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Carbon Capture Simulation Initiative

Tight Reformulation of Transshipment Model for Heat Integration Problems

Yang Chen [a], Ignacio Grossmann [a], David Miller [b]

a. Dept. of Chemical Engineering, Carnegie Mellon University

b. DOE, National Energy Technology Laboratory

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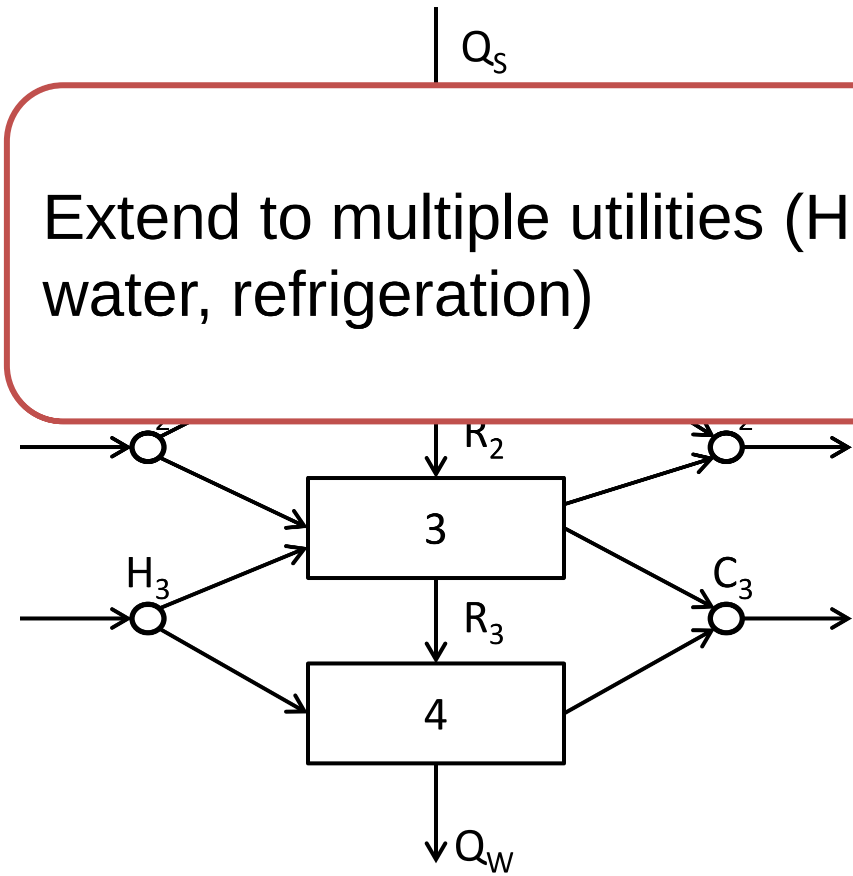
Introduction

- Heat integration plays an important role to reduce energy consumption and CO_2 emissions.
- Sequential procedures to synthesize heat exchanger networks:
  - **Step 1**: Minimize utility cost → LP Transshipment Model
  - **Step 2**: Predict optimal stream matches for minimizing the number of heat exchangers → MILP Transshipment Model
  - **Step 3**: Derive heat exchanger network structures for minimizing the investment cost → NLP Model
- Sequential approach is a practical way to solve large scale heat integration problems.

