

CCSI

Carbon Capture Simulation Initiative

Advanced Heat Integration Tool for Simulation-based Optimization Framework

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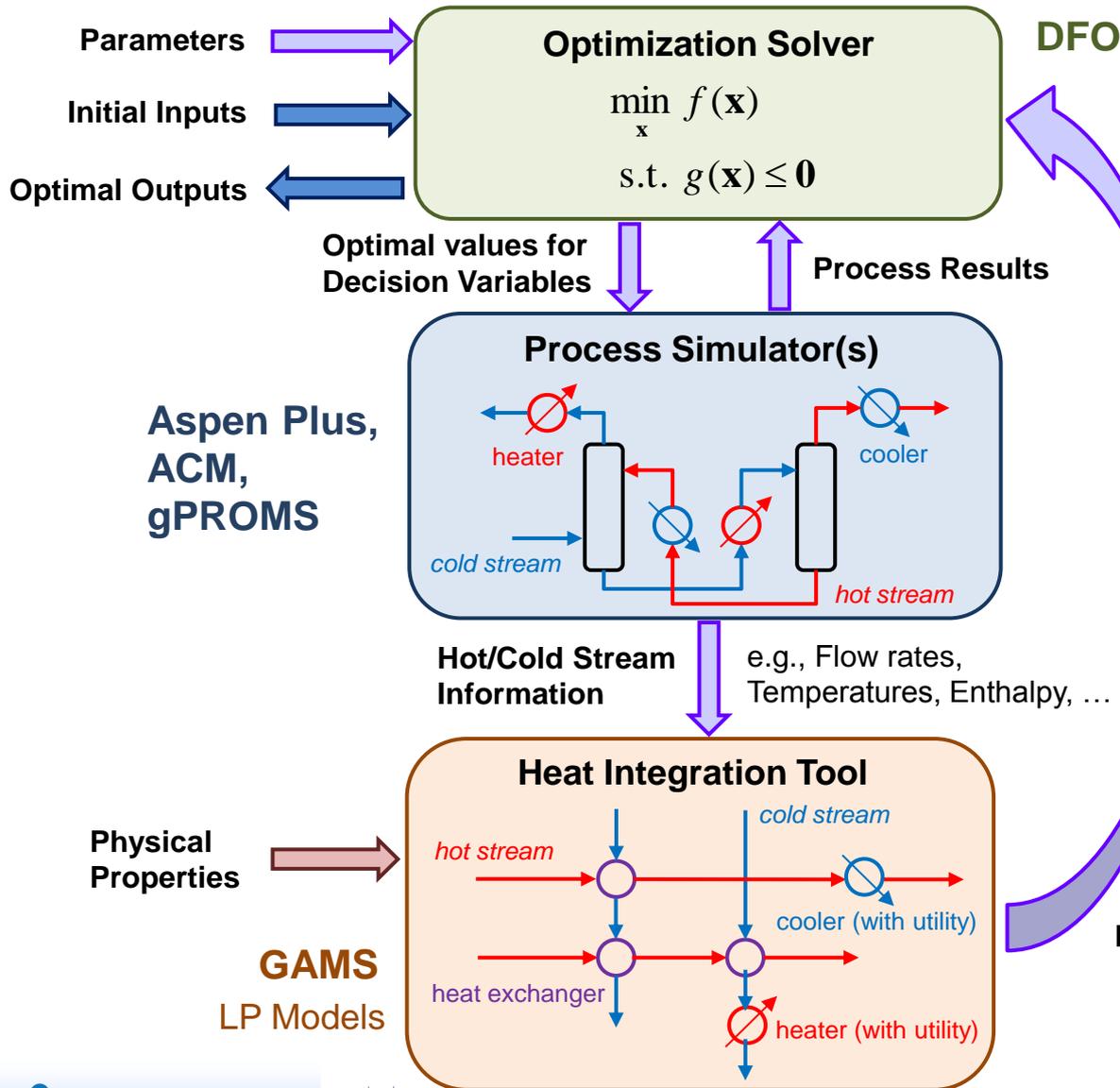


Simulation-Based Optimization

- + 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

Minimum Utility Cost (Consumption)

