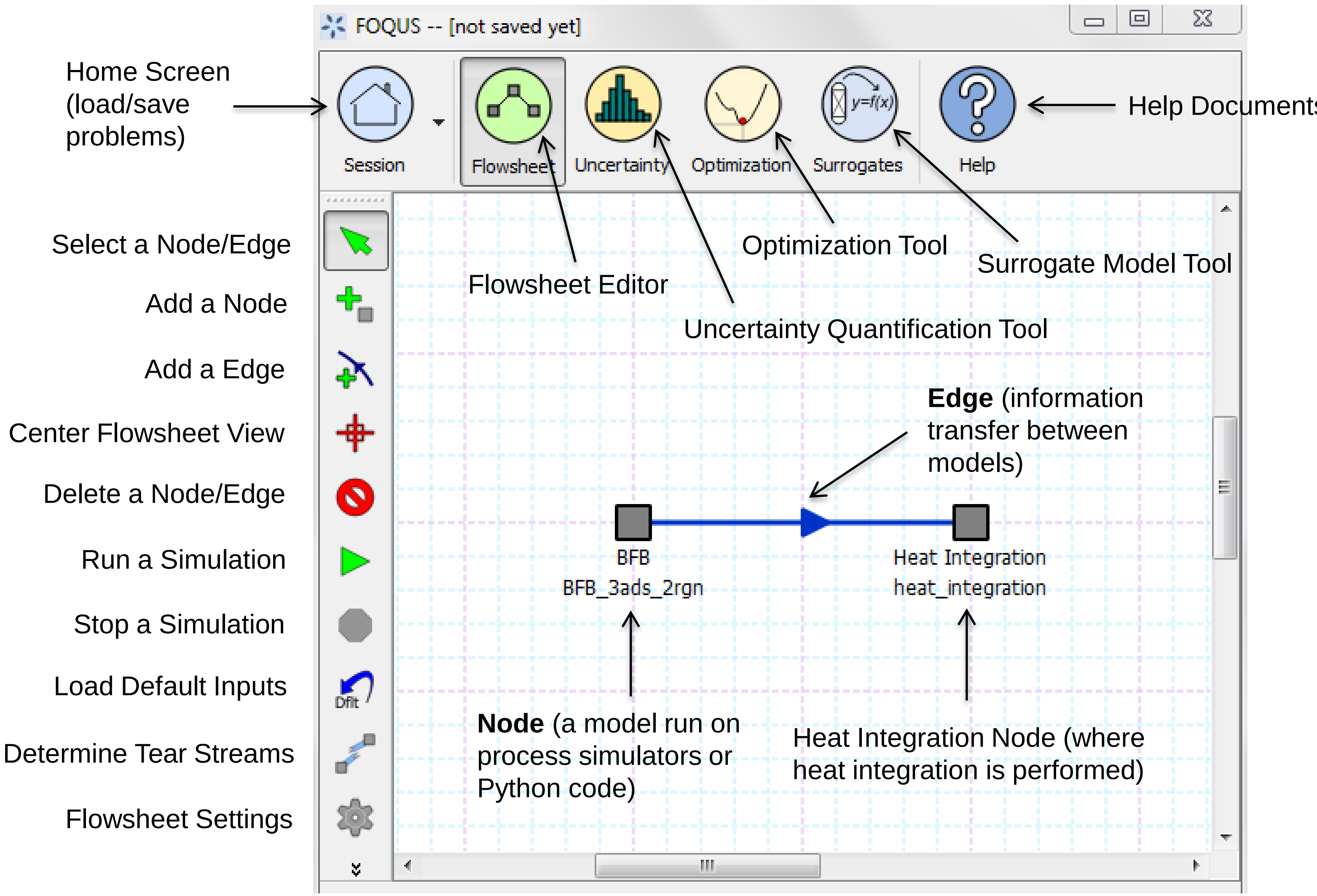
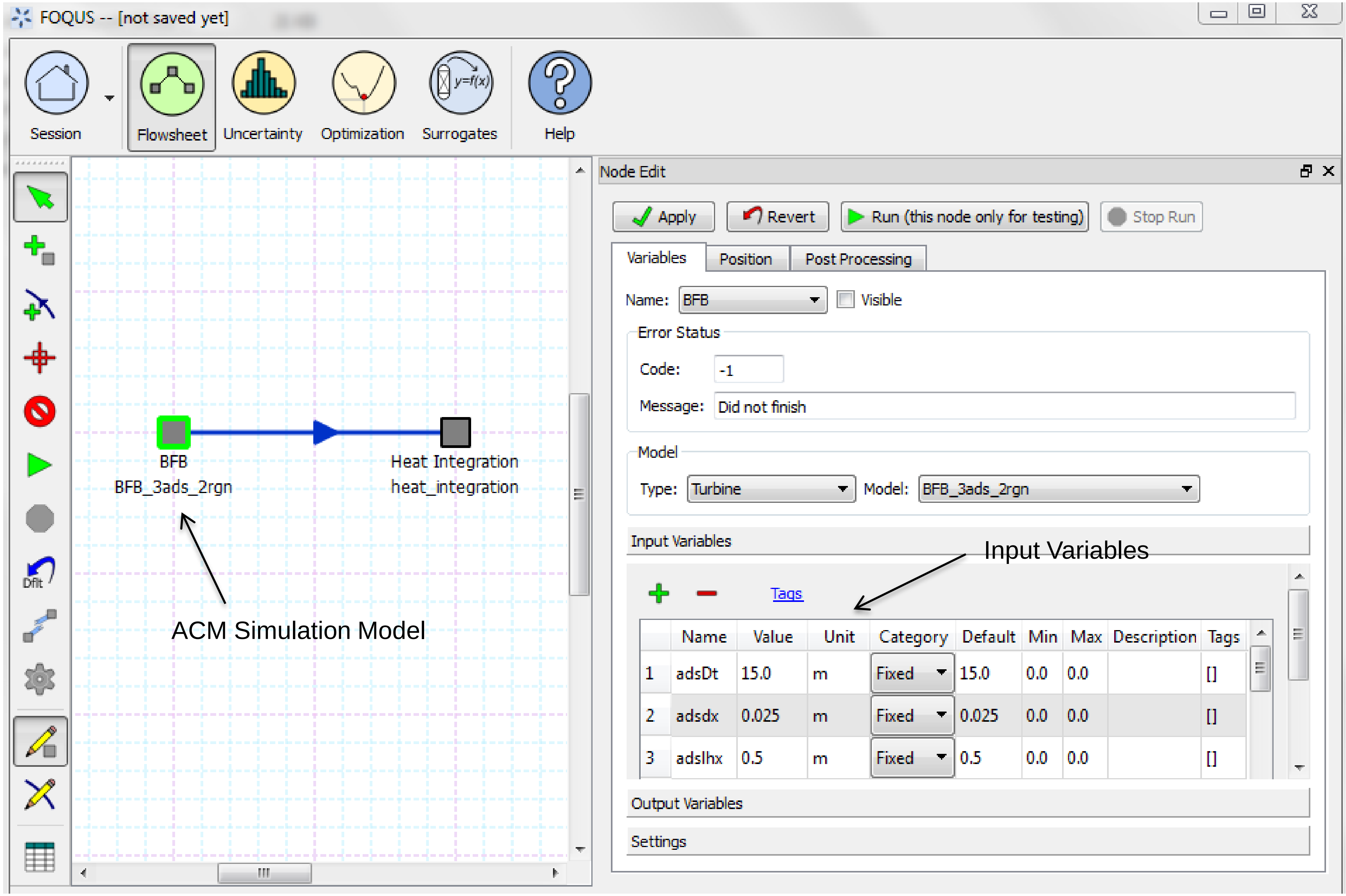
Implementation - Graphical User Interface

