Optimization and Heat Integration in Simulation Models

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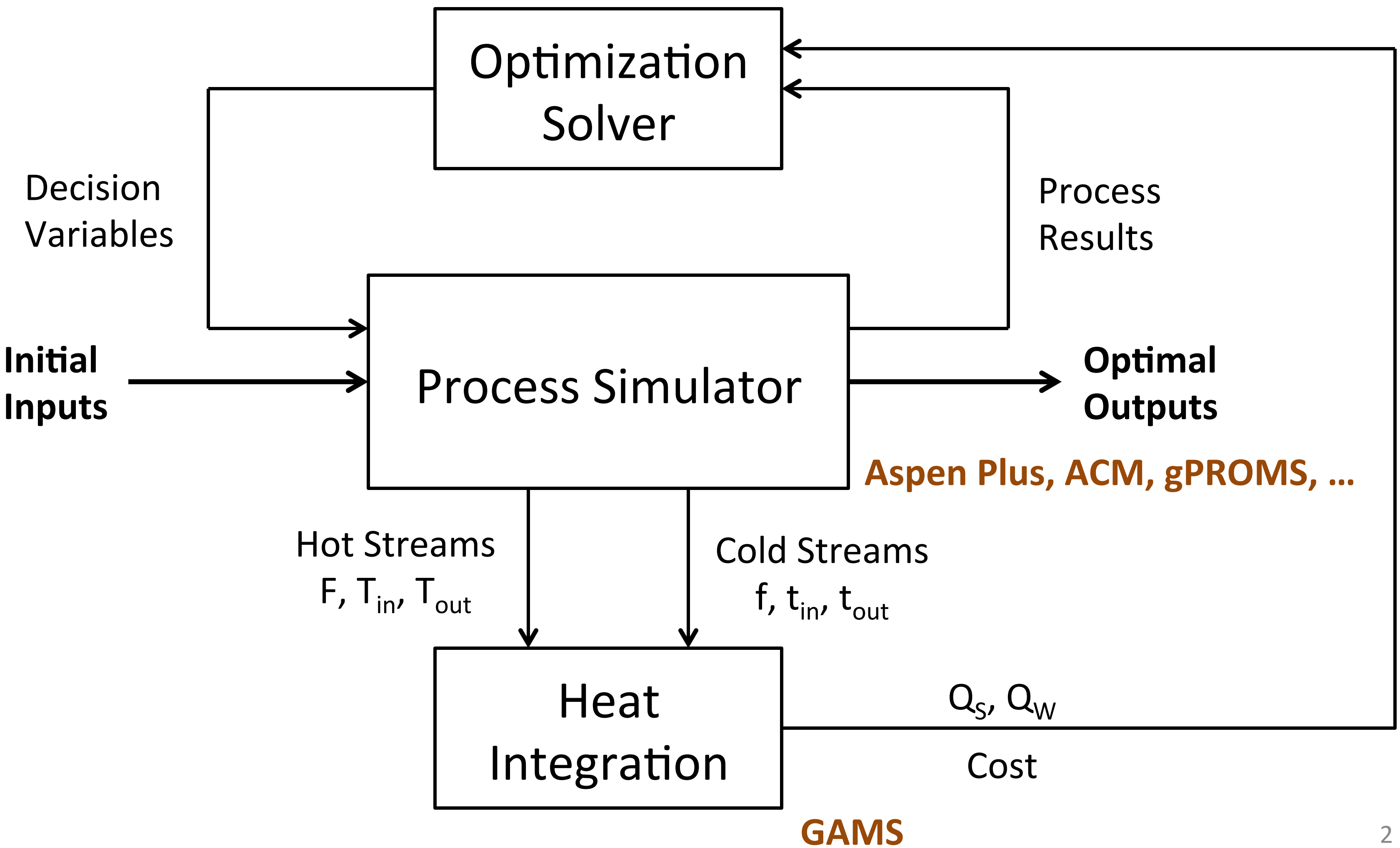
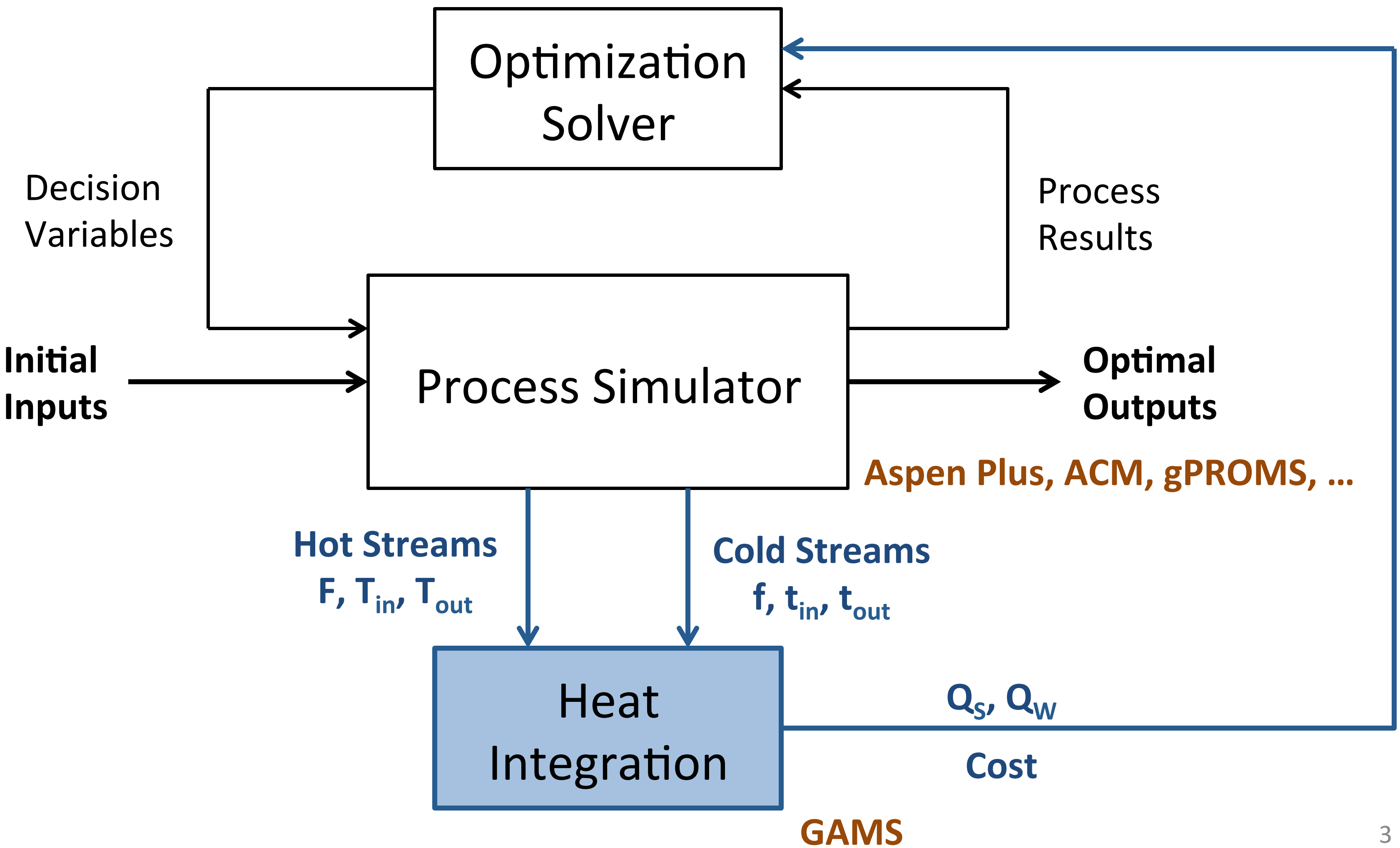
CCSI™
Carbon Capture Simulation Initiative

