A Modified Formulation of Optimal Source–Sink Matching in Carbon Capture and Storage Systems with Time, Injection Rate and Capacity Constraints

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Carbon capture and storage (CCS) is considered as one of the leading options in mitigating carbon dioxide emissions into the atmosphere. It involves collecting and compressing of relatively pure carbon dioxide from a given source, then storing it into a various locations or also called sinks. Multiple variables limits the implementation of CCS such as injection rate limit of sink, capacity of sink, start and end of operating life of source and sink, and other socio-economical aspects that the CCS retrofit will do to the existing carbon source facility. The proposed approach focuses on temporal issues where operating lives of sources and sink may not completely coincide. In 2012, Tan et al. developed an optimization model for optimal source sink matching in carbon capture and storage systems with time, injection rate, and capacity constraints. This paper improves the existing optimization model by eliminating inconsistencies in the optimization results. Previous case studies presented by Tan, et al. were re-evaluated and a new case study was added to further show improvement made by the modified model. The new model provides more accurate and robust results compared to the original model and eliminates inconsistencies that required human intervention in order to extract the correct conclusion. It also simplified the model, requiring lesser variables and solver iterations, and making it more suited for large scale set up optimization.

Keywords: Carbon capture and storage, source–sink matching, mixed integer linear programming

1. INTRODUCTION

In 2012, Tan et al.[1] developed an optimization model for optimal source sink matching in carbon capture and storage systems with time, injection rate, and capacity constraints. This paper aims to improve the existing optimization model and eliminate inconsistencies in the optimization results.

The summarized optimization model by Tan et al. is as follows (eq. 1 ~ 11):

$$\max \sum_k \sum_j \sum_i Q_{ik} s_{ijk} \qquad (1)$$

$$b_{ijk} S_i^L \le s_{ijk} \le b_{ijk} S_i^U \qquad \forall i,j,k \qquad (2)$$

$$b_{ijk} \in \{0,1\} \qquad \forall i,j,k \qquad (3)$$

$$b_{ijk} \le b_{ij(k+1)} \qquad \forall i,j \quad \forall k,k+1 \in K \qquad (4)$$

$$s_{ijk} \le s_{ij(k+1)} \qquad \forall i,j \quad \forall k,k+1 \in K \qquad (5)$$

$$s_{ij(k+1)} - s_{ijk} \le \left(b_{ij(k+1)} - b_{ijk}\right) S_i^U \qquad \forall i,j \quad \forall k,k+1 \in K \qquad (6)$$

$$b_{ij} T^L \le \sum_k Q_{ik} b_{ijk} \le b_{ij} T^U \qquad \forall i,j \qquad (7)$$

$$b_{ij} \in \{0,1\} \qquad \forall i,j \qquad (8)$$

$$\sum_j b_{ij} \leq 1 \qquad \forall i \qquad (9)$$
$$\sum_j \sum_i s_{ijk} Q_{ik} \leq D_j \qquad \forall j \qquad (10)$$
$$\sum_i s_{ijk} Q_{ik} \leq E_{jk} \qquad \forall j,k \qquad (11)$$

In the model by Tan et al., three decision variables were utilized namely b_{ij}, b_{ijk} and s_{ijk}. These variables dictate where the connection, b, will be from source i to sink j, on what period k they will connect, and what will be the allowed maximum CO_2 rate, s, will be obtained from the source. These variables are correlated by the following constraints:

$$b_{ijk} S_i^L \leq s_{ijk} \leq b_{ijk} S_i^U \qquad \forall i,j,k \qquad (2)$$
$$s_{ijk} \leq s_{ij(k+1)} \qquad \forall i,j \quad \forall k, k+1 \in K \qquad (5)$$
$$s_{ij(k+1)} - s_{ijk} \leq \left(b_{ij(k+1)} - b_{ijk}\right) S_i^U \qquad \forall i,j \quad \forall k, k+1 \in K \qquad (6)$$
$$b_{ij} T^L \leq \sum_k Q_{ik} b_{ijk} \leq b_{ij} T^U \qquad \forall i,j \qquad (7)$$