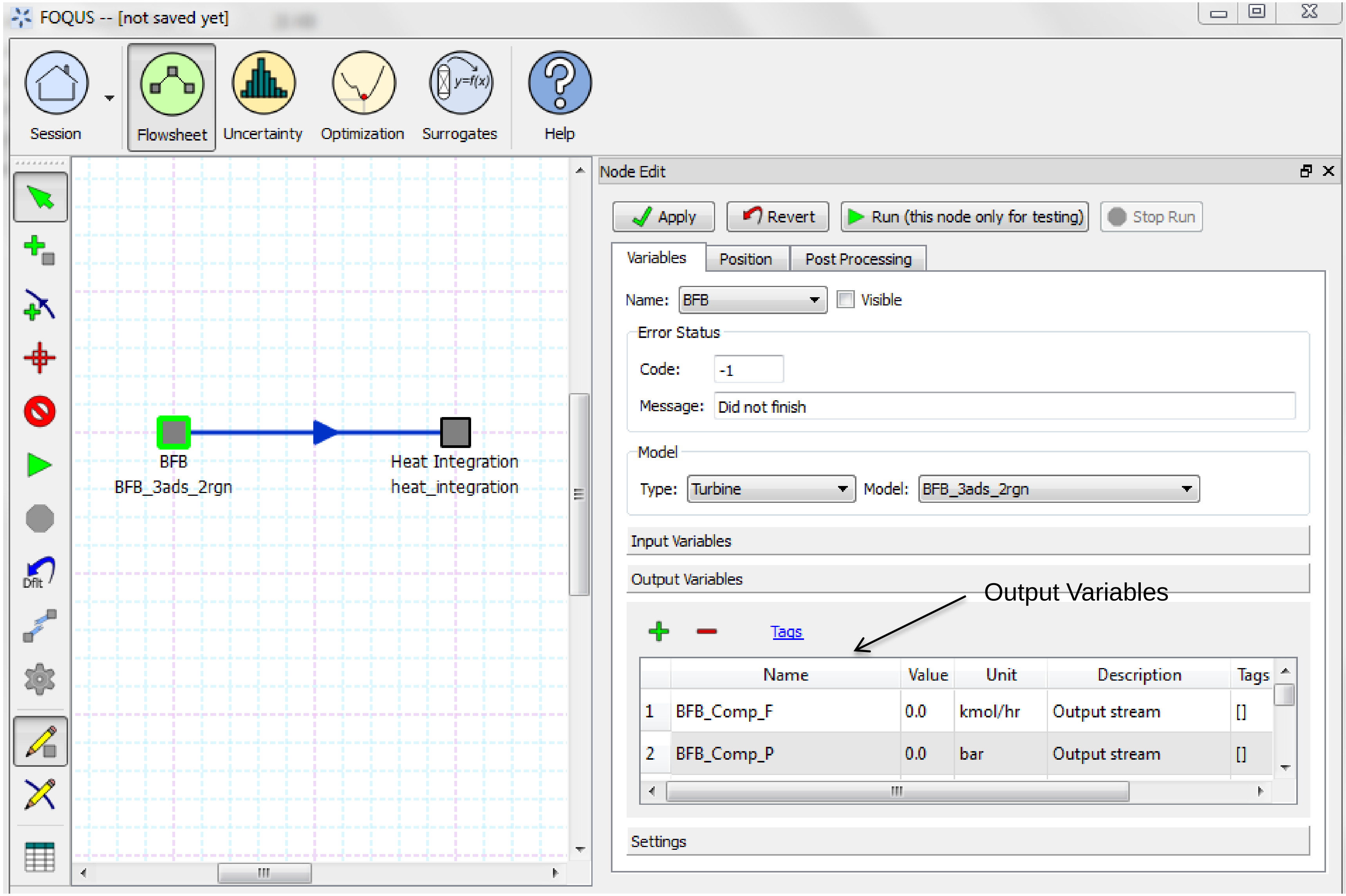


Framework for Optimization and Quantification of