

CCSI

Carbon Capture Simulation Initiative

Simulation-Based Optimization Framework with Heat Integration

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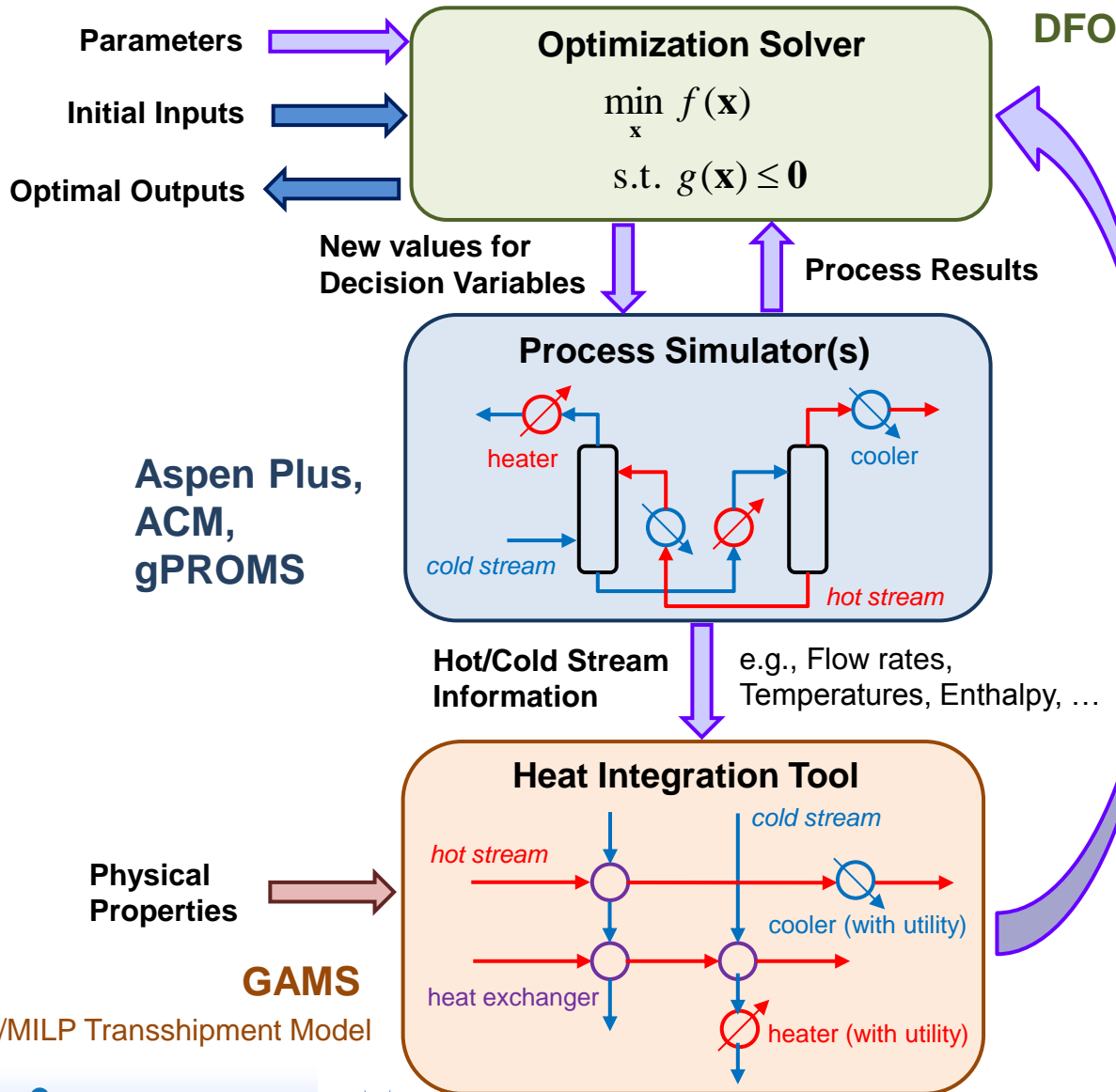
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Simulation-Based Optimization

- + 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 in optimization**
Superstructure optimization pre-determines best configuration