Equation 2 limits s_{ijk} so that it will only have a value between S_i^L and S_i^U while the multiplier b_{ijk} ensures that there will only be a flow rate when a connection is present between source and sink. Equations 6 and 5 combined limit the value of s_{ijk} such that it will retain a common value for the whole connection period between source and sink. Equation 7 ensures that sum of the periods where an active connection between source i to sink j for periods k ($\Sigma_k Q_{ik} b_{ijk}$) is within the minimum T^L and maximum T^U viable period considered for connection between source i to sink j to be established (b_{ij}=1).

Decision variables b_{ij} and b_{ijk} both represent a connection between source i to sink j with the latter having an additional dimension which is the specific period, k (every 5 years). It is therefore expected that the conclusions obtained from these variables must be consistent.

2. METHODOLOGY

CASE STUDY 1

Using Case Study 1 presented by Tan et al., the results were reproduced using Lingo v.14 platform[2]. The parameters and results are as follows:

Table 1: Case Study 1 Parameters (From Tan et al.)

Sources	Flow Rate (Mt/y)	Time of Flow (y)	Maximum Capture (Mt)
1	10	0-20	200
2	2.5	0-30	75
3	4	0-30	120
4	4	0-25	100
5	6	10-30	120
Total	26.5	n/a	615
Sinks	**Injection Limit (Mt/y)**	**Start Time (y)**	**Maximum Storage (Mt)**
A	10	0	400
B	10	5	500
Total	20	n/a	900

Table 2: Case Study 1 Results (From Tan et al.)

Source	Sink A	Sink B	Source Summary
1	10 Mt/y (t=0 to 20)	0	200 Mt (100%)
2	0	0	0 Mt (0%)
3	0	4 Mt/y (t=5 to 30)	100 Mt (83%)
4	0	0	0 Mt (0%)
5	0	6 Mt/y (t=10 to 30)	120 Mt (100%)
Sink Summary	200 Mt (50%)	220 Mt (44%)	420 Mt of CO2

Table 3: Case Study 1 b_{ij} Variable Results (Original Optimization Model Raw Results)

	j(1)	j(2)
i (1)	1	0
i (2)	0	0
i (3)	0	1
i (4)	0	0
i (5)	0	1

Table 4: Case Study 1 b_{ijk} Variable Results (Original Optimization Model Raw Results)

	Sink 1 (j=1)						Sink 2 (j=2)					
	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)
i (1)	1	1	1	1	1	1	0	0	0	0	0	1
i (2)	0	0	0	0	0	0	0	0	0	0	0	0
i (3)	0	0	0	0	0	0	0	1	1	1	1	1
i (4)	0	0	0	0	0	1	0	0	0	0	0	1
i (5)	0	0	0	0	0	0	0	0	1	1	1	1

Table 5: Case Study 1 s_{ijk} Variable Results (Original Optimization Model Raw Results)

	Sink 1 (j=1)						Sink 2 (j=2)					
j=1	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)
i (1)	10	10	10	10	10	10	0	0	0	0	0	**10**
i (2)	0	0	0	0	0	0	0	0	0	0	0	0
i (3)	0	0	0	0	0	0	0	4	4	4	4	4
i (4)	0	0	0	0	0	**4**	0	0	0	0	0	**4**
i (5)	0	0	0	0	0	0	0	0	6	6	6	6
$\Sigma_i s_{ijk}$	10	10	10	10	10	**14**	0	4	10	10	10	**24**
$\Sigma_i s_{ijk} Q_{ik}$	10	10	10	10	0	0	0	4	10	10	10	10

We can observe that only the variable b_{ij} was consistent with the optimization results presented by Tan et al. Although manual selection of values from the results can be done and the same optimized results can be obtained, such task is prone to human error and shows weakness in the optimization model since it cannot, by itself, provide the optimized solution to the problem.

