

# Flexible Superstructure Synthesis Approach for Multi-Region and Multi-Period Carbon Capture and Storage Network Design

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The use of Carbon Capture and Storage (CCS) systems is an important technology to consider for achieving net zero. Optimisation of the supply chain component of a CCS system in terms of layout, time constraints, and central storage has the potential to decrease system cost, increase flexibility, and promote the proliferation of CCS in industry. This work uses a superstructure approach to synthesise an optimal CCS supply chain network which accounts for node locations, time availability, variable production of CO<sub>2</sub> and stream quality. Additionally, a carbon hub was introduced to the superstructure, which allowed for temporary storage as well as mixing for incoming streams. Different pathing rules involving the carbon hub were investigated to quantify the benefit of a hub approach. A case study was investigated where it was shown that the inclusion of the carbon hub greatly improved system resilience in the event of constrained storage capacities and reduced the loss of profit by 3 %.

## 1. Introduction

The world's CO<sub>2</sub> emissions continue to grow year-on-year due to anthropogenic activities (IEA, 2012). Global treaties such as the Paris Agreement aim to achieve net zero by the middle of the 21st century. There are certain industries such as steel, cement, hydrogen, and ammonia production which produce carbon as part of their process and are challenging to decarbonise (Diamante et al., 2014). CCS provides an additional avenue for carbon emissions reduction and a tool to achieve net zero following the emissions targets prescribed by the Paris Agreement.

A CCS system consists of capture, transport, and storage components. Carbon is typically captured from flue gas or process output streams that have high concentrations of CO<sub>2</sub>. Carbon storage typically refers to geological sequestration, where CO<sub>2</sub> is pumped as a supercritical fluid into underground structures, such as spent coal mines and saline formations, for long-term storage. Alternative methods such as biochar production are also being studied as an alternative sequestration method. To aid in the optimisation of CCS supply chain networks, this work uses a superstructure approach to represent a model which can synthesise an optimal CCS distribution network. This is a method, where the model is solved simultaneously, and accounts for location, time availability, variable production of CO<sub>2</sub> and stream quality. Consolidating these factors into a single model allows for greater accuracy and flexibility in real-world scenarios.

Additionally, this work introduces a carbon hub to the proposed integrated network. This carbon hub allows for temporary storage as well as mixing for incoming streams. Different pathing rules involving the carbon hub were investigated to quantify the benefit of a hub approach.

## 2. Literature Review

There has been extensive work on adapting existing heat integration techniques to CCS network planning, such as Pinch Technology used by Tan and Foo (2007) for energy allocation with carbon constraints. These earlier sequential methods, especially graphical approaches, had the advantage of being intuitive. However, they can quickly become complex in larger systems and are tedious to iterate with new parameters (Isafiade et al., 2022). Simultaneous methods are also being adapted to CCS network synthesis. These methods can output the

optimal source-sink matching, accounting for multiple parameters in a single step, which makes them better suited for complex systems with multi-period and multi-region considerations. The work of Migo-Sumagang et al. (2022) presented a mini-review of P-graph to carbon management.

The time availability constraint was introduced in a CCS network synthesis model by Ooi et al. (2013) which collated the time availability constraint with flow rate and maximum sink capacity constraints. The objective was to maximise carbon captured and stored in the system and was solved numerically using mixed integer linear programming (MILP). To account for the novel temporal constraint, the overall system operation time was split into several segments where a set of binary variables determined if each source/sink operated in a particular segment. This model was then able to output the optimal stream matching of the specified CCS network. Tan further developed this model specifically for biochar deployment, a low-technology carbon sequestration technique (Tan, 2016). In addition to the time availability, flow rates, sink capacity constraints, transport costs, and carbon quality constraints were also introduced. Of particular interest was the introduction of stream splitting and blending as a possibility, bearing similarities to the stage-wise superstructure model developed by Yee and Grossmann (1990) for heat integration.

A hub concept developed by Chang et al. (2018) for heat integration may be of interest as an add-on to this model, where a geographical centre served as a hub for heat integration between process plants. The benefits of the hub approach as outlined in Chang et al. (2018) include increasing the flexibility of stream matching without a drastic increase in pipe lengths and the ability to rematch stream duties within the hub when some process plants are shut down. The application of this hub approach to a CCS network is envisioned to include centralised temporary storage at the hub to overcome bottlenecks, which cannot be done as easily at each carbon source due to space and regulatory restrictions. The hub will allow stream blending to meet quality constraints by splitting impurities between sinks, and the reduction of administrative costs by serving as a central monitoring point, which has been highlighted as a major concern in these emissions incentive programmes (Arp et al., 2018), for issuing carbon credits, carbon taxing, or the sale of carbon to other industries.