- LP Transshipment Model

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

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

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

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

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

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

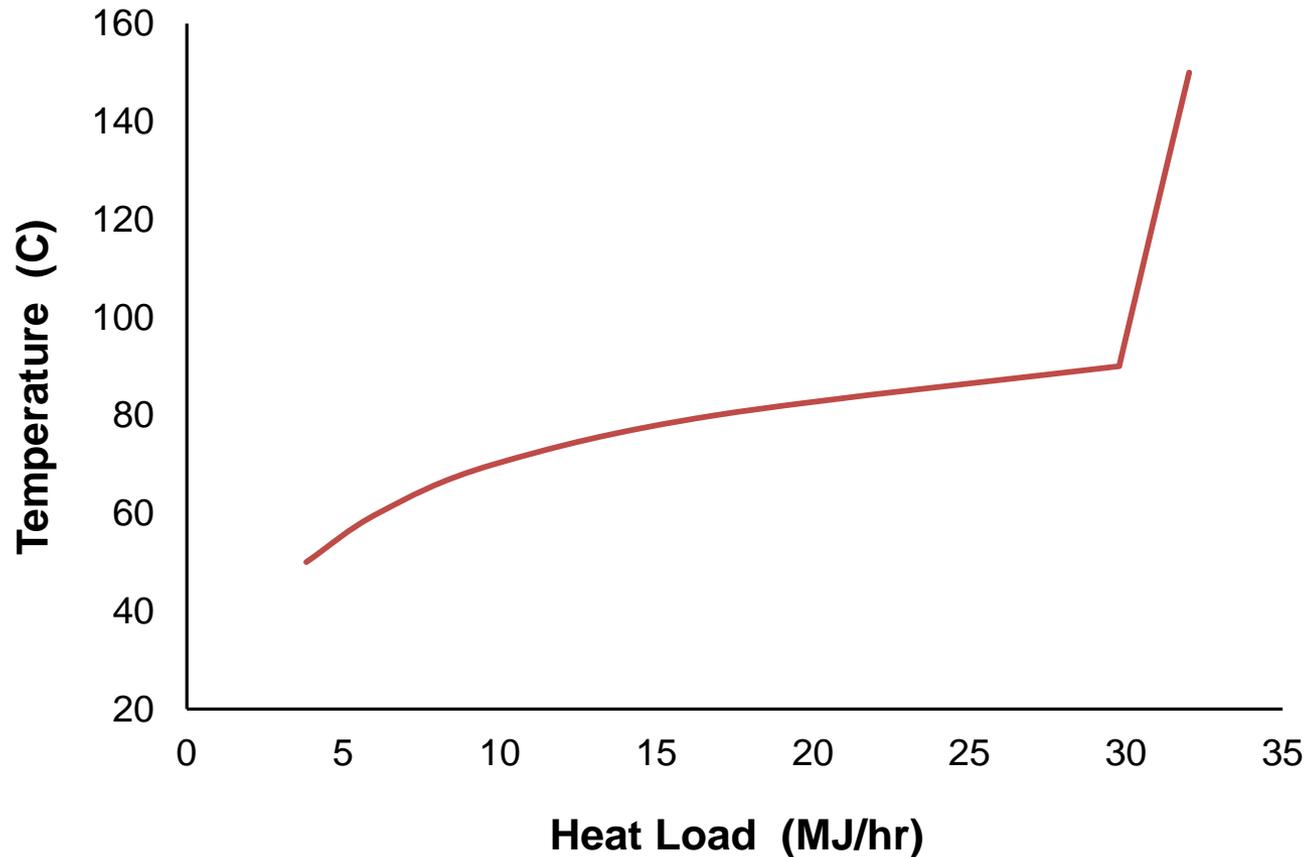
Q^S	heat load of hot utility
Q^W	heat load of cold utility
Q^H	heat load of hot process stream
Q^C	heat load of cold process stream
Q	exchange of heat
R	heat residual
c	unit cost of utility
k	temperature interval
i	hot process stream
j	cold process stream
m	hot utility
n	cold utility

- 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.