MODIFICATIONS OF THE OPTIMIZATION MODEL

The optimization model results show multiple inconsistencies between b_{ijk} and b_{ij} for Sources 1 and 4. It also violated restrictions set upon by equations 7 and 9 where a connection should only exist from one source to a sink with a minimum viable period of operation. This inconsistency was due to the lack of restriction on variable b_{ijk}. This can be traced back to equation 7 and 9.

$$b_{ij} T^L \leq \sum_k Q_{ik} b_{ijk} \leq b_{ij} T^U \quad \forall i,j \quad (7)$$

$$\sum_j b_{ij} \leq 1 \quad \forall i \quad (9)$$

The restriction in equation 7 has a loophole where when the value of b_{ij} and Q_{ik} happens to be both zero (0), b_{ijk} variables after last period of Q_{ik}=1 can obtain a value of 1 or 0 without violating any constraints. Equation 9 is also rendered useless in restraining the values of b_{ijk} due to the loophole in equation 7. This is what happened in Case study 1 where the last period of Source 1 and Source 4 obtained a value of 1. This loophole can be neutralized by modifying equation 7 and 9 to 7' and 9'.

$$b_{ijk_{(Last)}} T^L \leq \sum_k Q_{ik} b_{ijk} \leq b_{ijk_{(Last)}} T^U \quad \forall i,j \quad (7')$$

$$\sum_j b_{ijk_{(Last)}} \leq 1 \quad \forall i \quad (9')$$

The variable b_{ij} is eliminated from the model and replaced by $b_{ijk(Last)}$. The variable b_{ij} in equation 7 and 9 was used as a representative for the connection between source i to sink j. The variable $b_{ijk(Last)}$ can also be used as a representative since it is assumed that the connection between source i to sink j will be retained up to the end of the planning horizon (last period k). This is reinforced by equation 4. By this modification, even if Q_{ik} and b_{ijk} are zero (0), b_{ijk} will be forced to take a zero value since equation 4 will force all b_{ijk} before $_{(Last)}$ to also be zero (0).

$$b_{ijk} \leq b_{ij(k+1)} \quad \forall i,j \quad \forall k, k+1 \in K \quad (4)$$

The current constraints for the variable s_{ijk} allow it to have a positive value even if the source no longer provides CO_2 to the sink. This was allowed since s_{ijk} variable is multiplied by Q_{ik} which zeroes out the value when the source stops operating in equations 1, 10, and 11. This result to s_{ijk} values that are inconsistent with the final conclusion obtained from the optimization model. This is reflected in source 1 where s_{ijk} retains a value of 10 for periods k=5 and k=6 even if it is no longer operational. This inconsistency is eliminated by reformulating how s_{ijk} is constrained in the model. Refer to the following:

$$b_{ijk} S_i^L \leq s_{ijk} \leq b_{ijk} S_i^U \quad \forall i,j,k \quad (2)$$

$$b_{ijk} Q_{ik} S_i^L \leq s_{ijk} \leq b_{ijk} Q_{ik} S_i^U \quad \forall i,j,k \quad (2')$$

Equation 2 restricts s_{ijk} to have a value between S_i^L and S_i^U while the factor b_{ijk} dictates where it will be a positive or a zero value. The proposed equation 2' reinforces the restriction by including the factor Q_{ik}. This will force the variable s_{ijk} to have a positive value only during the time source i is operational. This will contradict with the existing equation 5 where it forces s_{ijk} to keep its positive value up to the end of the planning horizon. It is therefore necessary to modify this equation to equation 5' in order to allow s_{ijk} to have a zero value once source i stops operating before the end of the planning horizon.

$$s_{ijk} \leq s_{ij(k+1)} \quad \forall i,j \quad \forall k, k+1 \in K \quad (5)$$

$$s_{ijk} * Q_{i(k+1)} \leq s_{ij(k+1)} \quad \forall i,j \quad \forall k, k+1 \in K \quad (5')$$

$$s_{ij(k+1)} - s_{ijk} \leq (b_{ij(k+1)} - b_{ijk})S_i^U \quad \forall i,j \quad \forall k, k+1 \in K \qquad (6)$$

