A Superstructure-Based Mixed-Integer Programming Approach to Optimal Design of Pipeline Network for Large-Scale CO_2 Transport

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Pipeline transport is the major means for large-scale and long-distance CO_2 transport in a CO_2 capture and sequestration (CCS) project. But optimal design of the pipeline network remains a challenging problem, especially when considering allocation of intermediate sites, like pump stations, and selection of pipeline routes. A superstructure-based mixed-integer programming approach for optimal design of the pipeline network, targeting on minimizing the overall cost in a CCS project is presented. A decomposition algorithm to solve the computational difficulty caused by the large size and nonlinear nature of a real-life design problem is also presented. To illustrate the capability of our models. A real-life case study in North China, with 45 emissions sources and four storage sinks, is provided. The result shows that our model and decomposition algorithm is a practical and cost-effective method for pipeline networks design. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 2442–2461, 2014
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Introduction

Carbon dioxide capture and sequestration (CCS) is widely regarded as a major means to reduce carbon dioxide emissions from centralized industrial emission sources, for instance, power plants and chemical plants. However, although there has been increasing research interest in the capture side and sequestration side, research on the transport side, which connects the capture and sequestration, is still rather limited. Among other transport means, pipeline transport is ideal for large-scale and long-distance carbon dioxide transport, but its design remains a challenging problem. This is mainly due to the nature of this problem. In such problems, the number of carbon dioxide emissions sources and geologically suitable sites for sequestration, also known as sinks, is usually rather large. The number of suitable sites for intermediate sites, like pump stations which keep pressure of carbon dioxide above its critical point, and the number of possible routes of pipelines, which connect sources, intermediate sites, and sinks, is infinite. Moreover, complex fluid mechanics of carbon dioxide flow in pipelines and mass and energy balance over an entire pipeline network also make designing such a network a rather challenging problem.

Some approaches, although not many, have been made to tackle this problem. Most early trials use a source-sink matching method,[1–4] where a carbon dioxide emission source and a sequestration sink are linked by a pipeline. This method aims to minimize the sum of capture cost, sequestration cost, and pipeline cost. A major drawback of this method is that it does not allow any merges or splits of carbon dioxide flows, and all captured carbon dioxide should be transported from one source to a sink in a single pipeline. This method can provide useful guidance in an early stage of a CCS project where the total amount of captured carbon dioxide is not much and the numbers of capture sources and sequestration sites are relatively small. However, in later stages where both the amount of captured carbon dioxide and the number of sources and sinks are large, the source-sink matching method becomes less capable in dealing with the more complex situation. Egberts et al.[1] extended the method of source-sink matching by adding geographic information of a region obtained from a geographic information system. Dooley et al.[2] applied the method of source-sink matching in their study, requiring straight pipelines with a minimum and maximum length used to connect sources and

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sinks. In the topical report ILSGS,[3] sources and sinks are also matched in pairs and straight pipelines are used to connect the sources to the sinks matched with them, as well. In the work of Kazmierczak et al.,[4] the authors propose an iterative algorithm to solve a CO_2 pipeline network optimal design problem constructed using the source-sink matching method. While providing an efficient means to solve a nonlinear problem, the algorithm does not include hydraulic characteristics of pipelines, and it can guarantee a local optimum. In the work of Middleton and Bielicki,[5] the authors present a so-called SimCCS model to match sources and sinks. It takes California as an example, with 37 sources and 14 sinks, and works out the source-sink matching design of the pipeline network system. The study compares the cost of a point-to-point pipeline system and that of a pipeline network system, and it concludes that the latter one is more cost effective due to the scale effect of the network system. In the work of Zheng,[6] the author provides a superstructure based mixed-integer programming (MIP) approach to tackle the source-sink matching problem, and illustrates its application in a real-life case study. Through these applications, the source-sink matching method has become a relatively mature technique for addressing the pipeline design problem in a CCS project at its early stage, but its ability for pipeline network design is rather limited.

There are also studies focusing on other parts of the optimal designs of pipeline networks. In the work of McCollum and Ogden,[7] the authors present models to estimate costs occurred during compressing, transporting, and sequestrating CO_2. In the work of Dooley et al.,[8] the authors conduct analysis of distribution of CO_2 sources and sinks, and conclude that for each CO_2 emission source in the US, there are always sinks available for sequestration. It is also estimated that the sequestration costs are between $-7/ton, which indicates profitable, and $15/ton, and that prices of gas and petroleum can largely affect the sequestration costs of CO_2. In the work of Wilcox,[9] the authors study the thermodynamic properties of CO_2, which provide rather useful information for the pipeline design problem as pressure losses should be considered based on such studies.

In this article, we present a superstructure-based modeling and optimization framework to address the design problems of pipeline networks by considering all alternative sources, sinks, intermediate sites, and pipeline connections amongst them. The superstructure representation of the design problem and its mathematical formulation is first presented, followed by a real-life case study of optimal design of a CO_2 pipeline network in a region of North China.