Uncertainty and Sensitivity (FOQUS)

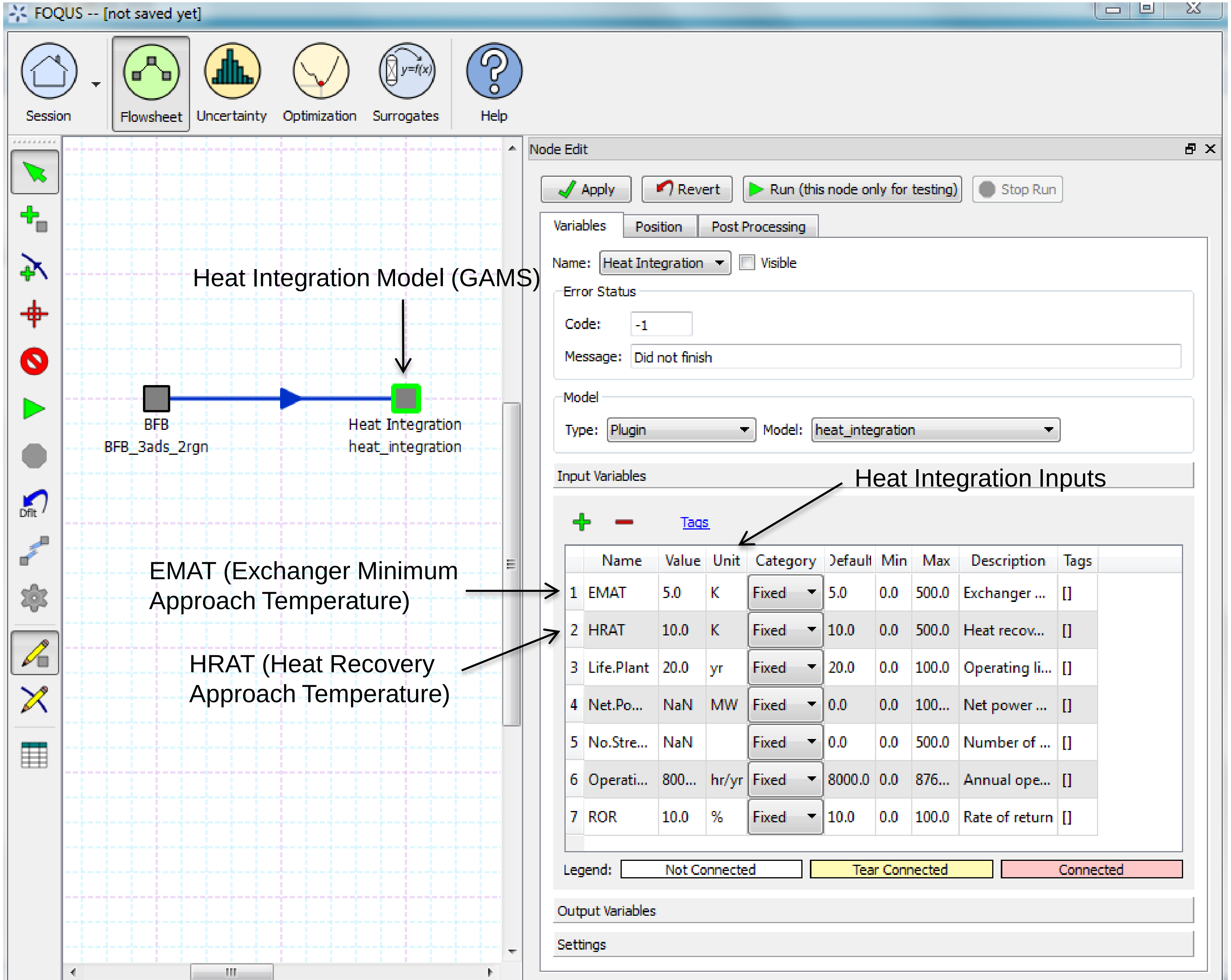
Simulation Model (1)