Another effect of equation 2' is the simplification of equations 1, 10, and 11 since the factor Q_{ik} will no longer be necessary. This results to equations 1', 10', and 11'.

$$\max \textstyle\sum_k \sum_j \sum_i s_{ijk} \qquad (1')$$

$$\textstyle\sum_j \sum_i s_{ijk} \leq D_j \quad \forall j \qquad (10')$$

$$\textstyle\sum_i s_{ijk} \leq E_{jk} \quad \forall j,k \qquad (11')$$

A comparison table of the original optimization model and the modified optimization model can be seen in table 6. Both the original model and the modified model are calculated as a Mixed Integer Linear Program (MILP).

Table 6: Optimization Model Comparison Summary

Original Model from Tan et al.			**Modified Model**		
MILP			MILP		
$\max \sum_k \sum_j \sum_i Q_{ik} s_{ijk}$		(1)	$\max \sum_k \sum_j \sum_i s_{ijk}$		(1')
$b_{ijk} S_i^L \leq s_{ijk} \leq b_{ijk} S_i^U$	$\forall i,j,k$	(2)	$b_{ijk} Q_{ik} S_i^L \leq s_{ijk} \leq b_{ijk} Q_{ik} S_i^U$	$\forall i,j,k$	(2')
$b_{ijk} \in \{0,1\}$	$\forall i,j,k$	(3)	$b_{ijk} \in \{0,1\}$	$\forall i,j,k$	(3)
$b_{ijk} \leq b_{ij(k+1)}$	$\forall i,j \ \forall k, k+1 \in K$	(4)	$b_{ijk} \leq b_{ij(k+1)}$	$\forall i,j \ \forall k, k+1 \in K$	(4)
$s_{ijk} \leq s_{ij(k+1)}$	$\forall i,j \ \forall k, k+1 \in K$	(5)	$s_{ijk} Q_{i(k+1)} \leq s_{ij(k+1)}$	$\forall i,j \ \forall k, k+1 \in K$	(5')
$s_{ij(k+1)} - s_{ijk} \leq (b_{ij(k+1)} - b_{ijk}) S_i^U$	$\forall i,j \ \forall k, k+1 \in K$	(6)	$s_{ij(k+1)} - s_{ijk} \leq (b_{ij(k+1)} - b_{ijk}) S_i^U$	$\forall i,j \ \forall k, k+1 \in K$	(6)
$b_{ij} T^L \leq \sum_k Q_{ik} b_{ijk} \leq b_{ij} T^U$	$\forall i,j$	(7)	$b_{ijk_{LAST}} T^L \leq \sum_k Q_{ik} b_{ijk} \leq b_{ijk_{LAST}} T^U$	$\forall i,j$	(7')
$b_{ij} \in \{0,1\}$	$\forall i,j$	(8)	*(deleted)*	*(deleted)*	(8)
$\sum_j b_{ij} \leq 1$	$\forall i$	(9)	$\sum_j b_{ijk_{LAST}} \leq 1$	$\forall i$	(9')
$\sum_j \sum_i s_{ijk} Q_{ik} \leq D_j$	$\forall j$	(10)	$\sum_j \sum_i s_{ijk} \leq D_j$	$\forall j$	(10')
$\sum_i s_{ijk} Q_{ik} \leq E_{jk}$	$\forall j,k$	(11)	$\sum_i s_{ijk} \leq E_{jk}$	$\forall j,k$	(11')

Presented in Tables 7 and 8 are the results of Case Study 1 using the Modified Optimization Model.