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

Simulation-Based Optimization with Heat Integration

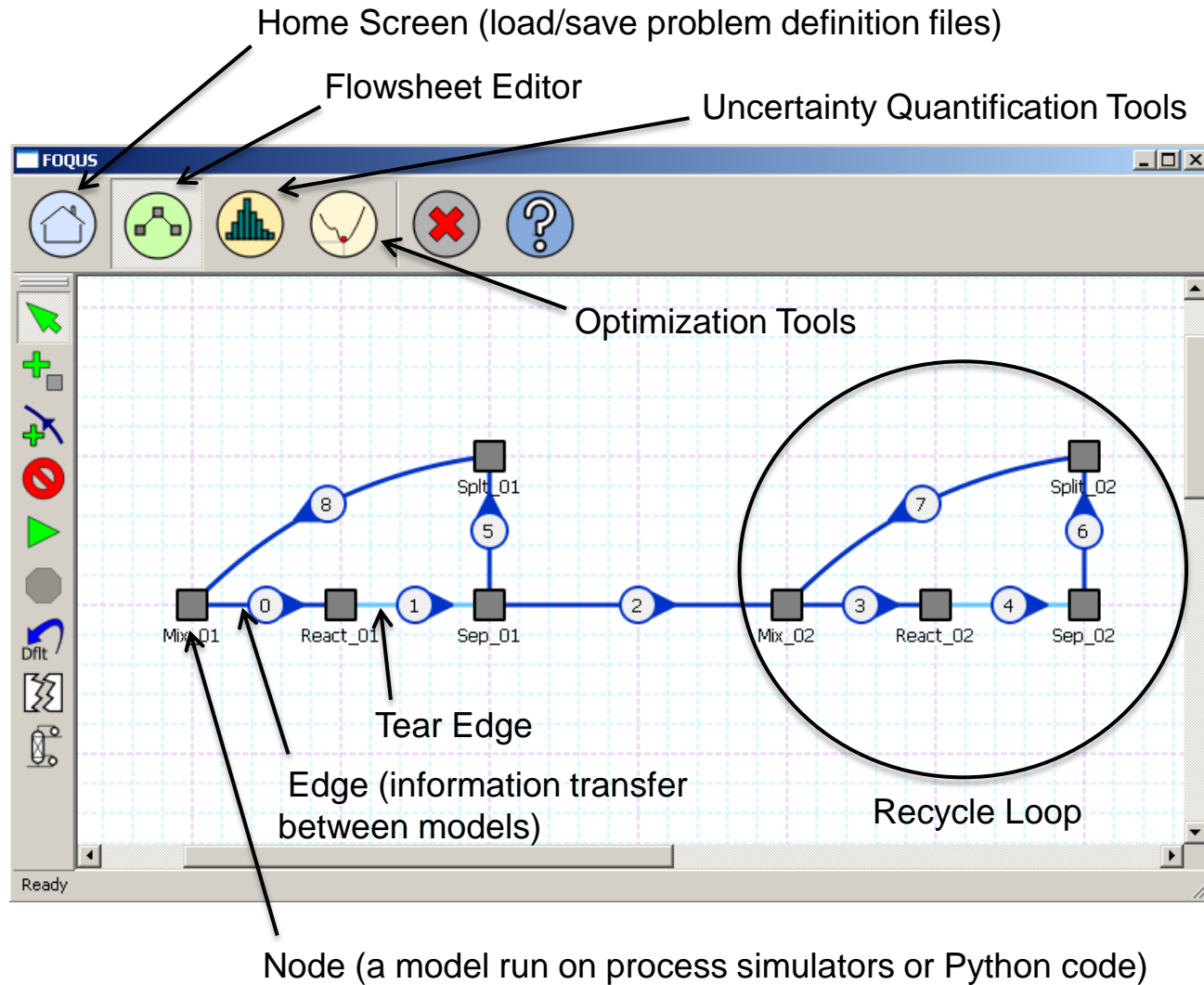


Simultaneous process optimization and heat integration are achieved in this framework

Heat Integration Results:

- Hot/cold utility consumptions
- Minimum utility cost
- Minimum number of heat exchangers
- Optimal matches between hot and cold streams

Graphic User Interface



Simulation/Calculation Task

FOQUS

Node Edit

✓ Apply ↶ Revert

Calculation Error Code (0 = okay): -1

Name:

Model:

x: y: z:

Input Variables

Name	Value	Unit	Category	Default	Min	Max	Description	Tags
1 FA_In1	1000	kmol/hr	Fixed	1000	0.0	100000.0	Flow rate of A in from stream 1	[]
2 FA_In2	100.0	kmol/hr	Fixed	100.0	0.0	100000.0	Flow rate of A in from stream 2	[]
3 FB_In1	0.0	kmol/hr	Fixed	0.0	0.0	100000.0	Flow rate of B in from stream 1	[]
4 FB_In2	0.0	kmol/hr	Fixed	0.0	0.0	100000.0	Flow rate of B in from stream 2	[]
5 FC_In1	0.0	kmol/hr	Fixed	0.0	0.0	100000.0	Flow Rate of C in from stream 1	[]
6 FC_In2	0.0	kmol/hr	Fixed	0.0	0.0	100000.0	Flow rate of C in from stream 3	[]

Output Variables

Name	Value	Unit	Description	Tags
1 FA_Out	1040.0			[]
2 FB_Out	5.0			[]
3 FC_Out	10.0			[]

Ready

Heat Integration Interface

The screenshot displays the FOQUS software interface. On the left is a process flow diagram on a grid, showing a 'BFB' unit connected to a 'Heat Integration' unit. On the right is the 'Node Edit' window for the 'Heat Integration' node.