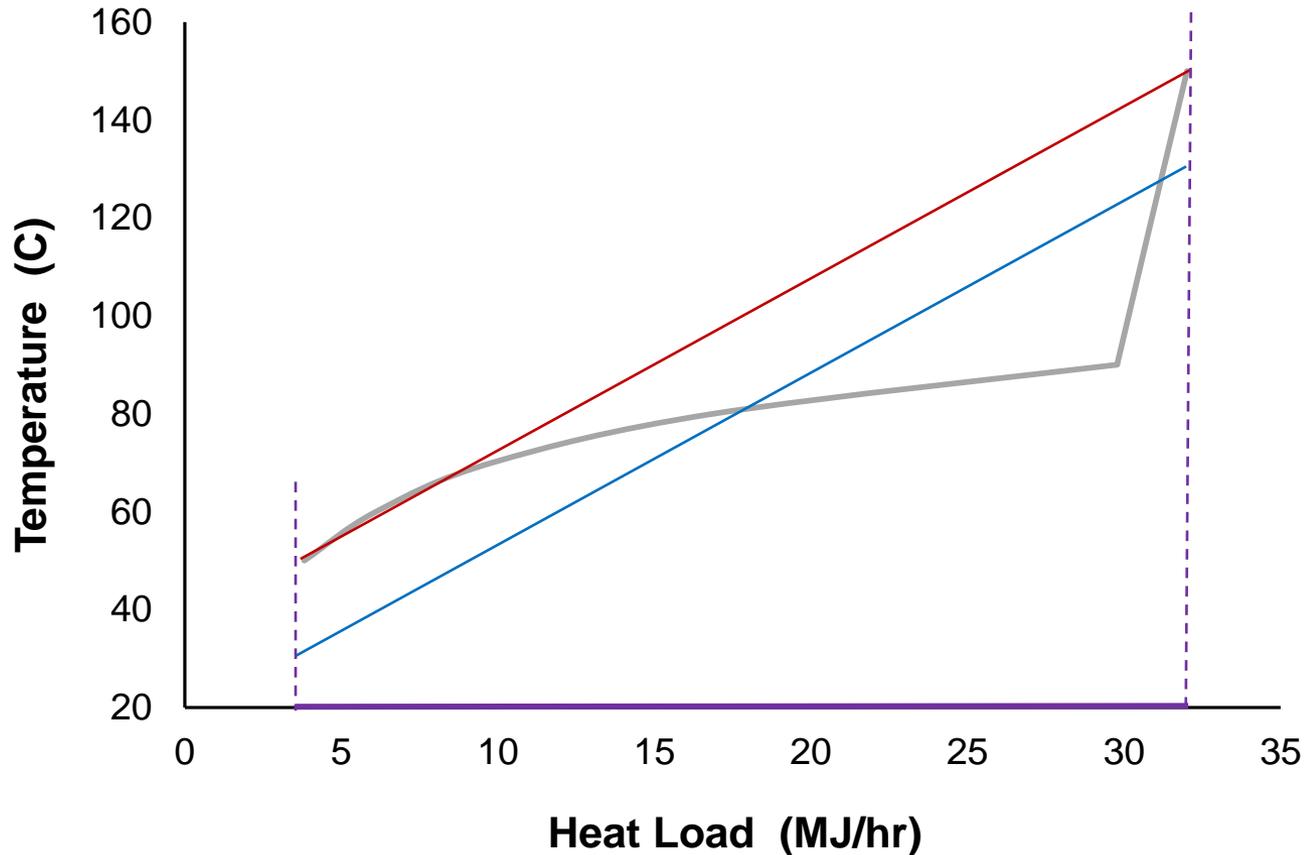
Stream with Variable FCp

- A process stream with phase change



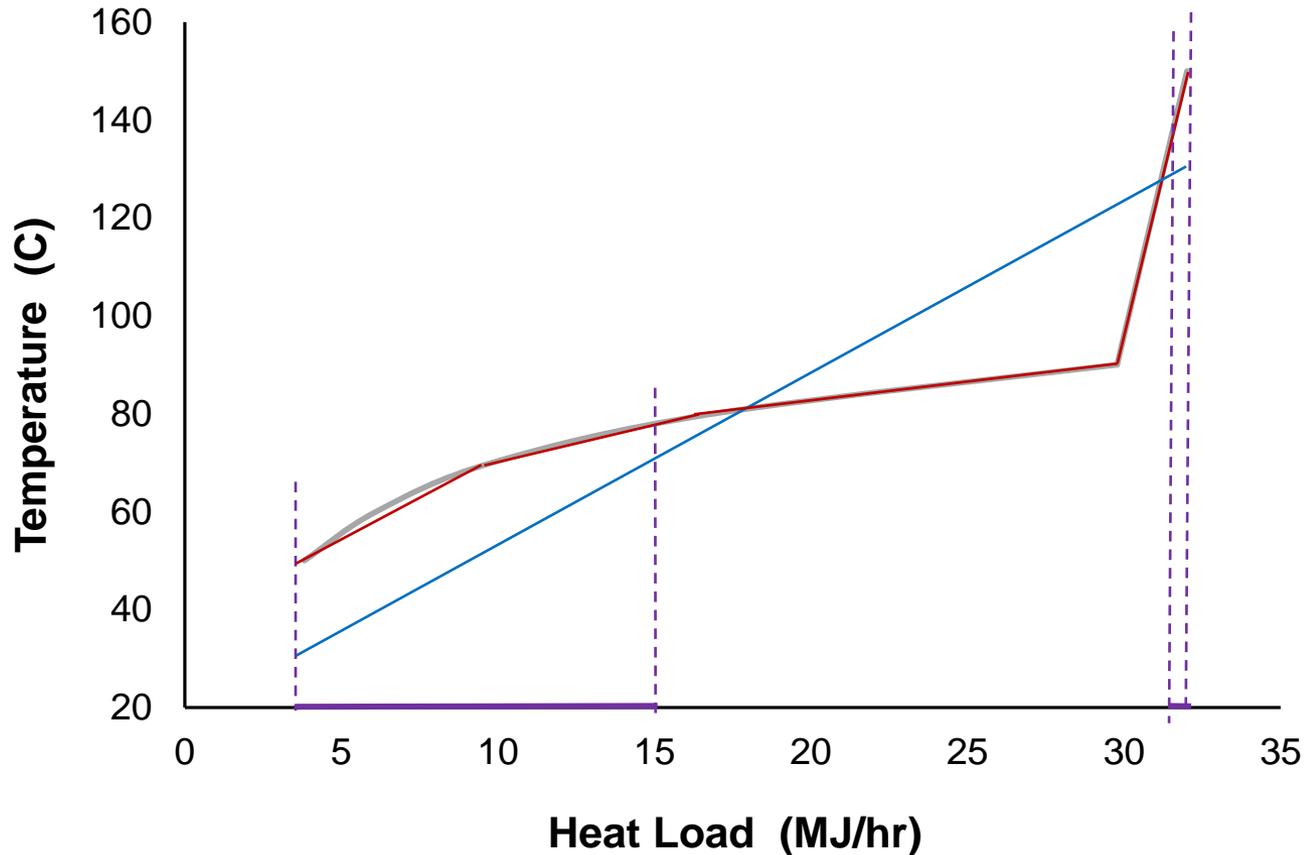
A mixture stream of CO₂ and H₂O (CO₂: 40%, H₂O: 60%; 1kmol/hr; 1 bar)

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)

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

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

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

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.

Implementation - Graphical User Interface

The screenshot displays the FOQUS software interface. At the top, a menu bar contains icons for Session, Flowsheet, Uncertainty, Optimization, Surrogates, and Help. Below this is a toolbar with icons for selecting nodes/edges, adding nodes and edges, centering the view, deleting elements, running and stopping simulations, loading default inputs, determining tear streams, and accessing settings. The main workspace shows a flowsheet with two nodes: 'BFB_3ads_2rgn' and 'Heat Integration heat_integration', connected by a blue arrow representing an edge. Labels with arrows identify these components and the various tools used to create them.

Home Screen (load/save problems) →

Session Flowsheet Uncertainty Optimization Surrogates Help ← Help Documents

Select a Node/Edge

Add a Node

Add a Edge

Center Flowsheet View

Delete a Node/Edge

Run a Simulation

Stop a Simulation

Load Default Inputs

Determine Tear Streams

Flowsheet Settings

Flowsheet Editor

Optimization Tool

Surrogate Model Tool

Uncertainty Quantification Tool

Edge (information transfer between models)

BFB_3ads_2rgn

Heat Integration heat_integration

Node (a model run on process simulators or Python code)

Heat Integration Node (where heat integration is performed)

Simulation Model (1)

The screenshot displays the FOQUS software interface. The main workspace shows a simulation model with two nodes: 'BFB' (labeled 'BFB_3ads_2rgn') and 'Heat Integration' (labeled 'heat_integration'). A blue arrow points from the BFB node to the Heat Integration node. A red arrow points to the BFB node with the label 'ACM Simulation Model'. The 'Node Edit' panel on the right shows the configuration for the 'BFB' node.