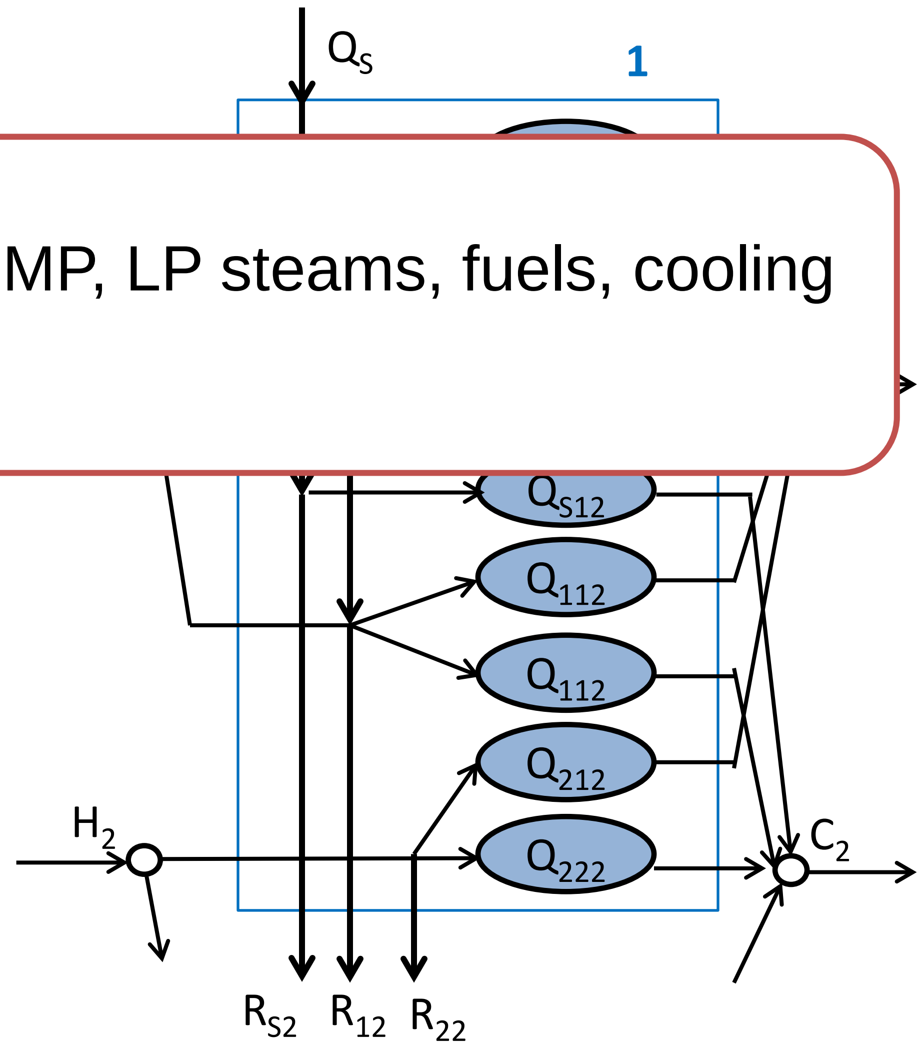
Goal: Study alternative approaches for solving MILP Transshipment model.

Transshipment Model

Compact



Expanded



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

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

Transshipment Model Formulations

LP Transshipment Model

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

$$\left.\begin{aligned}
\text{s.t.} \quad & R_{ik} - R_{i,k-1} + \sum_{j \in C_k} Q_{ijk} + \sum_{n \in W_k} Q_{ink} = Q_{ik}^H && i \in H_k' \\
& R_{mk} - R_{m,k-1} + \sum_{j \in C_k} Q_{mjk} - Q_m^S = 0 && m \in S_k' \\
& \sum_{i \in H_k} Q_{ijk} + \sum_{m \in S_k} Q_{mjk} = Q_{jk}^C && j \in C_k \\
& \sum_{i \in H_k} Q_{ink} - Q_n^W = 0 && n \in W_k \quad k = 1, \ldots, K
\end{aligned}\right\} \text{Heat Balances}$$

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

- 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

MILP Transshipment Model

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

$$\left.\begin{aligned}
\text{s.t.} \quad & R_{ik} - R_{i,k-1} + \sum_{j \in C_k} Q_{ijk} = Q_{ik}^H && i \in H_k' \\
& \sum_{i \in H_k} Q_{ijk} = Q_{jk}^C && j \in C_k \quad k = 1, \ldots, K_q
\end{aligned}\right\} \text{Heat Balances}$$

$$\left.\sum_{k=1}^{K_p} Q_{ijk} - U_{ij} y_{ij}^p \leq 0 \right\} \text{Match Constraints}$$

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

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

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MILP Transshipment model is difficult to solve

- Computational time increases exponentially with the problem size.