CAPD CENTER

Simulation-Based Optimization Framework

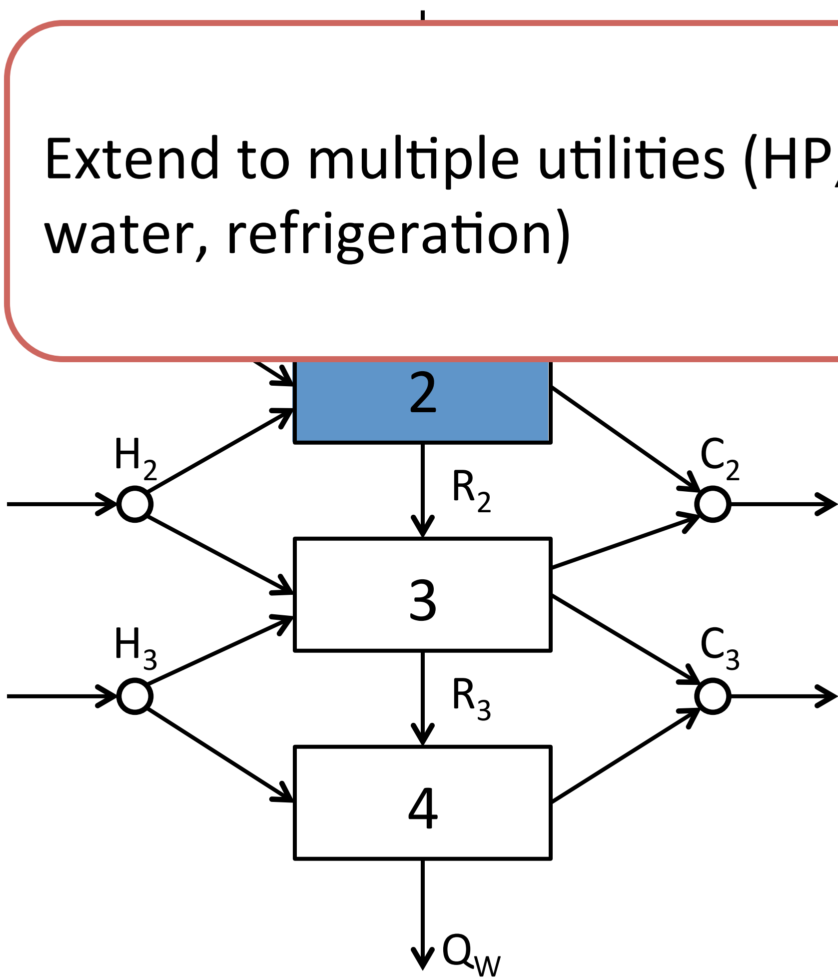


Simulation-Based Optimization Framework

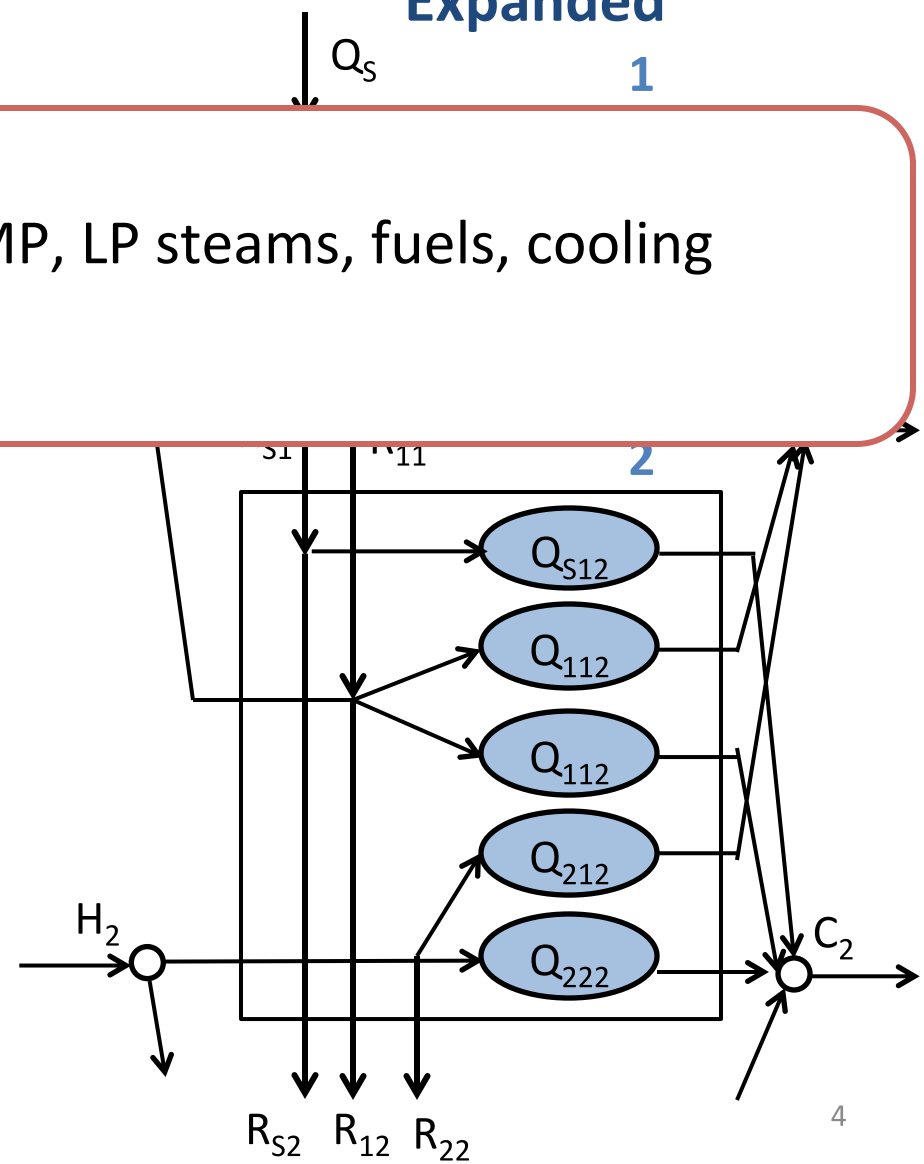


Transshipment Model

Compact



Expanded



Extend to multiple utilities (HP, MP, LP steams, fuels, cooling water, refrigeration)

Transshipment Model (LP Version)

- 1st Step: LP transshipment model
  - Minimum hot and cold utility consumption
  - Minimum utility cost

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

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

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

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

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

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

$$R_{i0} = R_{iK} = 0$$

Q^S	heat load of hot utility
Q^W	heat load of cold utility
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

Transshipment Model (MILP Version)

- 2nd Step: MILP transshipment model
  - Matches between process streams and utilities
  - Minimum number of heat exchangers
  - Minimum capital cost for heat exchange

network

$$\min \sum_{i \in H} \sum_{j \in C} y_{ij}^q$$

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

$$\sum_{i \in H_k} Q_{ijk} = Q_{jk}^C \qquad j \in C_k \qquad k = 1, \ldots, K_q$$

$$\sum_{k=1}^{K_q} Q_{ijk} - U_{ij} y_{ij}^q \leq 0$$

$$R_{ik},\ Q_{ijk} \geq 0$$

y	stream match
Q	exchange of heat
R	heat residual
U	upper bound of heat load
q	subnetwork
k	temperature interval
i	hot stream
j	cold stream

Case Study Problems – Similar Flows (FCp)