Superstructure Representation

The methodologies of superstructure-based modeling have been widely used in the optimal design of process configurations and operating conditions via mathematical programming.[10] Continuous variables as well as discrete variables are used to describe and capture all possible arrangements of devices, flow sequences, and interactions among them.[11] Previous studies have applied superstructure-based modeling in the optimal design of process-scale problems, including polygeneration energy system design,[12,13] distributed energy system design,[14] design and operation of combined cooling, heating and power systems,[15] and design of energy systems in commercial buildings,[16] as well as mega level problems and macrolevel problems, such as hydrogen infrastructure planning,[17] strategic planning of chemical centers,[18] and planning of the power sector of China.[19]

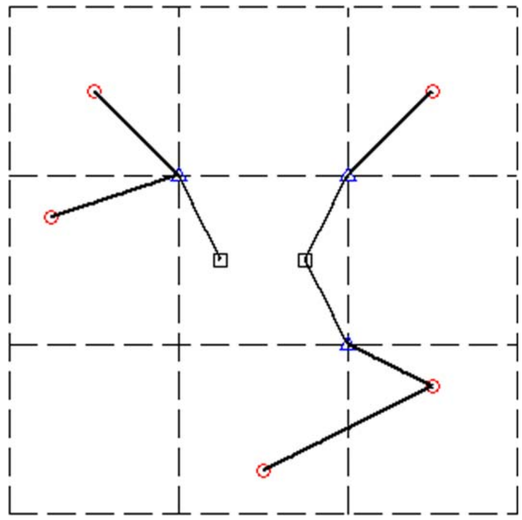

Figure 1. Superstructure representation of the pipelines network for CO_2 transport (circle source, square sink, triangle pump station).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

A superstructure representation of the optimal design problem of a carbon dioxide pipeline network is presented in Figure 1. In this superstructure representation, a region with a certain number of sources (represented by circles) and sinks (represented by squares) where the pipeline network is to be built is first meshed into a grid with a number of nodes. These nodes, sources, and sinks are potential locations for intermediate sites (represented by a triangle, including pump stations, and intersection sites with or without pumps), that is, an intermediate site can be built (or not built) at each node, source, or sink, but intermediate sites cannot be built in other places than these nodes, sources, or sinks. In this way, the distances between sources, sinks, and intermediate sites can be obtained directly. A pipeline can be built between sources, sinks, and intermediate sites. The main purpose of meshing the region into a grid is to limit the number of potential locations of intermediate sites to a finite number, and also to make the distances between sources, sinks, and intermediate sites available beforehand. Based on this superstructure representation, an MIP problem can be developed to formulate the mass flows from sources to intermediate sites and sinks, pressure drop along pipelines, pressure boost at pumps, and overall investment cost. Details of the model are presented next.

Mathematical Model

First, all sources, sinks, and nodes in the superstructure representation are denoted as sites

$$I,\ J = \{\text{Source 1, Source 2, Source 3}, \cdots, \text{Sink 1, Sink 2, Sink 3}, \cdots, \text{Node 1, Node 2, Node 3}, \cdots\}$$

Pipelines of various diameters are available for different ranges of mass flow rates of carbon dioxide, as follows

$$D = \{\text{Diameter 1, Diameter 2, Diameter 3}, \cdots\}$$

A binary variable is introduced to represent the existence (or not) of a pipeline of a certain diameter between two sites, as follows

$$y_{i,j,d}=\begin{cases}1 & \text{if a pipeline of diameter d is installed between node } i \text{ and node } j\\ 0 & \text{otherwise}\end{cases}$$

Other key variables include pressure rise of each CO_2 flow at the intermediate sites ($\text{rise}_{i,j}$), mass flow rate of CO_2 in each pipeline ($F_{i,j}$), and quantity of CO_2 captured (or sequestrated) at each source (or sink) (c_i, k_i). A nomenclature of all sets, parameters, and variables can be found in Appendix A.

The overall investment and operational costs of a pipeline network is selected as the objective function (see Section Objective function), and the MIP model of the optimal design problem can be formulated as follows

Minimize U obj = capture + storage + pipe + pump + carbon

s.t.

$$h^{\text{mc}}(x,y)=0, g^{\text{mc}}(x,y)\le 0\begin{cases}\text{CCS target (optional)}\\ \text{Conservation of mass}\\ \text{Capabilities of sources and sinks}\\ \text{Single pipe constraint}\end{cases}$$

$$h^{\text{sc}}(x,y)=0, g^{\text{sc}}(x,y)\le 0\begin{cases}\text{Pressure drop of carbon dioxide flow}\\ \text{Pressure drop constraints}\\ \text{Pressure rise constraints}\end{cases}$$

$$\boldsymbol{x}\in R^n, y\in \boldsymbol{Y}=\{0,1\}^m$$

where U is the objective function, h^{mc} and g^{mc} are mass constraints, h^{sc} and g^{sc} are pressure constraints, $\boldsymbol{x}$ is the vector of continuous real variables, and $\boldsymbol{Y}$ is the vector of binary variables.

Detailed specifications of the objective function and key constraints are to be illustrated next.