Simulation Model (2)

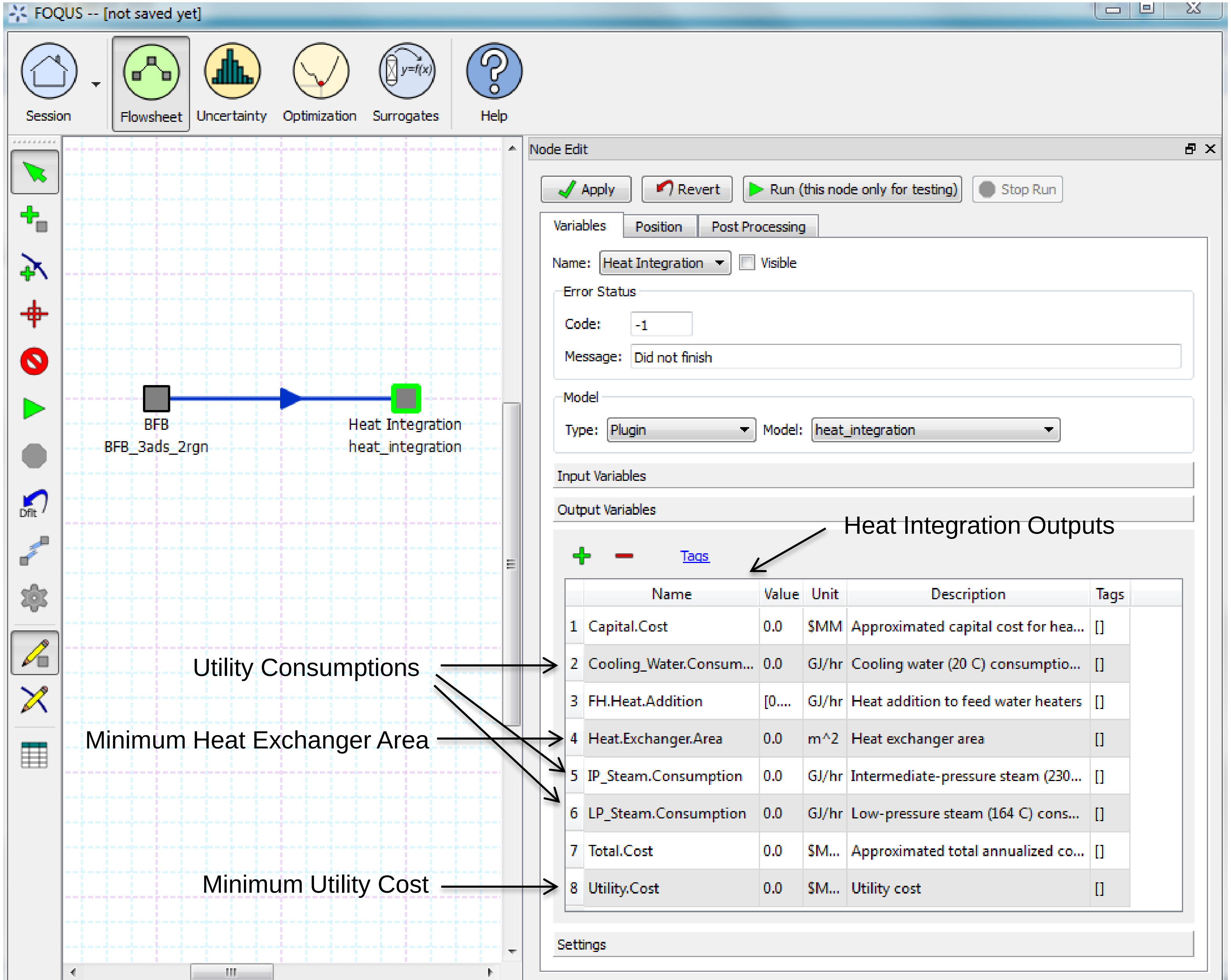


Heat Integration Tool (1)