	Hot Streams				Cold Streams		
	FCp (MW/°C)	Tin (°C)	Tout (°C)		FCp (MW/°C)	Tin (°C)	Tout (°C)
1	1	400	120	1	1.5	160	400
2	2	340	120	2	1.3	100	250
3	1.5	380	150	3	2.5	50	300
4	2.5	300	100	4	2.8	200	380
5	1.7	420	160	5	1.9	150	450
6	0.8	390	110	6	0.8	100	180
7	1.2	360	200	7	1.7	200	350
8	1.8	280	130	8	1.6	120	330
9	1.1	250	80	9	0.9	110	220
10	1.3	330	170	10	2.1	190	360
11	2.1	430	300	11	1.8	260	420
12	2.2	200	100	12	1.2	80	180
13	1.2	150	70	13	1.6	130	390
14	1.6	330	180	14	1.4	180	260
15	1.9	370	115	15	2	155	365
16	1.4	355	105	16	1	95	480
17	0.9	310	130	17	1.1	175	385
18	1.3	260	90	18	1.5	130	290
19	1.1	300	115	19	2.2	210	430
20	2.3	265	190	20	1.7	230	370

Steam: HP 500°C, MP 350°C

Cooling Water: 20 - 50°C

Case Study Problems – Dissimilar Flows (FCp)

	Hot Streams				Cold Streams		
	FCp (MW/°C)	Tin (°C)	Tout (°C)		FCp (MW/°C)	Tin (°C)	Tout (°C)
1	6	400	120	1	14	160	400
2	2	340	120	2	3	100	250
3	0.5	380	150	3	0.4	50	300
4	8	300	100	4	2.5	200	380
5	3	420	160	5	2	150	450
6	4	390	110	6	6	100	180
7	0.2	360	200	7	1.5	200	350
8	0.6	280	130	8	0.2	120	330
9	1.5	250	80	9	5.5	110	220
10	4	330	170	10	3	190	360
11	12	430	300	11	8	260	420
12	8	200	100	12	12	80	180
13	5	150	70	13	0.3	130	390
14	0.6	330	180	14	4.5	180	260
15	0.3	370	115	15	1	155	365
16	6	355	105	16	0.1	95	480
17	0.9	310	130	17	7	175	385
18	3	260	90	18	2	130	290
19	1	300	115	19	0.5	210	430
20	0.3	265	190	20	1.7	230	370

Steam: HP 500°C, MP 350°C

Cooling Water: 20 - 50°C

Case Study Results – Similar Flows (FCp)

Problem Size	LP Transshipment Model				MILP Transshipment Model			
# of Hot Streams * # of Cold Stream	# of Continuous Variables	QS (MW)	QW (MW)	CPU Time (seconds)	# of Continuous Variables	# of Binary Variables	Minimum Matches	CPU Time (seconds)
2 * 2	38	45	210	0.031	38	10	8	0.156
3 * 3	72	115	0	0.031	72	17	8	0.047
5 * 5	235	307	60	0.031	235	67	24	0.421
10 * 10	1057	474	197	0.031	1057	219	42	1059.309
15 * 15	2692	711	391.5	0.031	2692	421	(57)	------
20 * 20	6284	1473	684.5	0.031	6284	778	(83)	------

------ : global optimal solution was not obtained within 100,000 seconds.

Case Study Results – Dissimilar Flows (FCp)

Problem Size	LP Transshipment Model				MILP Transshipment Model			
# of Hot Streams * # of Cold Stream	# of Continuous Variables	QS (MW)	QW (MW)	CPU Time (seconds)	# of Continuous Variables	# of Binary Variables	Minimum Matches	CPU Time (seconds)
2 * 2	38	1910	220	0.047	38	12	9	0.187
3 * 3	72	1861	186	0.031	72	24	14	0.189
5 * 5	235	1105	760	0.031	235	67	26	0.311
10 * 10	1057	825	755	0.047	1057	196	39	23.104
15 * 15	2692	786	514.5	0.016	2692	392	55	760.583
20 * 20	6284	1351.5	1283	0.031	6284	712	(81)	------

------ : global optimal solution was not obtained within 100,000 seconds.

Next Step: Link Heat Integration Tool to Simulators

- Link the heat integration tool (GAMS model) to process simulators (including ACM and Aspen plus) and optimization solver through Python or C-based programs.

- Test some simple ACM models at first.

- Initial demonstration: solid sorbent absorber/regenerator ACM model for CO_2 capture

- Variable FCp: piecewise linear approximation

Disclaimer