Heat integration inputs (indicated by an arrow pointing to the 'Heat Integration' node in the diagram)

Minimum temperature difference (indicated by an arrow pointing to the 'Hrat' input variable in the table)

Heat integration outputs (indicated by an arrow pointing to the 'Cooling_Water.Consumption' output variable in the table)

Utility consumptions (indicated by arrows pointing to 'Cooling_Water.Consumption', 'HP_Steam.Consumption', and 'MP_Steam.Consumption' output variables)

of heat exchangers (indicated by an arrow pointing to the 'Min.No.HX' output variable)

Utility cost (indicated by an arrow pointing to the 'Utility.Cost' output variable)

Node Edit Window Details:

Calculation Error Code (0 = okay): -1

Name: Heat Integration

Model: Heat Integration

x: -200.0 y: 0.0 z: 0.0

Input Variables

Name	Value	Unit	Category	Default	Min	Max	Description	Tags
1 Hrat	10.0	K	Fixed	10.0	0.0	500.0	Minimum approach temperature	[]
2 Max.Time	60.0	second	Fixed	60.0	0.0	10000.0	Maximum allowable time for heat integration	[]
3 Net.Power	null	MW	Fixed	0.0	0.0	1000.0	Net power output without CCS	[]

Output Variables

Name	Value	Unit	Description	Tags
1 Cooling_Water.Consumption	null	GJ/hr	Cooling water (20 C) consumption (Cost: \$0.21/GJ)	[]
2 FH.Heat.Addition	null	GJ/hr	Heat addition to feed water heaters	[]
3 HP_Steam.Consumption	null	GJ/hr	High-pressure steam (230 C) consumption (Cost: \$8.04/GJ)	[]
4 MP_Steam.Consumption	null	GJ/hr	Medium-pressure steam (164 C) consumption (Cost: \$6.25/GJ)	[]
5 Min.No.HX	null	None	Minimum number of heat exchangers	[]
6 Utility.Cost	null	\$/hr	Total utility cost	[]

Optimization Problem Setting

Solver selection and parameters

Select decision variables

Variable Scaling Method
input variables are scaled
to be 0 at min and 10 at max

Min/Max constraints

Current Value
(initial guess)

Objective function
Python expression

Inequality constraint
Python expression
(enforced with penalty)

Variable	Scale	Min	Max	Value
1 <input checked="" type="checkbox"/> BFB.rgndx	Linear	0.014	0.026	0.02
2 <input checked="" type="checkbox"/> BFB.BFBads.T.Lb	Linear	2.8	4.2	4.0
3 <input checked="" type="checkbox"/> BFB.BFBrgn.T.Lb	Linear	2.8	4.2	4.0
4 <input checked="" type="checkbox"/> BFB.adslhx	Linear	0.25	0.55	0.5
5 <input type="checkbox"/> BFB.GHXfg.GasOut.T	None	25.0	40	40.0
6 <input checked="" type="checkbox"/> BFB.SolidIn.Fm	Linear	400000.0	900000.0	600000.0