As more emphasis is placed on carbon reductions in emerging economies, carbon sinks are being identified in these regions, which may only be ready for deployment years down the line or are limited in size. A more resilient CCS network will be beneficial to accommodate the scattered and uncertain sink capacity.

There currently exists a gap for a simultaneous CCS network synthesis model which optimises carbon source-sink matching in terms of maximum project profit and accounts for distance, time availability, stream quality, and cost of transportation constraints with a central hub. A carbon hub approach will be taken for the synthesis of this consolidated network, and its effectiveness in reducing network costs will be investigated.

### 3. Methodology

The detailed problem statement is as follows:

- Given a set of carbon sources  $so$ , carbon sinks  $si$ , and a central carbon hub  $nt$ .
- Given a project lifetime split into  $p$  time intervals.
- Carbon produced from each carbon source  $so$  contains undesirable impurities  $k$ .
- Each source  $so$  has a minimum and maximum production rate.
- Each sink  $si$  has a maximum carbon injection rate per year and a maximum total carbon capacity over project lifetime.
- Allow mixing and redistribution of carbon and impurities within the hub.
- The problem is to determine the optimal carbon flow in the network during each time interval to maximise profit over the entire project lifetime.

To investigate the impact of a carbon hub on the CCS network, three hub pathing options were investigated:

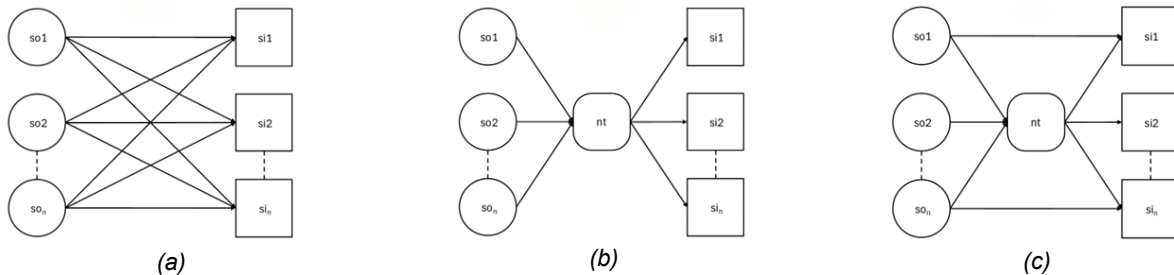


Figure 1: (a) Direct source-sink flow only (b) Forced flow through hub (c) No flow restrictions

To achieve the previously mentioned objectives, the flexible stage-wise superstructure method developed by Yee and Grossman (1990) was adapted for carbon transport. A superstructure comprising all possible stream connections was constructed.

Rather than the temperature stages in Yee and Grossman's (1990) superstructure, the system timeline  $t$  was broken down into  $p$  number of stages. Additionally, to aid in the formulation of the model, 2 helper parameters  $i$  and  $j$  were created, where  $i$  refers to any node carbon flows out of and  $j$  refers to any node carbon flows into. For each of these time interval  $p$ , the flow of carbon  $x$  (t/y) from  $i$  to  $j$  was optimised for maximum total project profit determined by:

$$\max(\text{net profit}) = \sum_{i, Si, p} (x_{i, Si, p} CI) - \sum_{i, Si, p} (x_{i, Si, p} AC) - \sum_{So, j, p} (x_{So, j, p} PC) - \sum_{i, j, p} (x_{i, j, p} TC_{i, j}) \quad (1)$$

where  $CI$ ,  $AC$ , and  $PC$  are Carbon Income, Application Cost, and Production Cost constants measured in \$/t and the transport cost  $TC$  being calculated by:

$$TC_{i, j} = (TCF)(\text{distance}_{i, j}) \left( \sum_{i, j, p} x_{i, j, p} \right) \quad (2)$$

where  $TCF$  is a constant cost coefficient given in \$/t.km.

The objective function remains the same for all 3 hub connection scenarios. As the helper parameters  $i$  and  $j$  can represent any node in the system, some undesired carbon flows such as flow into sources, backflow out of sinks, and nodes connecting to themselves can be eliminated from the superstructure to save computing power:

$$\sum_i x_{i, so, p} = 0 \quad (3)$$

where  $x_{i, so, p}$  represents the flow of carbon from node  $i$  to any source  $so$  in period  $p$ , setting this to 0 disables any backflow of carbon into production facilities.

$$\sum_j x_{si, j, p} = 0 \quad (4)$$

where  $x_{si, j, p}$  represents the flow of carbon from any sink  $si$  to any node  $j$  in period  $p$ , setting this to 0 prevents any backflow out from any carbon sinks.