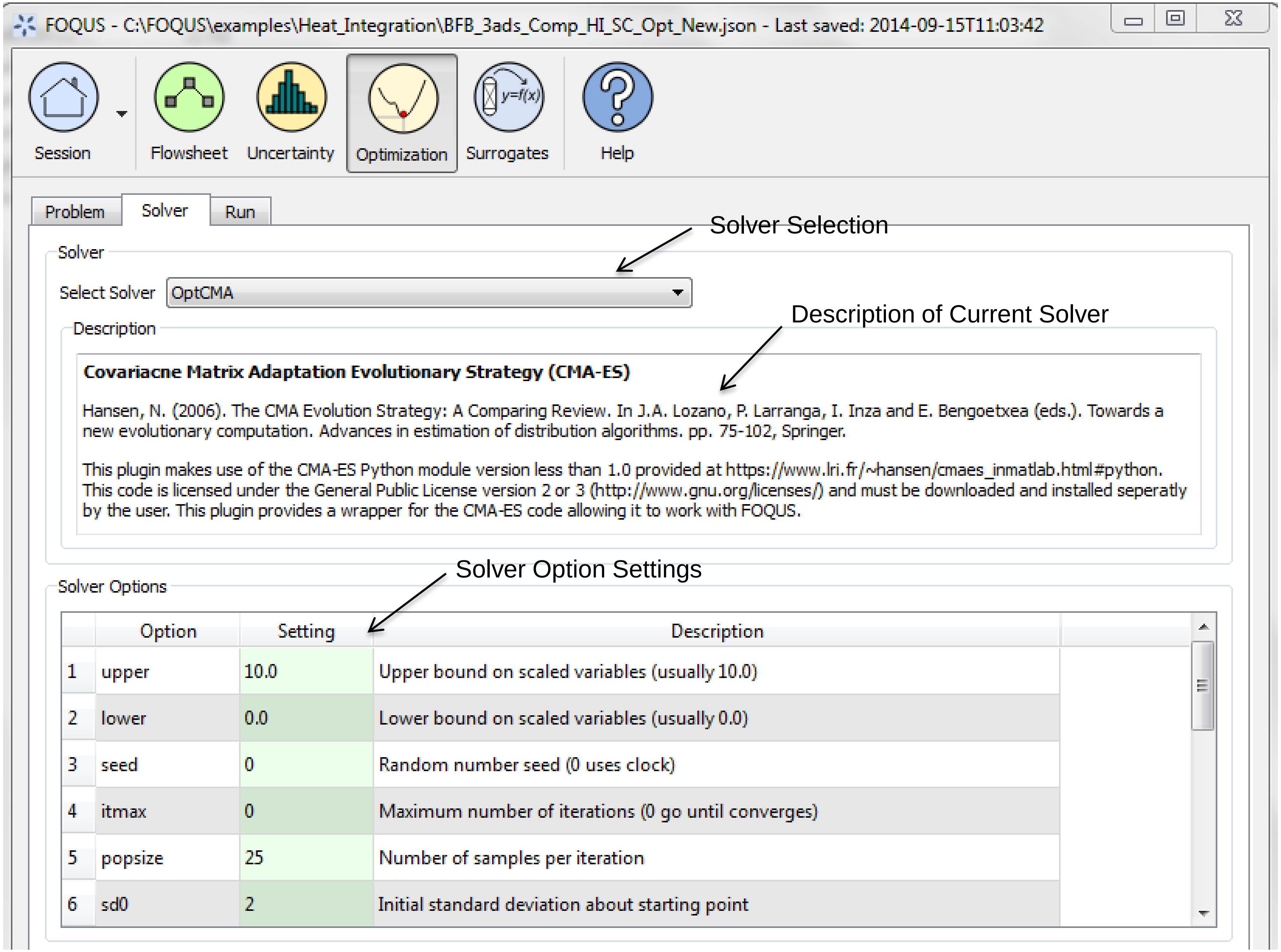
	Name	Value	Unit	Category	Default	Min	Max	Description	Tags
1	EMAT	5.0	K	Fixed	5.0	0.0	500.0	Exchanger ...	[]
2	HRAT	10.0	K	Fixed	10.0	0.0	500.0	Heat recov...	[]
3	Life.Plant	20.0	yr	Fixed	20.0	0.0	100.0	Operating li...	[]
4	Net.Po...	NaN	MW	Fixed	0.0	0.0	100...	Net power ...	[]
5	No.Stre...	NaN		Fixed	0.0	0.0	500.0	Number of ...	[]
6	Operati...	800...	hr/yr	Fixed	8000.0	0.0	876...	Annual ope...	[]
7	ROR	10.0	%	Fixed	10.0	0.0	100.0	Rate of return	[]

Heat Integration Tool (2)