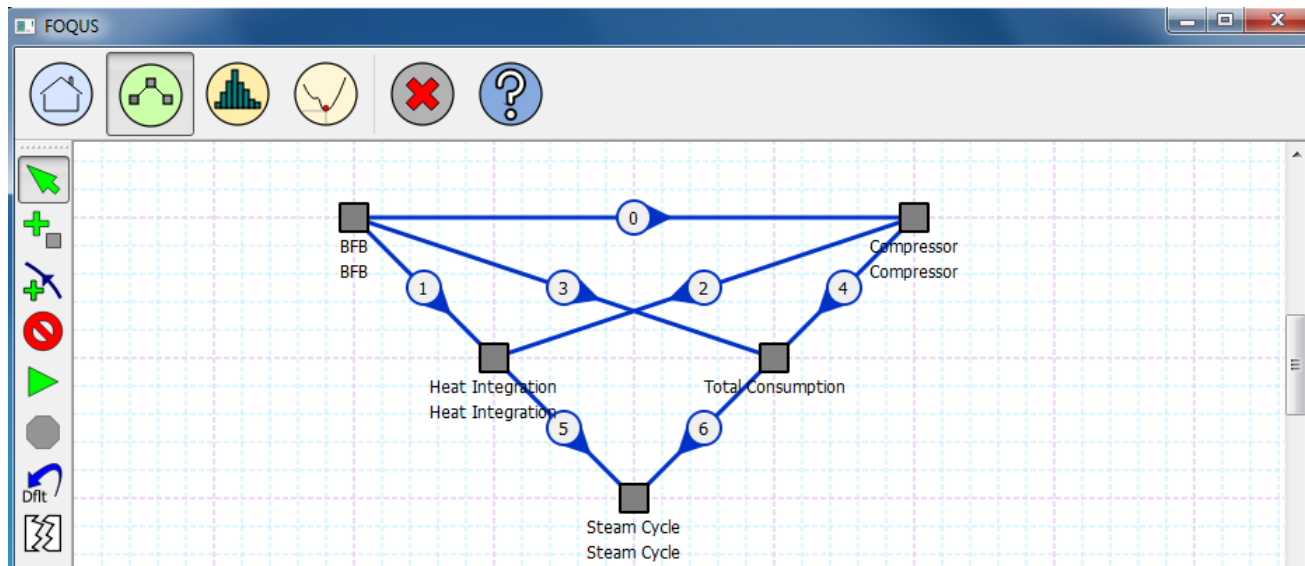
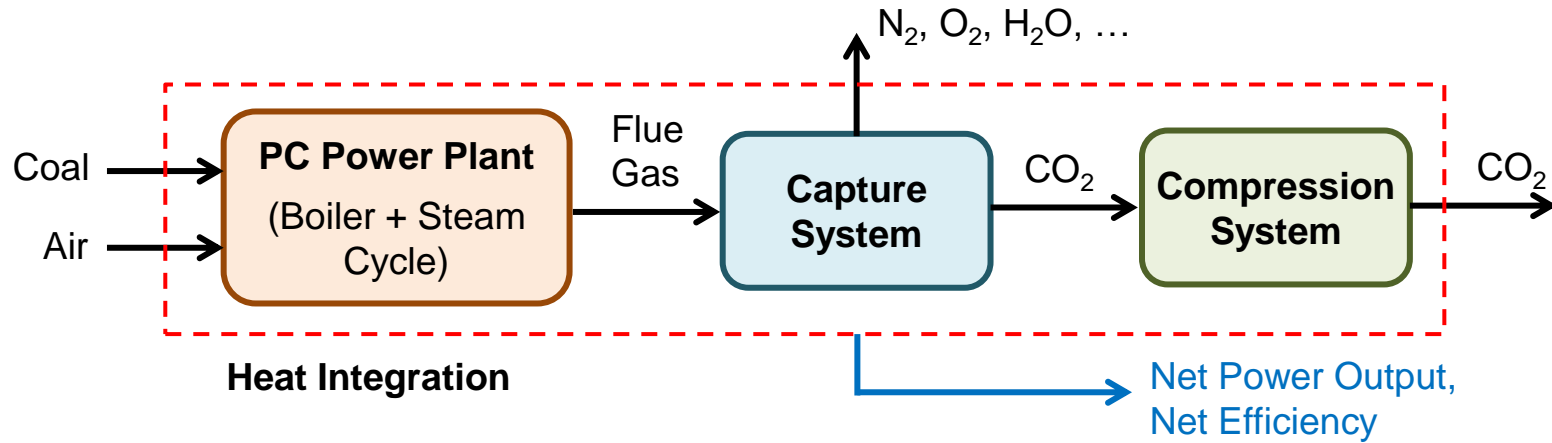
Expression	Penalty Scale	Value for Failure
1 f["BFBCost.B49"].value	1.0	1000.0

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

Start/Monitor Optimization

Problem Definition

Case Study



Case Study Results

Objective Function: Maximizing net efficiency

Constraint: CO₂ removal ratio ≥ 90%

Decision Variables (17): Bed length, diameter, sorbent and steam feed rate

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 (%)	32.6	31.8	30.0
Net power output (MW _e)	504.3	491.5	463.9
CO₂ removal ratio (%)	91.9	90.2	90.2
Electricity consumption (MW _e)	86.9	75.1	75.1
IP steam withdrawn from power cycle (kg/s)	0	0	0
LP steam withdrawn from power cycle (kg/s)	93.9	125.3	139.0
Cooling water consumption (m ³ /s)	12.8	10.4	20.7
Heat addition to feed water (MW _{th})	135.4	139.8	0

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

Software: FOQUS

Framework for Optimization and Quantification of Uncertainty and Sensitivity

- Builds on Sinter and the Turbine Gateway
- Common framework for model execution
 - simulation based optimization
 - uncertainty quantification (UQ)
 - steady state reduced model building (coming soon)

More information: <https://www.acceleratecarboncapture.org>

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