Objective function

Our objective function is the total cost of a CCS project, including capture cost, which occurs in the process of capturing carbon dioxide from the sources, sequestration cost, which occurs in the process of sequestrating carbon dioxide in the sinks, and transportation cost, which occurs in the process of transporting carbon dioxide from the sources to the sinks. The mathematical expression of the total cost function is as follows

$$\begin{aligned}\text{total cost}=&\text{pipe cost}+\text{pump cost}+\text{capture cost}\\ &+\text{storage cost}+\text{carbon cost}\end{aligned} \tag{1}$$

The CO_2 emission sources are different in terms of capture cost, because of different attributes of the carbon dioxide flows they emit.[4] The total capture cost also increases with the increase of the life span (*tm*) of the CCS project, because the carbon dioxide to be captured becomes larger. The total capture cost can be expressed as follows

$$\text{capture cost}=tm\cdot\sum_i \text{cap}_i\cdot c_i \tag{2}$$

Sinks are also different in terms of sequestration cost, because of their different geological attributes.[4] The total storage cost function can be expressed as follows

$$\text{storage cost}=tm\cdot\sum_i \text{sink}_i\cdot k_i \tag{3}$$

Transportation cost consists of pipe cost, pump cost, and extra carbon dioxide emission cost. The pipe cost is the sum of costs of rights of ways, materials, labor, O&M, and miscellaneous.[20] According to the work of NETL,[20] the pipe cost function in our model can be expressed as follows

$$\begin{aligned}\text{pipe cost}=\sum_{i,j,d}&[(73.2\cdot {L_d}^2+28.67\cdot L_d+23.79)\\ &\cdot dis_{i,j}+1.22]\cdot y_{i,j,d}\cdot 10^5,\ \ i\ne j\end{aligned} \tag{4}$$

Pump cost is actually the cost of electricity consumed by pumps used for pressurizing carbon dioxide flows in the pipeline system. Other costs are negligible compared with the electricity cost. According to the work of Fox et al.,[21] and White,[22] the total pump cost is proportional to the product of pressure rise and mass flow rate. To build up an MIP model, the bilinear term has been linearized as a piecewise linear function in our model, which can be expressed as follows

$$\begin{aligned}&\text{pump cost}=tm\cdot ep\cdot\sum_{i,j}(\theta_k^{\text{UB}}\cdot F_{i,j}),\ \ i\ne j\quad \text{if rise}_{i,j}\\ &\in\left[\theta_k^{\text{LB}},\ \theta_k^{\text{UB}}\right)\end{aligned} \tag{5}$$

Inaccuracy incurred through the proposed linearization depends on the lengths of the subintervals. The shorter each subinterval is, the more accurate the approximation can be. The magnitude of the relative gap between the approximation and the actual value of each interval is $\frac{\theta_k^{\text{UB}}-\theta_k^{\text{LB}}}{\theta_k^{\text{UB}}}$. In our model, the disjunction is managed with a binary indicator variable $r_{k,i,j}$, two big constants R and M, and two positive intermediate variables $pra_{k,i,j}$ and $prb_{k,i,j}$

$$r_{k,i,j}=\begin{cases}1 & \text{if rise}_{i,j}\in\left[\theta_k^{\text{LB}},\ \theta_k^{\text{UB}}\right)\\ 0 & \text{otherwise}\end{cases}$$

$$\sum_k r_{k,i,j}=1,\ \ i\ne j \tag{5.1}$$

$$pra_{k,i,j}\ge 0,\ \ i\ne j \tag{5.2}$$

$$prb_{k,i,j}\ge 0,\ \ i\ne j \tag{5.3}$$

$$pra_{k,i,j}\le \theta_k^{\text{UB}}-\theta_k^{\text{LB}},\ \ i\ne j \tag{5.4}$$

$$pra_{k,i,j}\le \text{rise}_{i,j}-\theta_k^{\text{LB}}+\left(1-r_{k,i,j}\right)\cdot R,\ \ i\ne j \tag{5.5}$$

$$pra_{k,i,j}\ge \text{rise}_{i,j}-\theta_k^{\text{LB}}-\left(1-r_{k,i,j}\right)\cdot R,\ \ i\ne j \tag{5.6}$$

$$prb_{k,i,j}\le r_{k,i,j}\cdot M,\ \ i\ne j \tag{5.7}$$

$$prb_{k,i,j}\le F_{i,j}+\left(1-r_{k,i,j}\right)\cdot M,\ \ i\ne j \tag{5.8}$$

$$prb_{k,i,j}\ge F_{i,j}-\left(1-r_{k,i,j}\right)\cdot M,\ \ i\ne j \tag{5.9}$$

$$\text{pump cost}=tm\cdot ep\cdot\sum_{k,i,j}(\theta_k^{\text{UB}}\cdot prb_{k,i,j}),\ \ i\ne j \tag{5.10}$$

For the sake of clarity and convenience, we summarize formulas 5.1–5.10 as formula (5) in the mathematical representation of the model. In our real-life case study in North China, we divide the pressure rise interval $[0,\ 6.4]$ into 14 subintervals, with R to be 13 (larger than the upper bound of $\text{rise}_{i,j}-\theta_k^{LB}$) and M to be 4600 (larger than the upper bound of $F_{i,j}$). It is worth mentioning that the bilinear term can also be linearized with other methods, for instance, McCormick envelopes.[23,24]

Extra carbon dioxide emission cost is the cost of carbon emission caused by electricity consumption by the pumps of CCS[25] and measured by the price of the permit for carbon dioxide emission. Accordingly, the function to calculate the total extra carbon dioxide emission cost is similar to that used for calculating the total pump cost [formula (5)], which can thus be expressed as follows

$$\text{carbon cost} = tm \cdot cp \cdot \sum_{i,j} (\theta_k^{UB} \cdot F_{i,j}),\ \ i \neq j \quad \text{if rise}_{i,j} \in \left[\theta_k^{LB},\ \theta_k^{UB}\right) \tag{6}$$