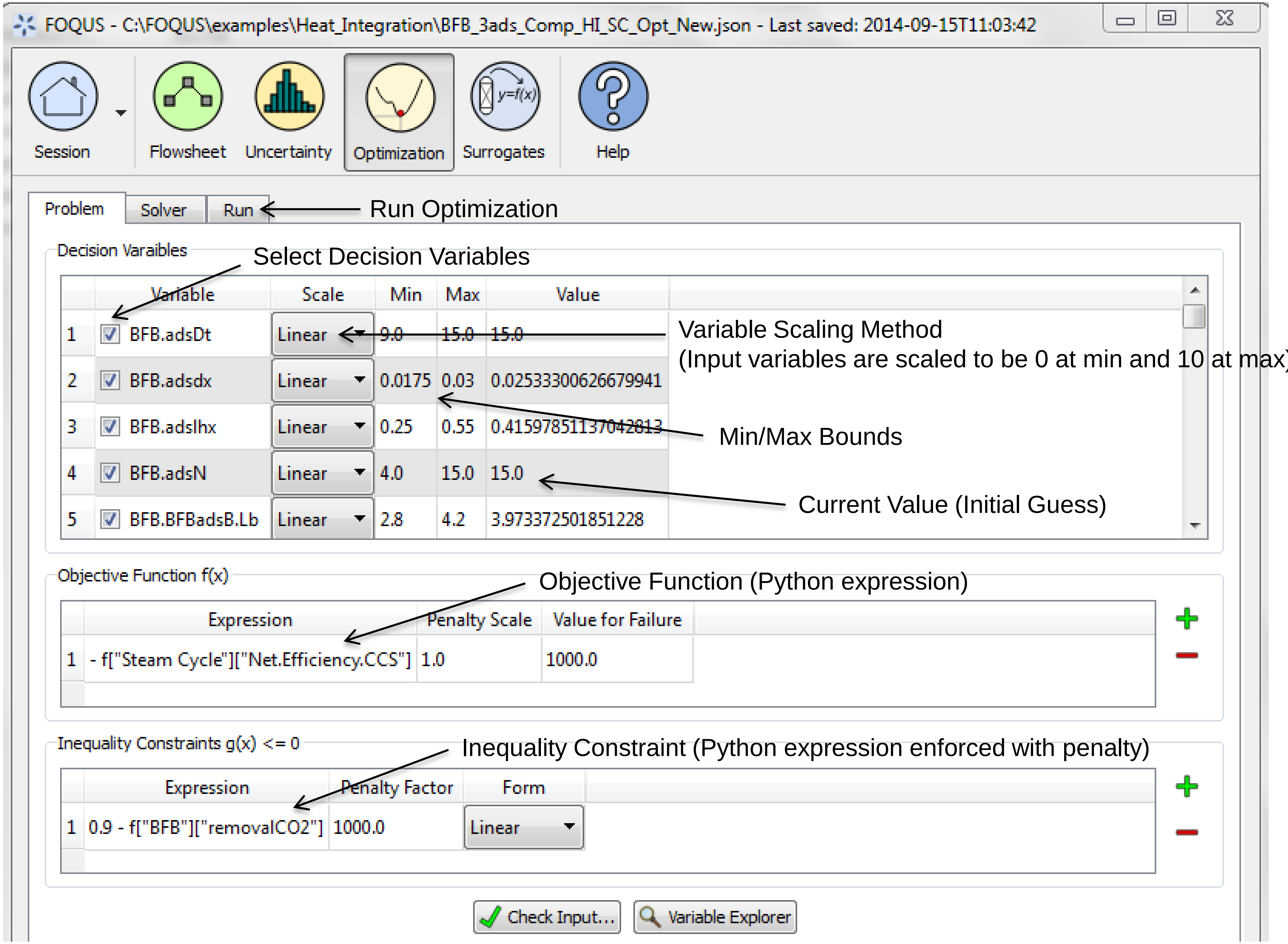


	Name	Value	Unit	Description	Tags
1	Capital.Cost	0.0	$MM	Approximated capital cost for hea...	[]
2	Cooling_Water.Consum...	0.0	GJ/hr	Cooling water (20 C) consumptio...	[]
3	FH.Heat.Addition	[0....	GJ/hr	Heat addition to feed water heaters	[]
4	Heat.Exchanger.Area	0.0	m^2	Heat exchanger area	[]
5	IP_Steam.Consumption	0.0	GJ/hr	Intermediate-pressure steam (230...	[]
6	LP_Steam.Consumption	0.0	GJ/hr	Low-pressure steam (164 C) cons...	[]
7	Total.Cost	0.0	$M...	Approximated total annualized co...	[]
8	Utility.Cost	0.0	$M...	Utility cost	[]