Node Edit Panel:

- Buttons: Apply, Revert, Run (this node only for testing), Stop Run
- Variables: Position, Post Processing
- Name: BFB, Visible:
- Error Status: Code: -1, Message: Did not finish
- Model: Type: Turbine, Model: BFB_3ads_2rgn
- Input Variables:

	Name	Value	Unit	Category	Default	Min	Max	Description	Tags
1	adsDt	15.0	m	Fixed	15.0	0.0	0.0		[]
2	adsdx	0.025	m	Fixed	0.025	0.0	0.0		[]
3	adslhx	0.5	m	Fixed	0.5	0.0	0.0		[]

Output Variables

Settings

Simulation Model (2)

FOQUS -- [not saved yet]

Session Flowsheet Uncertainty Optimization Surrogates Help

Node Edit

Apply Revert Run (this node only for testing) Stop Run

Variables Position Post Processing

Name: BFB Visible

Error Status

Code: -1

Message: Did not finish

Model

Type: Turbine Model: BFB_3ads_2rgn

Input Variables

Output Variables

Output Variables

+ - Tags

	Name	Value	Unit	Description	Tags
1	BFB_Comp_F	0.0	kmol/hr	Output stream	[]
2	BFB_Comp_P	0.0	bar	Output stream	[]

Settings

Heat Integration Tool (1)

FOQUS -- [not saved yet]

Session Flowsheet Uncertainty Optimization Surrogates Help

Heat Integration Model (GAMS)

BFB BFB_3ads_2rgn Heat Integration heat_integration

EMAT (Exchanger Minimum Approach Temperature)

HRAT (Heat Recovery Approach Temperature)

Node Edit

Apply Revert Run (this node only for testing) Stop Run

Variables Position Post Processing

Name: Heat Integration Visible

Error Status

Code: -1

Message: Did not finish

Model

Type: Plugin Model: heat_integration

Input Variables Heat Integration Inputs

	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	[]

Legend: Not Connected Tear Connected Connected

Output Variables

Settings

Heat Integration Tool (2)

FOQUS -- [not saved yet]

Session Flowsheet Uncertainty Optimization Surrogates Help

Node Edit

Apply Revert Run (this node only for testing) Stop Run

Variables Position Post Processing

Name: Heat Integration Visible

Error Status

Code: -1

Message: Did not finish

Model

Type: Plugin Model: heat_integration

Input Variables

Output Variables

Heat Integration Outputs

	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	[]

Settings

BFB BFB_3ads_2rgn Heat Integration heat_integration

Utility Consumptions

Minimum Heat Exchanger Area

Minimum Utility Cost

Optimization Solver

FOQUS - C:\FOQUS\examples\Heat_Integration\BFB_3ads_Comp_HI_SC_Opt_New.json - Last saved: 2014-09-15T11:03:42

Session Flowsheet Uncertainty **Optimization** Surrogates Help

Problem Solver Run

Solver Selection

Select Solver: OptCMA

Description of Current Solver

Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES)

Hansen, N. (2006). The CMA Evolution Strategy: A Comparing Review. In J.A. Lozano, P. Larranga, I. Inza and E. Bengoetxea (eds.). Towards a new evolutionary computation. Advances in estimation of distribution algorithms. pp. 75-102, Springer.

This plugin makes use of the CMA-ES Python module version less than 1.0 provided at https://www.lri.fr/~hansen/cmaes_inmatlab.html#python. This code is licensed under the General Public License version 2 or 3 (<http://www.gnu.org/licenses/>) and must be downloaded and installed separately by the user. This plugin provides a wrapper for the CMA-ES code allowing it to work with FOQUS.

Solver Option Settings

	Option	Setting	Description
1	upper	10.0	Upper bound on scaled variables (usually 10.0)
2	lower	0.0	Lower bound on scaled variables (usually 0.0)
3	seed	0	Random number seed (0 uses clock)
4	itmax	0	Maximum number of iterations (0 go until converges)
5	popsize	25	Number of samples per iteration
6	sd0	2	Initial standard deviation about starting point

Optimization Problem Setting

FOQUS - C:\FOQUS\examples\Heat_Integration\BFB_3ads_Comp_HI_SC_Opt_New.json - Last saved: 2014-09-15T11:03:42