Mass balance constraints

As to the mass balance constraints, each site should be subject to the mass conservation law, and the total quantity of carbon dioxide being sequestrated should not be smaller than the target value, if there is a target quantity of carbon dioxide to be sequestrated. The following function stipulates the quantity of CO_2 captured in the system (CCS target), it is included in our model only when there is a target quantity of CO_2 to be captured

$$\sum_i c_i \geq T \tag{7}$$

Each site in the model should be subject to the law of conservation of mass (Conservation of mass), which can be expressed as follows

$$\sum_{j \neq i} F_{j,i} + c_i = \sum_{j \neq i} F_{i,j} + k_i \tag{8}$$

Our model stipulates that there can only be at most one pipeline connecting any two sites (Single pipe constraints). Thus, the following functions are included in our model

$$\sum_d y_{i,j,d} = \begin{cases} 1 & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases},\ \ i \neq j \tag{9}$$

The disjunction is also managed with binary indicator variables, big constants, positive intermediate variables, and similar techniques as above.

The last parts of the mass constraints pertain to capabilities of sources and sinks, carbon dioxide captured (or sequestrated) at each source (or sink) should not exceed its capacity, these constraints (Capabilities of sources and sinks) can be expressed as follows

$$c_i \leq e_i \tag{10}$$

$$k_i \leq u_i \tag{11}$$

Pressure constraints

As to the pressure constraints, they pertain to pressure drop of CO_2 flows in pipelines. As gaseous CO_2 has a small density and the mass flow rate would be rather small if CO_2 is transported in gas phase, thus CO_2 in pipelines is usually transported as supercritical fluid or dense-phase liquid to guarantee an efficient mass flow rate.[26] The temperature of CO_2 in pipelines is usually in the range of -15 to 40°C.[26] Thus, the pressure of CO_2 should be kept above 8.6 MPa to avoid vaporization.[26] Otherwise, the volume of CO_2 would be exploded and accidents could happen. Because of this, pipes with different diameters can be selected to adjust pressure drop of CO_2 flows in the pipeline, and pumps are also used in our model to pressurize CO_2 flows according to the constraints, which should be set at the nodes, sources, or sinks in our model. On the other hand, there should also be an upper bound for the pressure of the carbon dioxide flows to ensure sealing. In our model, the upper bound of the pressure is 15 MPa.[26] According to the works of Fox et al.,[21] White,[22] and Hendriks et al.,[27] pressure drop of carbon dioxide transported in pipelines is proportional to the square of mass flow rate. To build up an MIP model, the quadratic term has been linearized as a piecewise linear function in our model, which can be expressed as follows (Pressure drop of CO_2 flow)

$$pd_{i,j} \geq f \cdot \frac{(\alpha_p \cdot F_{i,j} + \beta_p) \cdot \text{dis}_{i,j}}{2\rho \cdot L_d \cdot S_d^2},\ \ i \neq j \quad \text{if } y_{i,j,d}=1,\ \ F_{i,j} \in \left[\delta_p^{LB},\ \delta_p^{UB}\right) \tag{12}$$

The accuracy of the approximation also increases with the decrease of the length of each subinterval. The magnitude of the relative gap between the approximation and the actual value of each interval is $\left(\frac{\delta_p^{UB}-\delta_p^{LB}}{2\cdot\delta_p^{LB}}\right)^2$. The disjunction is also managed with binary indicator variables, big constants, positive intermediate variables, and similar techniques as above. In our real-life case study in North China, we divide the interval of the mass flow rate of CO_2 $[0,\ 2306.26]$ into nine subintervals, with the big constants to be 4600 (larger than the upper bound of $F_{i,j}-\delta_p^{LB}$) and 1.07×10^7 (larger than the upper bound of $\alpha_p \cdot F_{i,j}+\beta_p$) respectively.

The equality holds up if there are no throttle valves or other devices used for depressurization. Engineering estimates for the value of f of CCS pipeline networks are adopted in our study. It suggests that f should be less than 0.015 for perfectly smooth pipeline walls and 0.02 for new untreated steel.[27]

The outlet pressure and the inlet pressure of each pipeline are subject to the following constraint (Pressure drop constraint)

$$pd_{i,j} = \begin{cases} (po_{i,j} - pi_j) & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases},\ \ i \neq j \tag{13}$$

The disjunction is also managed with binary indicator variables, big constants, positive intermediate variables, and similar techniques as above.

We assume that different CO_2 inlet flows of a site will be mixed at the site, and thus have a united inlet pressure. We also assume that different CO_2 outlet flows of a site can be pressurized separately, and thus have different outlet pressures.