Balanced Streams

Case	Solution	CPU Time (s)
5H, 5C	24	0.5
8H, 8C	35	35.9
10H, 10C	42	1017.9
12H, 12C	48	68688.6
15H, 15C	57	> 100000

Absolute Gap = 0.99

FCp: 0.8 ~ 2.8 MW/°C

Unbalanced Streams

Case	Solution	CPU Time (s)
5H, 5C	26	0.3
10H, 10C	39	25.7
15H, 15C	55	660.1
17H, 17C	67	> 100000
20H, 20C	78	> 100000

Absolute Gap = 0.99

FCp: 0.1 ~ 14 MW/°C

Somewhat easier to solve!

- Reasons for slow computational speed:
  - Large LP relaxation gap
  - Unit coefficients in the objective function

Approaches to Reduce Computation

Model Reformulation

- Disaggregated Models
- Additional Integer Cuts
- Priority for Integer Variables

Model Modification

- Weighted Factors in Objective Function

Approximate Approaches

- Relative Optimality Gap
- Heuristic for Reduced MILP Model
- NLP Reformulation

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Disaggregated Models

Original Transshipment Model

$$\sum_{k=1}^{K_p} Q_{ijk} - U_{ij} y_{ij}^{p} \le 0, \quad \forall i \in H,\ j \in C \qquad U_{ij} = \min\left\{ \sum_{k=1}^{K_p} Q_{ik}^{H},\ \sum_{k=1}^{K_p} Q_{jk}^{C} \right\}$$

Disaggregated Transshipment Model

$$Q_{ijk} - U_{ijk} y_{ij}^{p} \le 0, \quad \forall i \in H,\ j \in C, k \in K \qquad U_{ijk} = \min\left\{ \sum_{l=1}^{k} Q_{il}^{H},\ Q_{jk}^{C} \right\}$$

Transportation Model

$$q_{iljk} - U_{iljk} y_{ij}^{p} \le 0, \quad \forall i \in H,\ j \in C, l \in K, k \in K$$

$$U_{iljk} = \min\left\{ Q_{il}^{H}, Q_{jk}^{C} \right\}$$

$$\sum_{l=1}^{k} q_{iljk} = Q_{ijk}$$

y	stream match
Q, q	exchange of heat
Q^H	heat load of hot process stream
Q^C	heat load of cold process stream
U	upper bound of heat load
p	subnetwork
k, l	temperature interval
i	hot stream
j	cold stream

LP Relaxations of Disaggregated Models

Case	Solution	LP Relaxation		
		Original Transshipment Model	Disaggregated Transshipment Model	Transportation Model
Balanced Streams				
5H, 5C	24	16.302	16.718	16.802
8H, 8C	35	24.357	24.755	24.791
10H, 10C	42	28.848	30.075	30.103
12H, 12C	48	32.135	33.395	33.629
15H, 15C	57	40.390	42.388	42.576
Unbalanced Streams				
5H, 5C	26	17.931	20.072	20.645
10H, 10C	39	29.969	31.899	32.609
15H, 15C	55	41.424	43.477	44.640
17H, 17C	67	48.839	52.636	53.551
20H, 20C	78	56.593	61.848	63.231

Disaggregated models: tighter LP relaxations.

Computational Performance of Disaggregated Models

Case	Solution	CPU Time (s)		
		Original Transshipment Model	Disaggregated Transshipment Model	Transportation Model
Balanced Streams				
5H, 5C	24	0.5	0.5	0.4
8H, 8C	35	35.9	34.9	91.1
10H, 10C	42	1017.9	1011.4	3075.1
12H, 12C	48	68688.6	36356.6	> 100000
15H, 15C	57	> 100000	> 100000	> 100000
Unbalanced Streams				
5H, 5C	26	0.3	0.2	0.4
10H, 10C	39	25.7	21.1	150.1
15H, 15C	55	660.1	1043.1	> 100000
17H, 17C	67	> 100000	76676.2	> 100000
20H, 20C	78	> 100000	> 100000	> 100000

Transshipment MILP model outperforms Transportation MILP model.

Disaggregated Transshipment model: shorter computational times than the original model in most of cases.