Table 7: Case Study 1 b_{ijk} Variable Results (Modified Optimization Model Raw Results)

	Sink 1 (j=1)						Sink 2 (j=2)					
	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)
i (1)	1	1	1	1	1	1	0	0	0	0	0	0
i (2)	0	0	0	0	0	0	0	0	0	0	0	0
i (3)	0	0	0	0	0	0	0	1	1	1	1	1
i (4)	0	0	0	0	0	0	0	0	0	0	0	0
i (5)	0	0	0	0	0	0	0	0	1	1	1	1

Table 8: Case Study 1 s_{ijk} Variable Results (Modified Optimization Model Raw Results)

	Sink 1 (j=1)						Sink 2 (j=2)					
j=1	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)
i (1)	10	10	10	10	0	0	0	0	0	0	0	0
i (2)	0	0	0	0	0	0	0	0	0	0	0	0
i (3)	0	0	0	0	0	0	0	4	4	4	4	4
i (4)	0	0	0	0	0	0	0	0	0	0	0	0
i (5)	0	0	0	0	0	0	0	0	6	6	6	6
$\Sigma_i s_{ijk}$	10	10	10	10	0	0	0	4	10	10	10	10

The same objective value of 420 Mt of CO2 was obtained using the modified optimization model. We can also observe that all the inconsistencies between the results of Tan et al. and the raw data from the model have been eliminated. This eliminates the need for human intervention to properly pick out the correct results from the model.

CASE STUDY 2

Case 2 from Tan, et al. was also evaluated to test consistency of results of the modified optimization model. Both original and modified model obtained an objective value of 530 MT of CO2. The modified model has also successfully eliminated the inconsistencies in the results.

CASE STUDY 3

To further magnify the problem of the original optimization model, Case Study 3 is presented below. Case study 3 considers a longer planning horizon of 40 years.

Table 9: Case Study 3 Parameters

Sources	Flow Rate (Mt/y)	Time of Flow (y)	Maximum Capture (Mt)
1	10	0-20	200
2	2.5	0-30	75
3	4	0-35	140
4	4	0-25	100
5	6	10-40	180
Total	26.5	n/a	695
Sinks	**Injection Limit (Mt/y)**	**Start Time (y)**	**Maximum Storage (Mt)**
A	10	0	400
B	10	5	500
Total	20	n/a	900

Table 10: Case Study 3 Results

Sources	Sink A	Sink B	Source Summary
1	10 Mt/y (t=0 to 20)	0	200 Mt (100%)
2	0	0	0 Mt (0%)
3	0	4 Mt/y (t=5 to 35)	120 Mt (86%)
4	0	4 Mt/y (t=5 to 25)	80 Mt (80%)
5	6 Mt/y (t=20 to 40)	0	120 Mt (67%)
Sink Summary	320 Mt (80%)	200Mt(40%)	520 Mt of CO2

Table 11: Case Study 3 b_{ij} Variable Results (Original Optimization Model Raw Results)

	j(1)	j(2)
i (1)	1	0
i (2)	0	0
i (3)	0	1
i (4)	0	1
i (5)	1	0

Table 12: Case Study 3 b_{ijk} Variable Results (Original Optimization Model Raw Results)

	Sink 1 (j=1)								Sink 2 (j=2)							
	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)
i (1)	1	1	1	1	1	1	1	1	0	0	0	0	0	1	1	1
i (2)	0	0	0	0	0	0	1	1	0	0	0	0	0	0	1	1
i (3)	0	0	0	0	0	0	0	1	0	1	1	1	1	1	1	1
i (4)	0	0	0	0	0	1	1	1	0	1	1	1	1	1	1	1
i (5)	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0

Table 13: Case Study 3 s_{ijk} Variable Results (Original Optimization Model Raw Results)

	Sink 1 (j=1)								Sink 2 (j=2)							
j=1	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)
i (1)	10	10	10	10	10	10	10	10	0	0	0	0	0	10	10	10
i (2)	0	0	0	0	0	0	2.5	2.5	0	0	0	0	0	0	2.5	2.5
i (3)	0	0	0	0	0	0		4	0	4	4	4	4	4	4	4
i (4)	0	0	0	0	0	4	4	4	0	4	4	4	4	4	4	4
i (5)	0	0	0	0	6	6	6	6	0	0	0	0	0	0	0	0
$\Sigma_i s_{ijk}$	10	10	10	10	10	20	22.5	26.5	0	8	8	8	8	18	20.5	20.5
$\Sigma_i s_{ijk} Q_{ik}$	10	10	10	10	6	6	6	6	0	8	8	8	8	4	4	0