The last parts of the pressure constraints pertain to calculation of pressure rises of CO_2 flows at each site. The pressure rises at each site can be calculated by the following constraint (Pressure rise constraint)

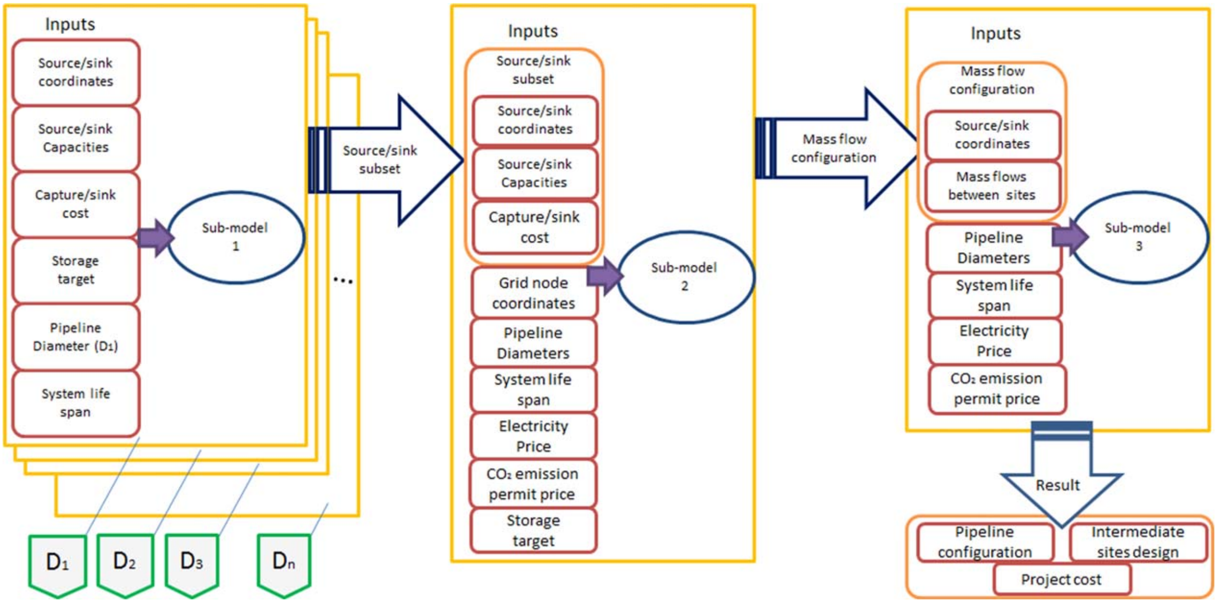

Figure 2. Decomposition algorithm.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

$$\text{rise}_{i,j}=\begin{cases} po_{i,j}-pi_i & \text{if } F_{i,j}>0 \\ 0 & \text{otherwise} \end{cases},\quad i\neq j \tag{14}$$

The disjunction is also managed with binary indicator variables, big constants, positive intermediate variables, and similar techniques as above.

Model summary

To sum up, our model can be summarized as follows:

To work out the optimal design of pipeline network for CO_2 transport, our model should finish the following tasks, which are also the outputs of our model:

1. Select the sources to capture carbon dioxide from, and decide on the quantity of carbon dioxide to be captured at each selected source.
2. Select the sinks to sequestrate carbon dioxide in, and decide on the quantity of carbon dioxide to be sequestrated at each selected sink.
3. Decide on the number of intermediate sites, with their positions and values of pressure rise.
4. Decide on whether to construct a pipeline between any two sites, with the diameter of the pipeline.
5. Decide on the mass flow rates in the pipelines.
6. Guarantee that the pressure of the carbon dioxide is within the safe range throughout the pipeline network system, which is from 8.6 to 15 MPa.

As prerequisites of our model, some assumptions have to be held, which are as follow:

1. The range of pressure rise of a pump is from 0 to 6.4 MPa. The upper bound is derived from the difference of 15 MPa and 8.6 MPa. Carbon dioxide newly captured at sources has the pressure of 15 MPa.
2. The cost of pumps is mainly electricity cost, and other costs are negligible in magnitude. The electricity price is 0.6 yuan/(kWh). The cost of extra carbon dioxide emission caused by electricity consumption by the pumps is measured by the price of the permit for carbon dioxide emission, which is 17 euros/ton (137.7 yuan/ton). The carbon dioxide intensity of electricity is 0.977kg/kWh.
3. The pipe cost is a function of pipe length and pipe diameter. The expression is as shown above.
4. The pressures of different inlet flows of a certain site must be a constant. This assumption requires the inlet flow with pressure higher than the constant to depressurize before flowing into the node, through throttles valves or other devices. On the other hand, the pressures of outlet flows of a certain site can be different because they can be pressurized separately.
5. The region under consideration is homogenous in geography. This assumption allows us to neglect differences in costs of constructing pipelines and intermediate sites in regions with different geographies.
6. The density of CO_2 in our model is regarded to be 731kg/m^3 as a constant. Our model neglects the density variance of carbon dioxide in the pipeline network due to the temperature changes and pressure changes.

Besides, inputs of the model are as listed below:

1. Geographic coordinates of the sources and the sinks.
2. Geographic coordinates of the nodes of the grids.
3. The capacities of the sources and the sinks.
4. Capture/storage costs of the sources/sinks.
5. Alternative diameters of the pipelines.
6. Electricity price and carbon emission permit price.
7. Life span of the system.
8. Target quantity of carbon dioxide to be sequestrated. (optional)

Adjustment, Reform, and Disassembling of the Model

Generally, the memory and computational ability of a PC cannot satisfy the requirements of the optimal design of a model with a reasonable number of grids. Take the case shown in Figure 3[26] as an example. With the region under