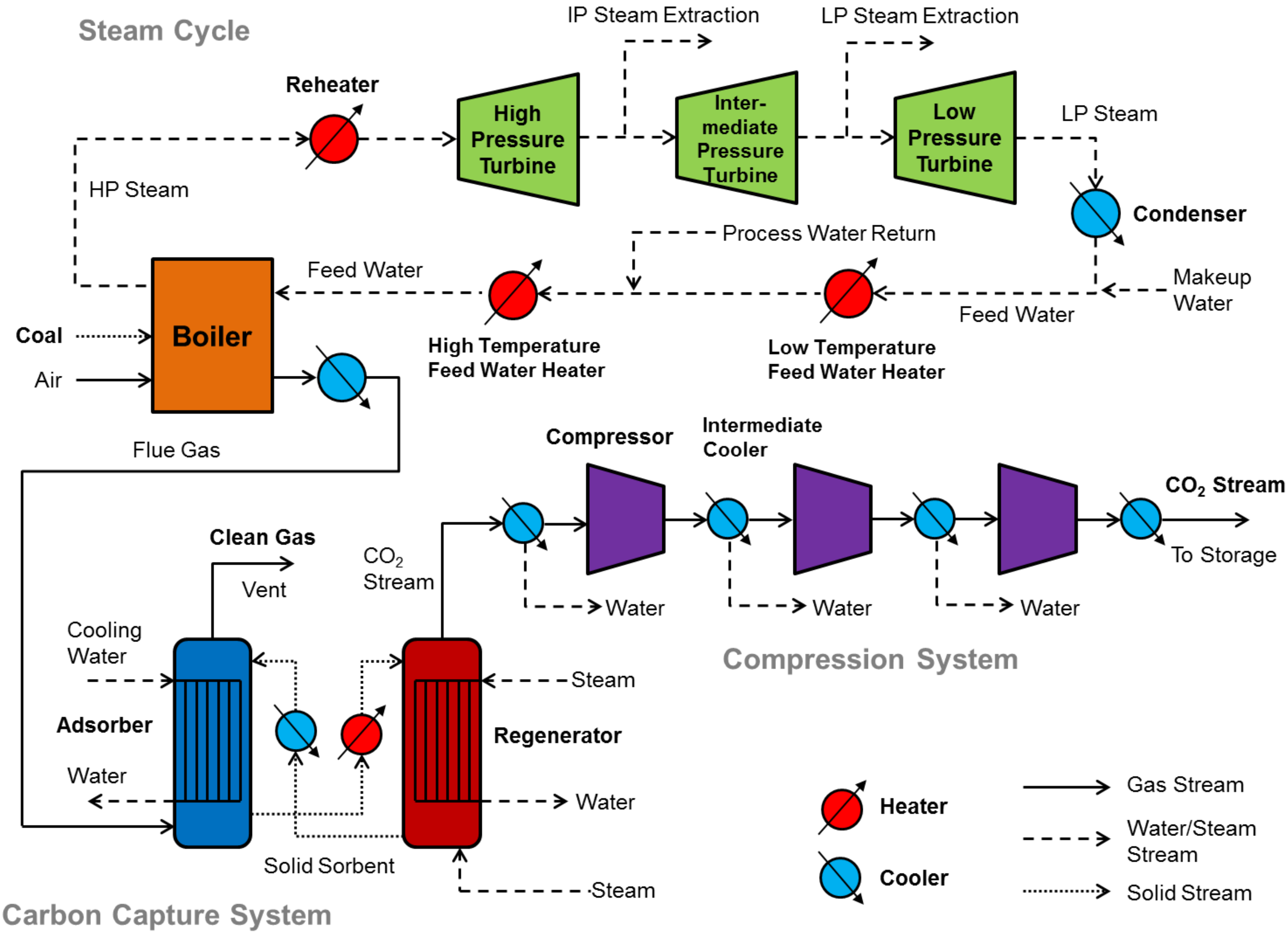
Optimization Solver



Optimization Problem Setting



Case Study – A Power Plant with CO_2 Capture



Problem Statement

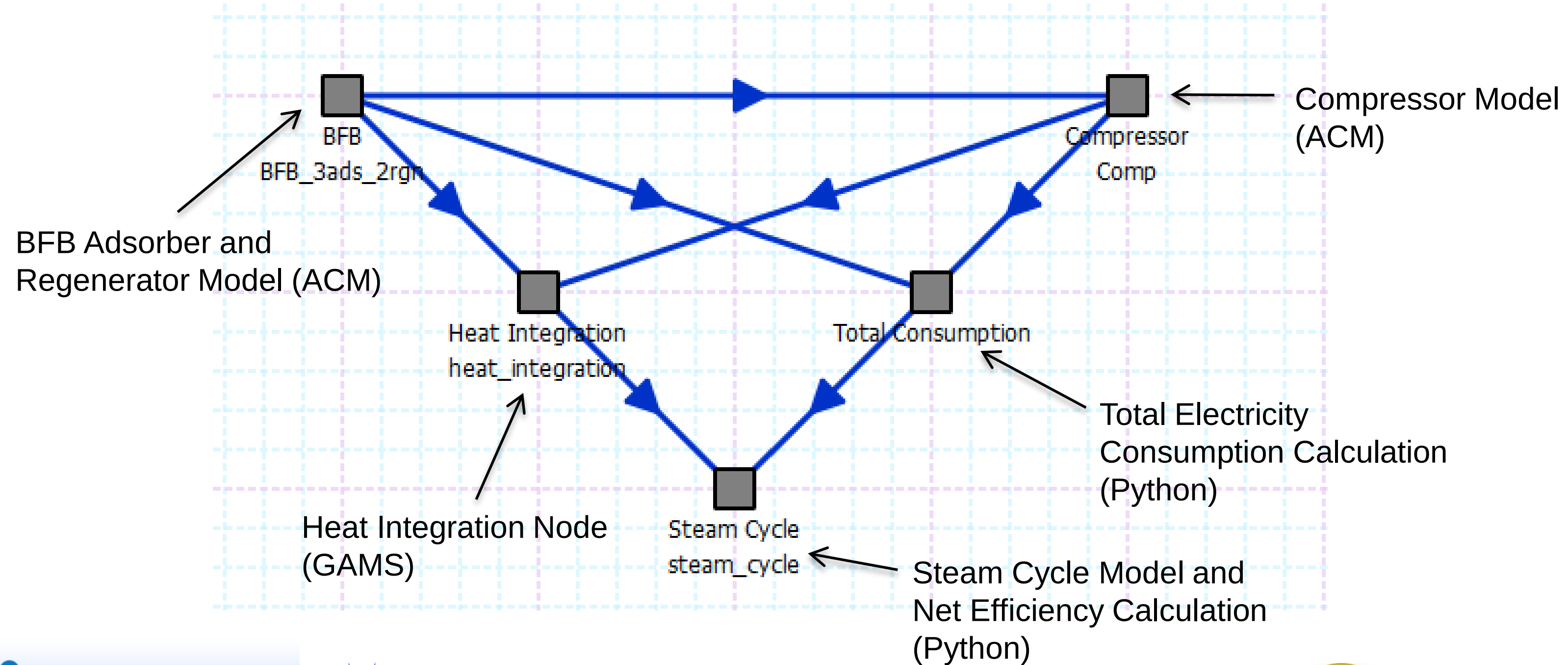
Objective Function: Maximizing **Net efficiency**

Constraint: **CO_2 removal** ratio ≥ 90%

Flowsheet evaluation (via process simulators)

Minimum utility and area target (via heat integration tool)

Decision Variables (23): Bed length, diameter, sorbent and steam feed rates, temperatures



Case Study Results (1)

Base case w/o CCS: 650 MW_e, **42.1 %** with CCS: 419.6 MW_e, **27.2 %**	**Simultaneous** optimization and heat integration approach	**Sequential** optimization and heat integration approach	Optimization **w/o** heat integration
Net power efficiency (%)	**33.8**	**32.2**	**30.5**
Net power output (MW_e)	522.2	497.9	471.1
CO_2 removal ratio (%)	**90.2**	**90.1**	**90.1**
Electricity consumption (MW_e)	85.2	73.8	73.8
IP steam withdrawn (GJ/hr)	0	0	0
LP steam withdrawn (GJ/hr)	768.5	1113.7	1231.9
Cooling water consumption (GJ/hr)	1820.3	1594.2	3333.6
Heat addition to feed water (GJ/hr)	562.9	467.4	0
Heat exchanger area (million m^2)	0.751	1.125	

Note: Constant FCps are assumed here and piecewise linear approximation is not used.

Optimization and heat integration significantly increased the net efficiency of the power plant with CCS.

Case Study Results (2)