Additional Integer Cuts

$$\sum_{j\in C} y_{ij}^p \geq \left\lceil \frac{\sum_{k=1}^{K_p} Q_{ik}^H}{\max_{j\in C}\left\{\sum_{k=1}^{K_p} Q_{jk}^C\right\}} \right\rceil, \ \forall i \in H \qquad \sum_{i\in H} y_{ij}^p \geq \left\lceil \frac{\sum_{k=1}^{K_p} Q_{jk}^C}{\max_{i\in H}\left\{\sum_{k=1}^{K_p} Q_{ik}^H\right\}} \right\rceil, \ \forall j \in C \qquad \sum_{i\in H}\sum_{j\in C} y_{ij}^p \leq \sum_{i\in H} N_i^p + \sum_{j\in C} N_j^p$$

y stream match
Q^H,Q^C heat load of hot/cold stream
p subnetwork
k temperature interval
i hot stream
j cold stream
N number of streams

Case	Solution	LP Relaxation			
		Original Transshipment Model		Disaggregated Transshipment Model	
		w/o cuts	w/ cuts	w/o cuts	w/ cuts
Balanced Streams					
5H, 5C	24	16.302	17.383	16.718	17.642
8H, 8C	35	24.357	24.416	24.755	24.850
10H, 10C	42	28.848	29.852	30.075	30.876
12H, 12C	48	32.135	32.854	33.395	34.268
15H, 15C	57	40.390	40.633	42.388	42.662
Unbalanced Streams					
5H, 5C	26	17.931	18.178	20.072	20.645
10H, 10C	39	29.969	30.067	31.899	32.609
15H, 15C	55	41.424	41.604	43.477	44.669
17H, 17C	67	48.839	49.246	52.636	53.674
20H, 20C	78	56.593	56.816	61.848	63.301

Computational Performance with Additional Integer Cuts

Case	Solution	CPU Time (s)			
		Original Transshipment Model		Disaggregated Transshipment Model	
		w/o cuts	w/ cuts	w/o cuts	w/ cuts
Balanced Streams					
5H, 5C	24	0.5	0.5	0.5	0.5
8H, 8C	35	35.9	33.0	34.9	33.2
10H, 10C	42	1017.9	1039.9	1011.4	878.3
12H, 12C	48	68688.6	65506.2	36356.6	33869.2
15H, 15C	57	> 100000	> 100000	> 100000	> 100000
Unbalanced Streams					
5H, 5C	26	0.3	0.3	0.2	0.3
10H, 10C	39	25.7	16.5	21.1	30.7
15H, 15C	55	660.1	919.2	1043.1	749.8
17H, 17C	67	> 100000	> 100000	76676.2	28682.359
20H, 20C	78	> 100000	> 100000	> 100000	> 100000

Integer cuts: increase computational speed in most of cases.

Disaggregated Transshipment model: the best MILP formulation.

Branching Priority for Binary Variables

$y_{ij}.prior = 1/UB_{ij}$ Branch y_{ij} with largest upper bound (UB_{ij}) first

Case	Solution	CPU Time (s)			
		Original Transshipment Model		Disaggregated Transshipment Model	
		w/o priority	w/ priority	w/o priority	w/ priority
Balanced Streams					
5H, 5C	24	0.5	0.5	0.5	0.5
8H, 8C	35	33.0	27.6	33.2	29.6
10H, 10C	42	1039.9	680.0	878.3	607.0
12H, 12C	48	65506.2	39856.9	33869.2	24400.8
15H, 15C	57	> 100000	> 100000	> 100000	> 100000
Unbalanced Streams					
5H, 5C	26	0.3	0.4	0.3	0.3
10H, 10C	39	16.5	6.9	30.7	31.3
15H, 15C	55	919.2	648.2	749.8	1527.2
17H, 17C	67	> 100000	> 100000	28682.359	> 100000
20H, 20C	78	> 100000	> 100000	> 100000	> 100000

Branching priority: improves the performance in most of cases.

Disaggregated Transshipment model with additional integer cuts and branching priority : the base model in the following studies.