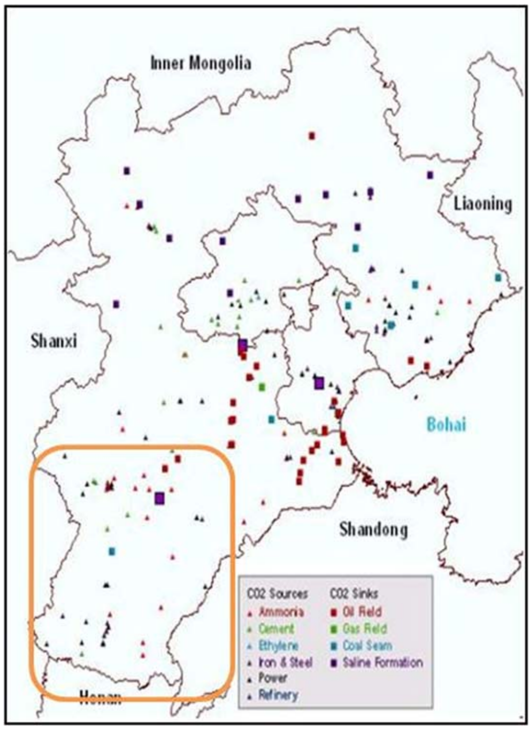

Figure 3. Map of region under consideration.[26]

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

consideration meshed into 6×6 grid, the problem will be formulated with 203,726 variables and 373,778 constraints, when there is no requirement for the quantity of carbon dioxide to be sequestrated. With CPLEX/GAMS,[28] feasible solutions cannot be obtained within 24 h on a computer with Core i5 CPU of 2.50 GHz and 4-GB memory. To make the optimal problem solvable with a reasonable number of nodes, we have to make some adjustments to the original model. Actually, we disassemble the original model into three submodels, to solve the optimization problem gradually, trying to decrease the scale of the problem while keeping the results effective. For the same case as aforementioned, the optimal design can be achieved within 1 h with our decomposition algorithm of three submodels. Figure 2 is the graphic illustration of the "three sub-model" decomposition algorithm. More details of the submodels can be found in the following subsections.

The first submodel: select potential sources and sinks

The first issue that makes the problem scale large is that the number of sources and sinks in the region under consideration is huge. Generally, not all the sources and sinks will be involved for sequestrating a certain amount of carbon dioxide. The optimizing process is trading off among the three components of the objective function, while selecting sources to capture carbon dioxide from and sinks to sequestrate carbon dioxide in: capture costs of the sources, sequestration costs of the sinks, and unit transportation costs from sources to sinks. Thus, sources and sinks with large capabilities, low costs, and location advantages, are most likely the ones involved in a CCS project.

Our first submodel is developed to select the sources and sinks potentially involved in the CCS project. With the first submodel, the scale of the dataset can be reduced reasonably, and thus the scale of the optimization problem can also be largely reduced. The first submodel is developed from the classic source-sink matching model, which can be outlined as follows

$$\text{Minimize } U\,\text{obj} = \text{capture} + \text{storage} + \text{pipe}$$

s.t.

$$h(x,y)=0,\, g(x,y) \leq 0 \begin{cases} \text{CCS target (optional)} \\ \text{Conservation of mass} \\ \text{Single pipe constraint} \\ \text{Capabilities of sources and sinks} \end{cases}$$

$$\boldsymbol{x} \in R^n,\, y \in \boldsymbol{Y} = \{0,1\}^m$$

Symbols here have the same meanings as above. In this model, carbon dioxide will be transported from sources to sinks without intermediate sites, and any source or sink can be used for merging carbon dioxide flows from different sources or distributing carbon dioxide flows to different sinks. Thus, we do not need to mesh the region under consideration at this stage. This submodel will also trade off among the same targets as above: capture costs, sink costs, and unit transportation costs, and can thus simulate the source and sink selection process of the original model. By changing the weights of unit transportation costs in the total costs, different bundles of sources and sinks can be worked out. These sources and sinks can be regarded as the ones possibly involved in CCS project, while we do not need to take the others into consideration. As the results of the submodels with different weights of unit transportation costs can be worked out quite easily with computers, the scale of the problem can be reduced quite efficiently, while the accuracy of the final design result will also be kept in this way. Details of the first submodel are shown in Appendix B.

The second submodel: optimal design of pipeline network

All the sources and sinks selected by the first submodel will be used as database of the second submodel. The target of the second model is to optimally design the configuration of the pipeline network. The outline of the second model is the same as the complete model

$$\text{Minimize } U\,\text{obj} = \text{capture} + \text{storage} + \text{pipe} + \text{pump} + \text{carbon}$$

s.t.

$$h^{mc}(x,y)=0,\, g^{mc}(x,y) \leq 0 \begin{cases} \text{CCS target (optional)} \\ \text{Conservation of mass} \\ \text{Capabilities of sources and sinks} \\ \text{Single pipe constraint} \end{cases}$$

$$h^{sc}(x,y)=0,\, g^{sc}(x,y) \leq 0 \begin{cases} \text{Pressure drop of carbon dioxide flow} \\ \text{Pressure drop constraints} \\ \text{Pressure rise constraints} \end{cases}$$

$$\boldsymbol{x} \in R^n,\, y \in \boldsymbol{Y} = \{0,1\}^m$$

Symbols here have the same meanings as above. According to the linear relationship between pressure drop and the