Session Flowsheet Uncertainty **Optimization** Surrogates Help

Problem Solver Run ← Run Optimization

Decision Variables Select Decision Variables

	Variable	Scale	Min	Max	Value
1	<input checked="" type="checkbox"/> BFB.adsDt	Linear ←	9.0	15.0	15.0
2	<input checked="" type="checkbox"/> BFB.adsdx	Linear	0.0175	0.03	0.02533300626679941
3	<input checked="" type="checkbox"/> BFB.adslhx	Linear	0.25	0.55	0.41597851137042813
4	<input checked="" type="checkbox"/> BFB.adsN	Linear	4.0	15.0	15.0
5	<input checked="" type="checkbox"/> BFB.BFBadsB.Lb	Linear	2.8	4.2	3.973372501851228

Variable Scaling Method (Input variables are scaled to be 0 at min and 10 at max)

Min/Max Bounds

Current Value (Initial Guess)

Objective Function $f(x)$ Objective Function (Python expression)

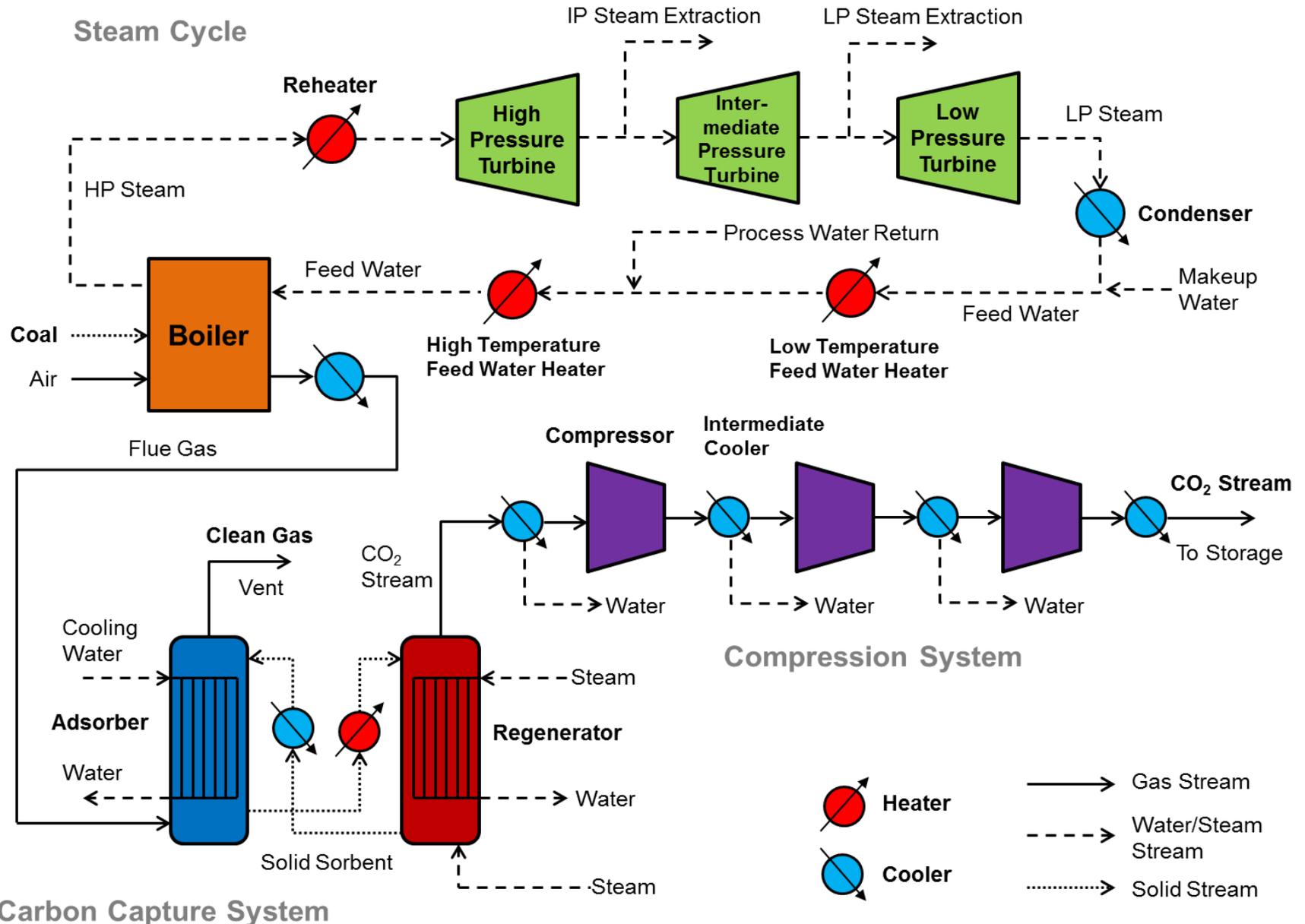
	Expression	Penalty Scale	Value for Failure
1	- f["Steam Cycle"]["Net.Efficiency.CCS"]	1.0	1000.0