Base case w/o CCS: 650 MW_e, **42.1 %** with CCS: 419.6 MW_e, **27.2 %**	Heat integration with **constant** FCps	Heat integration with **variable** FCps (5 segments)	**w/o** heat integration
Net power efficiency (%)	**33.8**	**31.9**	**30.5**
Net power output (MW_e)	522.2	493.4	471.1
CO_2 removal ratio (%)	**90.2**	**90.0**	**90.1**
Electricity consumption (MW_e)	85.2	72.0	73.8
IP steam withdrawn (GJ/hr)	0	0	0
LP steam withdrawn (GJ/hr)	768.5	1089.7	1231.9
Cooling water consumption (GJ/hr)	1820.3	1700.8	3333.6
Heat addition to feed water (MW_{th})	562.9	313.9	0
Heat exchanger area (million m^2)	0.751	0.923	

After considering variable FCps and using piecewise linear approximation of the composite curve, the net efficiency is somewhat decreased but the obtained results become much more **realistic**.

Conclusions

- Simulation-based optimization framework with heat integration is a suitable tool for optimization of large-scale high-fidelity process models.
- This framework can be easily implemented in the software FOQUS.
- Performance of power plant with CCS can be significantly increased by simultaneous optimization and heat integration.
- More accurate heat integration results are obtained by using piecewise linear approximation for the composite curve of process streams.

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DOE: Carbon Capture Simulation Initiative (CCSI)

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