Table 1. Database of Sources

Source Type	Code Name	Longitude	Latitude	CO_2 Emission (Mton/yr)	Capture Cost (yuan/ton)
Ammonia	A01	114.48	38.03	1.96	67.29
	A04	114.48	38.03	0.78	78.68
	A08	115.33	37.34	0.42	91.57
	A12	114.56	38.13	0.39	93.7
	A13	114.48	38.03	0.35	96.88
	A14	115.32	38.01	0.32	99.02
	A15	114.48	38.03	0.32	99.02
	A17	114.84	38.03	0.26	106.53
	A18	114.5	36.77	0.26	106.53
	A19	114.5	37.74	0.26	106.53
	A20	115.02	38.02	0.23	111.61
	A24	114.47	36.6	0.20	118.11
	A26	115.18	36.84	0.16	126.75
	A27	114.48	38.03	0.16	126.75
	A28	114.96	38.16	0.13	138.94
	A30	114.94	36.37	0.98	157.75
	A32	114.94	36.49	0.82	171.79
Cement	C13	114.15	36.38	1.46	443.17
	C14	114.33	38.07	1.42	443.45
	C16	114.48	37.61	0.71	453.34
	C19	114.75	37.35	1.42	436.45
	C25	114.3	38.09	3.51	436.04
Iron and steel	IS03	113.89	36.75	4.07	348.21
	IS04	114.48	37.05	4.07	348.21
	IS08	114.48	37.05	1.63	355.03
	IS10	114.48	36.68	1.22	358.25
	IS12	114.2	36.7	0.81	364.04
	IS23	114.47	36.6	6.11	346.34
Power	P02	114.5	36.64	0.23	382.18
	P04	114.43	36.47	0.23	382.18
	P05	114.43	36.47	0.25	379.17
	P10	114.52	38.03	0.37	361.06
	P16	114.16	37.96	0.51	347.59
	P19	113.68	36.47	0.94	320.34
	P20	115.44	36.56	0.98	317.83
	P23	114.5	36.64	1.87	310.05
	P25	114.53	38.06	2.34	308.16
	P26	115.66	37.73	2.81	304.25
	P28	114.46	37.06	2.81	304.25
	P29	115.66	37.73	2.81	304.25
	P31	114.43	36.47	3.74	306.05
	P33	113.93	38.34	5.61	288.59
	P36	114.21	38.06	6.08	288.01
	P37	114.15	36.48	6.18	284.5
Refinery	R03	114.48	38.03	0.54	519.28
	Number of plants = 45			Total emission = 72.73	

distance of transportation, the movement of the pumps along the pipelines is applicable for a particular configuration of pipeline networks, which would not bring about changes in the total cost, as long as the pressures of carbon dioxide flows in the pipelines are subject to the pressure constraints. Besides, according to the linear relationship between the cost of a pump and the value of its pressure rise, the division of the pumps along the pipelines is applicable for a particular configuration of pipeline networks, which would not bring about changes in the total cost, either, as long as the pressures of carbon dioxide flows in the pipelines are subject to the pressure constraints. Therefore, the second submodel can be solved without the upper bound of the pressure constraints, and we can just manually "move" the parts higher than the upper bound of the pressure constraints of the pipeline system in the design result to other places along the pipelines, until the pressures of carbon dioxide flows throughout the pipeline system are subject to the pressure constraints, without changing the total cost. In this way, it takes much less time to solve the optimization problem in the second submodel, because the carbon dioxide flows do not have to be pressurized halfway at the pump stations, and

Table 2. Database of Sinks

Sink Type	Code Name	Longitude	Latitude	Storage Capacity (Mton)	Sequestration Cost (yuan/ton)
Saline formation	AQU15	115.13	37.9	1417	0
Coal seam	ECBM08	114.53	37.38	27.78	−327.3
Oil field	EOR18	115.23	38.21	10.77	−700
	EOR27	115.4	38.3	28.42	−700
	Number of sinks = 4			Total capacity = 1483.97	

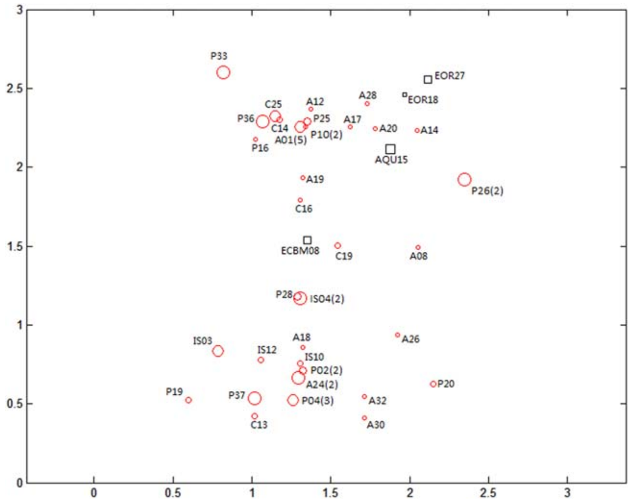

Figure 4. Region under consideration.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

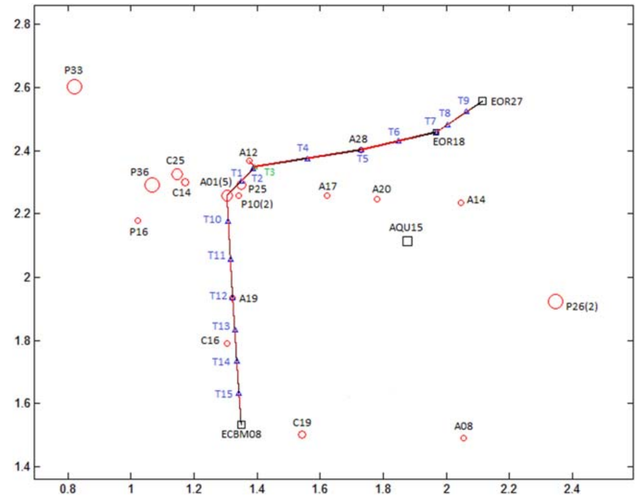

Figure 6. Design without requirement (enlarged).