Inequality Constraints $g(x) \leq 0$ Inequality Constraint (Python expression enforced with penalty)

	Expression	Penalty Factor	Form
1	0.9 - f["BFB"]["removalCO2"]	1000.0	Linear

Check Input... Variable Explorer

Case Study – A Power Plant with CO₂ Capture



Problem Statement

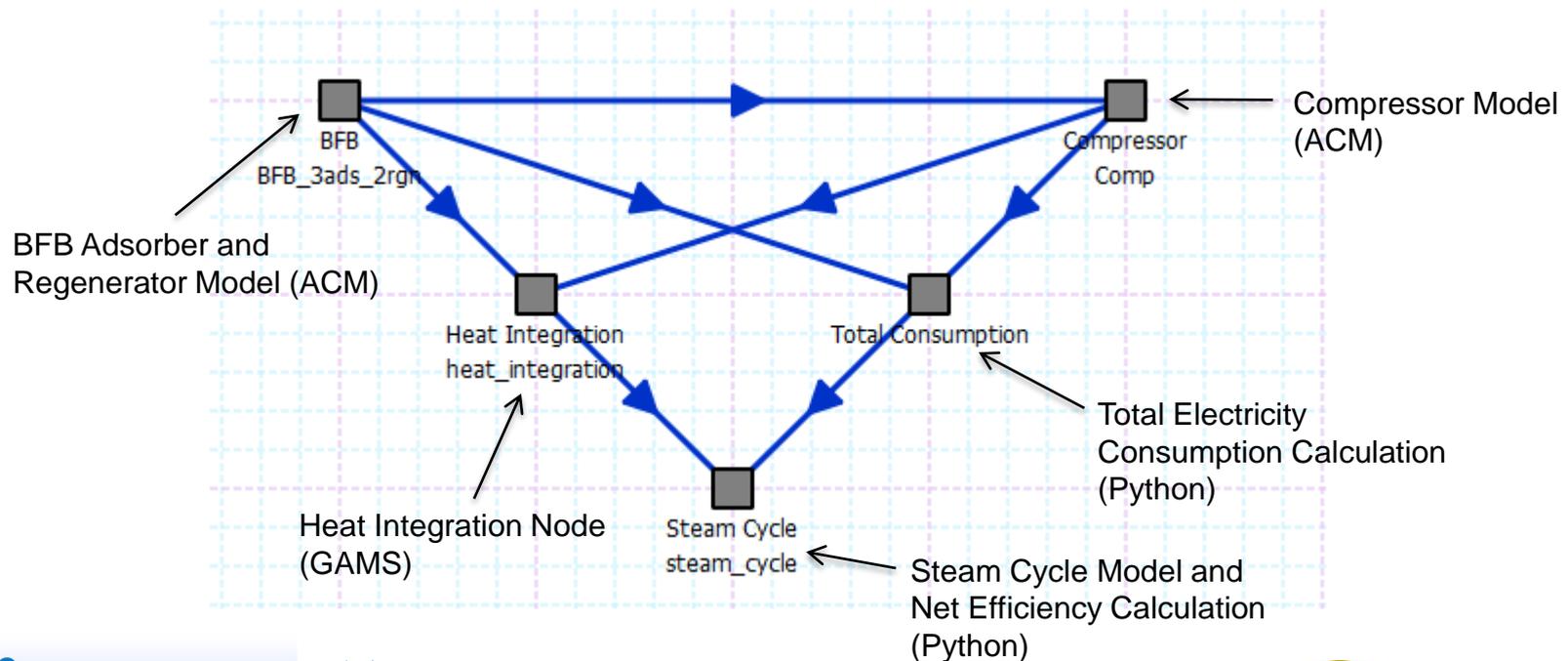
Objective Function: Maximizing **Net efficiency**

Constraint: **CO₂ removal** ratio $\geq 90\%$

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
CO₂ 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
CO₂ 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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