Approaches to Reduce Computation

Model Reformulation

- Disaggregated Models
- Additional Integer Cuts
- Priority for Integer Variables

Model Modification

- Weighted Factors in Objective Function

Approximate Approaches

- Relative Optimality Gap
- Heuristic for Reduced MILP Model
- NLP Reformulation

Weighted Factors in Objective Function

Objective Function:

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

$$\downarrow$$

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

i	hot stream
j	cold stream
y	stream match
w	weighting factor
U	upper bound of heat load
ΔT	mean temperature difference
ΔT_{in}	inlet temperature difference
ΔT_{out}	outlet temperature difference

$$w_{ij} = \frac{U_{ij}}{\Delta T_{ij}}$$

$$\Delta T_{ij} = \frac{\Delta T_{\mathrm{out},ij} - \Delta T_{\mathrm{in},ij}}{\ln \dfrac{\Delta T_{\mathrm{out},ij}}{\Delta T_{\mathrm{in},ij}}}$$

$$\Delta T_{ij} \cong \left(\Delta T_{\mathrm{in},ij} \Delta T_{\mathrm{out},ij} \frac{\Delta T_{\mathrm{in},ij} + \Delta T_{\mathrm{out},ij}}{2} \right)^{1/3}$$

Computational Performance of Weighted Model

Case	Base Model		Weighted Model	
	Solution	CPU Time (s)	Solution	CPU Time (s)
Balanced Streams				
5H, 5C	24	0.5	25	0.4
8H, 8C	35	29.6	38	22.9
10H, 10C	42	607.0	47	642.8
12H, 12C	48	24400.8	53	18608.8
15H, 15C	57	> 100000	65	> 100000
Unbalanced Streams				
5H, 5C	26	0.3	26	0.2
10H, 10C	39	31.3	43	3.2
15H, 15C	55	1527.2	61	145.4
17H, 17C	67	> 100000	75	1901.0
20H, 20C	78	> 100000	85	> 100000

Absolute Gap = 0.99 Relative Gap = 1%

Investment Cost of Weighted Model

Minimize the investment cost of heat exchanger networks for both models in SYNHEAT, by fixing all stream matches in previous results.

Case	Base Model			Weighted Model		
	# of Heat Exchangers	Total Area (m^2)	Investment Cost ($/yr)	# of Heat Exchangers	Total Area (m^2)	Investment Cost ($/yr)
Balanced Streams						
5H, 5C	24	250.6	67330	25	179.0	61630
Unbalanced Streams						
5H, 5C	26	672.9	141613	26	595.3	124451

Weighted model: smaller exchanger area and investment cost, but possibly more stream matches.

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Model Modification

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Approximate Approaches

– Relative Optimality Gap
– Heuristic for Reduced MILP Model
– NLP Reformulation

Different Optimality Gap

Case	Absolute Gap = 0.99 (Base)		Relative Gap = 5%		Relative Gap = 10%	
	Solution	CPU Time (s)	Solution	CPU Time (s)	Solution	CPU Time (s)
Balanced Streams						
5H, 5C	24	0.5	24	0.5	24	0.5
8H, 8C	35	29.6	35	29.6	35	18.3
10H, 10C	42	607.0	42	607.0	42	187.5
12H, 12C	48	24400.8	48	24400.8	48	3877.9
15H, 15C	57	> 100000	57	> 100000	57	> 100000
Unbalanced Streams						
5H, 5C	26	0.3	26	0.3	26	0.3
10H, 10C	39	31.3	39	31.3	40	4.5
15H, 15C	55	1527.2	55	1442.9	56	109.8
17H, 17C	67	> 100000	67	>100000	69	6414.2
20H, 20C	78	> 100000	78	>100000	78	30682.8

10% of relative gap is acceptable for most of cases.