Table 14: Case Study 3 b_{ijk} Variable Results (Modified Optimization Model Raw Results)

	Sink 1 (j=1)								Sink 2 (j=2)							
	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)
i (1)	1	1	1	1	1	1	1	1	0	0	0	0	0	0	0	0
i (2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
i (3)	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1
i (4)	0	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1
i (5)	0	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0

Table 15: Case Study 3 s_{ijk} Variable Results (Modified Optimization Model Raw Results)

	Sink 1 (j=1)								Sink 2 (j=2)							
j=1	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)	k(1)	k(2)	k(3)	k(4)	k(5)	k(6)	k(7)	k(8)
i (1)	10	10	10	10	0	0	0	0	0	0	0	0	0	0	0	0
i (2)	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
i (3)	0	0	0	0	0	0	0	0	0	4	4	4	4	4	4	0
i (4)	0	0	0	0	0	0	0	0	0	4	4	4	4	0	0	0
i (5)	0	0	0	0	6	6	6	6	0	0	0	0	0	0	0	0
$\Sigma_i s_{ijk}$	10	10	10	10	6	6	6	6	0	8	8	8	8	4	4	0

As we can see in Case Study 3, the problem with the inconsistent results increases with the increase of inactive period of the source after the connection. Both original model and modified model obtained an objective value of 520 Mt of CO2.

3. RESULTS AND DISCUSSION

In terms of calculation speed and complexity, please refer to Table 16 for Model Statistics. The optimization is done using B-and-B solver in Lingo version 14 on a Core i3, 2.3 GHz processor. The modified model involves lesser variables due to removal of b_{ij} variable. It can be noticed that there are lesser iterations for Case 2 which is the largest system compared to Case 1 and 3. This indicates easier convergence of model for larger systems. Although computational time for original and modified model is negligible, it can be assumed that the modified model can handle larger systems better.

Table 16: Comparison of Original and Modified Model Statistics

	Original			Modified		
Model Statistics	CS 1	CS 2	CS 3	CS 1	CS 2	CS 3
Objective Value	420	530	520	420	530	520
Solver Iteration	0	344	20	19	246	19
Total Variables	126	186	166	116	171	156
Integer Variables	65	95	85	55	80	75
Total Constraints	311	463	415	311	463	415
Total Nonzeros	894	1326	1164	886	1315	1164
Computational Time, (s)	<1	<1	<1	<1	<1	<1

4. CONCLUSIONS

A modified optimization model for optimal source sink matching in carbon capture and storage systems with time, injection rate, and capacity constraints has been formulated. It provides more accurate and robust results compared to the original model and eliminates inconsistencies that required human intervention in order to extract the correct conclusion.

5. NOMENCLATURE (1)

Indices

I Set of CO_2 sources (i = 1, 2,. . . m)
J Set of CO_2 sinks (j = 1, 2,. . . n)
K Set of Planning Periods (k = 1. 2,. . . o)

Parameters

D_j CO_2 storage limit of sink j
E_{jk} CO_2 injection rate limit of sink j in period k
Q_{ik} Binary parameter denoting the existence of source i in period k
S_i^L Lower limit for CO_2 flowrate from source i
S_i^U Upper limit for CO_2 flowrate from source i
T^L Minimum viable duration of connectivity
T^U Duration of planning horizon

Variables

b_{ij} Binary variable denoting the existence CO2 stream from source i to sink j at any time within the planning horizon
b_{ijk} Binary variable denoting the existence CO2 stream from source i to sink j in period k
s_{ijk} CO2 flowrate from source i to sink j in period k

6. REFERENCES

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