The remainder of the mass balance equations for the sources and sinks are as follows:

$$SL_{so, p} \leq S_{so, p} \leq SU_{so, p} \quad (5)$$

$$\sum_j x_{so, j, p} = S_{so, p} \quad (6)$$

$$\sum_i x_{i, si, p} \leq D_{si, p} \quad (7)$$

$$\sum_{i, p} x_{i, si, p} \leq L_{si} \quad (8)$$

where  $SL$  and  $SU$  represent the lower and upper limits of source production rate (t/y) and  $S$  represents the optimal source production rate (t/y). The sink maximum injection rate and total carbon capacity are represented by  $D$  (t) and  $L$  (t/y) respectively.

The mass balances for the hub storage and mixing are as follows:

$$Stor_{nt, p} = \sum_{So} x_{so, nt, p} - \sum_{Si} x_{nt, si, p} + Stor_{nt, p-1} \quad (9)$$

$$\sum_{Si} x_{nt, si, p} \leq \sum_{So} x_{so, nt, p} + Stor_{nt, p-1} \quad (10)$$

$$Qnt_{nt,k,p} \left( Stor_{nt,p-1} + \sum_{so} x_{so,nt,p} \right) = Qnt_{nt,k,p-1} Stor_{nt,p-1} + \sum_{so} Q_{so,k,p} x_{so,nt,p} \quad (11)$$

where  $Stor$  represents the amount of carbon stored (t) at the hub in time interval and  $Qnt$  represents the contaminant concentration (g/t) leaving the hub. Eq(9) determines the amount of carbon stored in the hub, Eq(10) limits the maximum carbon flow out of the hub, and Eq(11) determines the concentration of contaminants leaving the hub after mixing.

$Qnt$  is calculated by dividing the total amount of contaminants in the hub by the total amount of carbon stored in the hub. The total amount of contaminants in the hub is then brought to the same side as  $Qnt$  to avoid dividing by zero.

The maximum concentration limits for each sink are enforced by:

$$\sum_{so} x_{so,si,p} Q_{so,k,p} + \sum_{nt} x_{nt,si,p} Qnt_{nt,k,p} \leq D_{si,p} Q_{si,k}^* \quad (12)$$

where  $Q^*$  (g/t) is the maximum concentration of contaminants at each sink. The first term on the left-hand side calculates the contaminants coming directly from the sources and the second term on the left-hand side calculates the contaminants coming from the hub. In the scenario where there are no direct carbon flows from sources or hub to the sinks, the  $x$  would go to 0 and the relevant term will fall away.

For the direct flow scenario, this is achieved by restricting the set  $j$  in Eq(6) to  $si$  nodes only:

$$\sum_j x_{so,si,p} = S_{so,p} \quad (13)$$

For the forced hub flow scenario, the same Eq(6) is modified to exclude  $so$  nodes from the summation set and forces all sources to flow into the hub  $nt$  as shown in Eq(14).

$$\sum_j x_{so,nt,p} = S_{so,p} \quad (14)$$

#### 4. Case Study

The model was tested using a modified case study from a potential biochar-based CCS system in the Philippines (Belmonte et al., 2018). In addition to the parameters listed in the problem statement, this case study introduced an additional carbon product, bio oil, which can be sold for additional income. The existing index  $k$  for calculating contaminant concentrations and mixing was expanded to include this additional carbon product. To reflect this new  $k$  species as an additional income source and not a harmful contaminant, no maximum concentration limit for bio oil has been included at the sinks and the carbon income term in the objective function has been split to describe the additional income from bio oil sales:

$$\begin{aligned} \max(\text{net profit}) = & \sum_{i,si,p} (x_{i,si,p} BC) + C_{fso} \sum_{so,si,p} (x_{so,si,p} BO) + Qnt_1(x_{nt,si,p} BO) \\ & - \sum_{i,si,p} (x_{i,si,p} AC) - \sum_{so,j,p} (x_{so,j,p} PC) - \sum_{i,j,p} (x_{i,j,p} TC_{i,j}) \end{aligned} \quad (15)$$

where  $C_f$  is the conversion factor of bio oil (t bio oil per t biochar) from each carbon source, and  $BO$  is the selling price of bio oil. The first entry of  $k$  is now reserved for bio oil concentration (t/t) instead of undesired contaminants. The hub was placed in San Antonio, and the distance from the hub to each source was obtained via Google Earth. The original case study model included a mechanism to exclude sources from the system if minimum viable productions cannot be met; as this exclusion mechanism does not exist in this model. The minimum carbon production rates were relaxed to keep the system feasible:

Table 1: Modified case study carbon production rates

	Original case study (t/y)	Modified base case (t/y)
so1 lower limit	6,000	6,000
so2 lower limit	20,000	12,000
so3 lower limit	10,000	8,000

The base case source and sink data are as follows:

*Table 2 : Base case source data*

	Minimum production (t/y)	Maximum production (t/y)	Contaminant 1 concentration (g/t)	Contaminant 2 concentration (g/t)	Contaminant 3 concentration (g/t)	Cf (t/t)
so1	6,000	8,000	80	150	4,600	1.55
so2	12,000	26,000	2,900	10,400	5,000	0.86
so3	8,000	13,000	4,600	5,000	2,600	1.82

*Table 3 : Base case sink data*

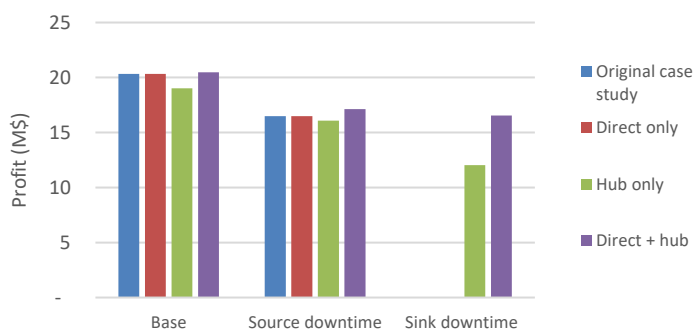
	Total capacity (t)	Maximum injection rate (t/y)	Maximum contaminant 1 concentration (g/t)	Maximum contaminant 2 concentration (g/t)	Maximum contaminant 3 concentration (g/t)
si1	67,270	6,727	750	2,600	1,250
si2	84,600	8,460	7,250	26,000	12,500
si3	215,000	21,500	1,500	5,200	2,500
si4	94,830	9,483	2,900	10,400	5,000

Additionally, to assess system resilience, both source and sink downtime were simulated by reducing the maximum source production and sink injection rates. For the source downtime scenario, Source 1's production is set to 0 for year 3, and its maximum production is halved from years 4-10. For the sink downtime scenario, Sink 1's injection rate for years 1-3 is set to 0, and Sink 4's injection rate for years 5-10 is set to 0.

## 5. Results

The base case yielded an objective value of \$ 20,336,817. Forcing all streams to pass through the hub first increased the total transport distance and yielded a lower profit of \$ 19,009,970.

In the sink and source outage scenarios, the inclusion of mixing and temporary storage features of the hub improved system resilience, particularly for sink outages (as shown in Figure 3), where the direct flow only models failed due to carbon production exceeding maximum sink flowrate. However, due to the temporary storage available at the hub, models which included the hub continued to return feasible solutions.



*Figure 2: Hub model output comparison*

This suggests the carbon hub concept can be beneficial for CCS networks with unstable or speculative supply and demand, such as those involving potential carbon sequestration sites which have not been fully characterised. The inclusion of the carbon hub may also be valuable for risk mitigation, derisking CCS projects and attracting more investors.

## 6. Conclusion

A MINLP model for CCS network synthesis was developed. This model consolidates distance, time availability, stream quality, and cost of transportation to optimise carbon flow for maximum project profit. The model additionally contains a central hub capable of rerouting, temporary storage, and mixing incoming streams to satisfy sink quality constraints and improve system resilience against source and sink outages. It was determined that the central hub negatively impacts CCS system profit when there are no fluctuations in carbon supply and demand, however, the

central hub significantly improves system resilience and reduces the loss of profit when fluctuations exist, particularly for scenarios which reduce carbon sink capacities. Additional work is recommended to consider the additional operating costs associated with the hub as well as mixing considerations.

### Nomenclature

#### Indices

*so* – Carbon Sources

*si* – Carbon Sinks

*nt* – Carbon hubs

*i* – Flow origin

*j* – Flow destination

*p* – Time interval

*k* – Contaminant species

*TC* – Transport cost

*TCF* – Transport cost constant

*SL* – Lower production limit

*SU* – Upper production limit

*D* – Sink yearly injection limit

*L* – Sink total carbon capacity

*Q* – Contaminant concentration from sources

*Q\** – Contaminant limit at sinks

#### Parameters

*CI* – Carbon income

*BC* – Biochar price

*Cf* – Bio oil conversion factor

*BO* – Bio oil price

*AC* – Application cost

*PC* – Production cost

#### Variables

*x* – Carbon flow

*S* – Carbon production rate

*Stor* – Carbon stored at hub

*Q<sub>nt</sub>* – Contaminant concentration from hub

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