Heuristic Approach to Solve Reduce MILP Model

- **Step 1**: Solve the relaxed LP model (Transshipment or Transportation).
- **Step 2**: Fix y_{ij} = 0 in the full MILP model if its relaxed value = 0 in the LP model. The set for these y_{ij} is defined as Y_0^{rx}. Solve the reduced MILP model (Disaggregated Transshipment).
- **Step 3**: In the full MILP model, fix all $y_{ij} \notin Y_0^{rx}$ as the solution of the reduced MILP model.
- **Step 4**: Fix one of $y_{ij} \in Y_0^{rx}$ to be 1, and leave other $y_{ij} \in Y_0^{rx}$ as variables. Solve the test MILP problem.
- **Step 5**: Check the value of Q_{ij} for the above y_{ij}. If Q_{ij} = 0, keep y_{ij} in Y_0^{rx}. If Q_{ij} > 0, remove y_{ij} from Y_0^{rx}.
- **Step 6**: Relax the above y_{ij} to variable. Go to the next y_{ij}.
- **Repeat** Step **4** - **6** for every $y_{ij} \in Y_0^{rx}$.
- **Step 7**: Fix y_{ij} = 0 for all $y_{ij} \in Y_0^{rx}$ in the full MILP model. Solve the final reduced MILP model (Disaggregated Transshipment) and obtain the approximate solution.

Heuristic for Reduced MILP Model

Case	**Full Model (Base)**		**Reduced Model** by LP Relaxation of **Original Transshipment** Model		**Reduced Model** by LP Relaxation of **Disaggregated Transshipment** Model		**Reduced Model** by LP Relaxation of **Transportation** Model	
	Solution	CPU Time (s)	Solution	CPU Time (s)	Solution	CPU Time (s)	Solution	CPU Time (s)
Balanced Streams								
5H, 5C	24	0.5	25	2.8	24	2.9	24	2.8
8H, 8C	35	29.6	35	8.6	35	6.4	36	6.6
10H, 10C	42	607.0	44	8.0	43	92.0	43	68.8
12H, 12C	48	24400.8	51	168.7	48	348.2	48	1121.7
15H, 15C	57	> 100000	58	> 100000	59	> 100000	59	> 100000
Unbalanced Streams								
5H, 5C	26	0.3	26	2.4	26	2.4	26	2.7
10H, 10C	39	31.3	42	4.3	41	4.5	41	5.9
15H, 15C	55	1527.2	61	9.9	56	147.0	55	521.9
17H, 17C	67	> 100000	72	52.2	70	23645.9	70	10157.0
20H, 20C	78	> 100000	86	63.9	79	> 100000	82	> 100000

Reduced MILP models:

- **Good approximate solutions**
- **CPU times reduced by at least one order of magnitude**

NLP Reformulation

$$y_{ij} \in \{0,1\} \longrightarrow y_{ij} \in [0,1]$$

Option 1:

Adding to Constraints:

$$y_{ij}(1 - y_{ij}) \le \varepsilon, \quad \forall i \in H,\ j \in C$$

Option 2:

Objective Function:

$$\sum_{i \in H} \sum_{j \in C} y_{ij} + K \sum_{i \in H} \sum_{j \in C} y_{ij}(1 - y_{ij})$$

Computational Performance of NLP Model

Case	MILP Model (Base)		NLP Model	
	Solution	CPU Time (s)	Solution	CPU Time (s)
Balanced Streams				
5H, 5C	24	0.5	26	82.0
8H, 8C	35	29.6	39	233.6
10H, 10C	42	607.0	48	202.5
12H, 12C	48	24400.8	53	458.5
15H, 15C	57	> 100000	70	1291.9
Unbalanced Streams				
5H, 5C	26	0.3	26	81.9
10H, 10C	39	31.3	46	864.8
15H, 15C	55	1527.2	66	1242.7
17H, 17C	67	> 100000	79	1674.1
20H, 20C	78	> 100000	95	14804.0

NLP Solver: OQNLP

NLP Models: Faster but worse solutions

Conclusions

- MILP Transshipment model is computational expensive for large-scale problems.
- Disaggregate Transshipment model is the best formulation for most of case studies.
- Additional integer cuts and branching priority for binary variables are helpful to improve computational performance.
- Weighted factors can be added into the objective function to reduce solution times and obtain designs with lower investment costs.
- An appropriate relative optimality gap (10%) can be used to get near-optimal solutions in relatively short times.
- Reduced MILP models obtained by a heuristic approach achieves near-optimal solutions while reducing solution times by at least one order of magnitude.
- NLP formulations obtained approximate solutions in relatively short times.

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