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the model can compensate all the pressure drop by just assigning pumps of arbitrarily large pressure rise values at the sources and the intersection sites. In other words, the grid nodes now are just potential intersection sites for merging carbon dioxide flows from different sites or distributing carbon dioxide flows to different sites, and thus the optimal solution can be obtained with much shorter computation time. On the other hand, an optimization problem with a much larger grid number can be solved within acceptable computation time. Details of the second submodel can be found in Appendix C.

The third submodel: optimize locations of the intersection sites

The positions of the intersection sites of the design result of the second submodel can hardly be the global optimal ones exactly, because the grid number in the second submodel is rather limited, while the global optimal positions of these intersection sites can be anywhere in the region under consideration. Thus, we build up the third submodel to optimize the positions of these intersection sites in the design result of the second submodel to make the final design result as close to the optimal one as possible, which can be outlined as follows:

$$\text{Minimize } U\,\text{obj} = \text{pipe} + \text{pump} + \text{carbon}$$

s.t.

$$h(x,y)=0,\, g(x,y)\leq 0 \begin{cases} \text{Single pipe constraint} \\ \text{Distance equations} \\ \text{Pressure drop of carbon dioxide flow} \\ \text{Pressure drop constraints} \\ \text{Pressure rise constraints} \end{cases}$$

$$\boldsymbol{x}\in R^n,\, y\in \boldsymbol{Y}=\{0,1\}^m$$

Symbols here have the same meanings as above. In this MINLP model, we fix the mass flow configuration in this

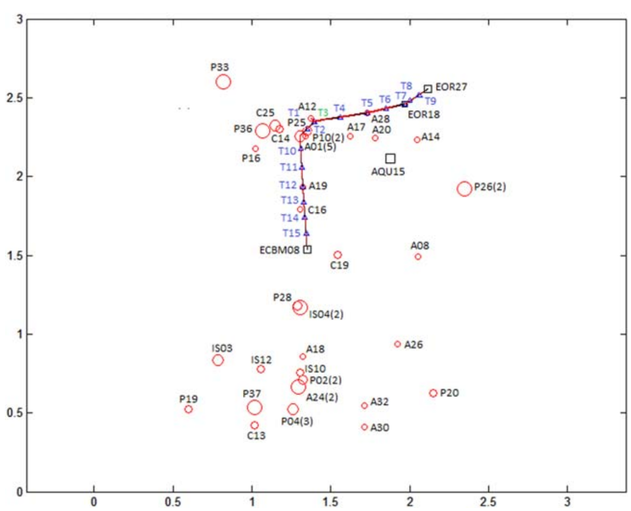

Figure 5. Design without requirement.

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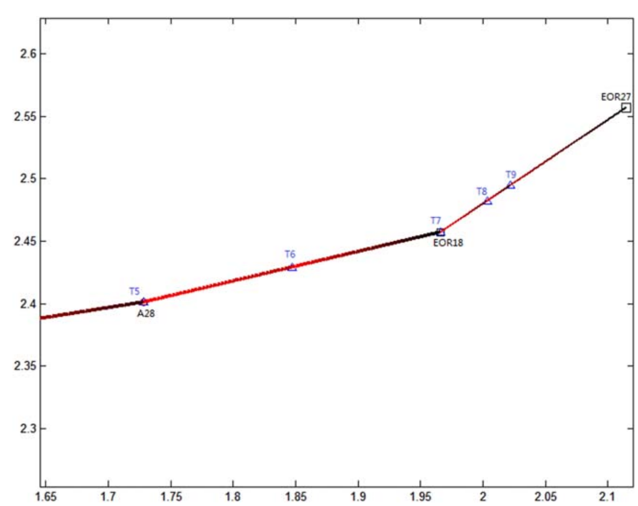

Figure 7. Design without requirement (enlarged).

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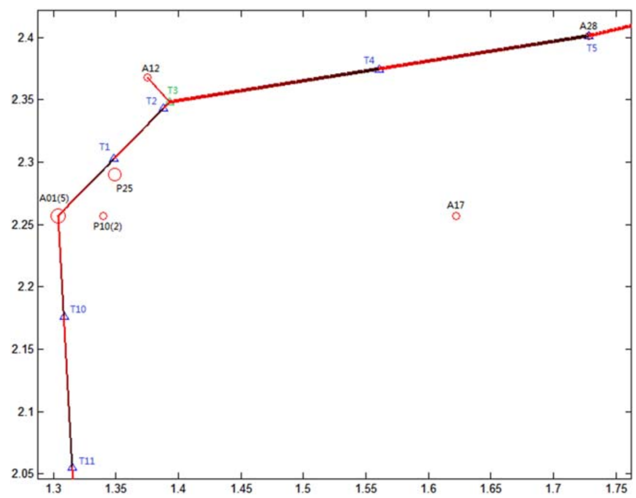

Figure 8. Design without requirement (enlarged).

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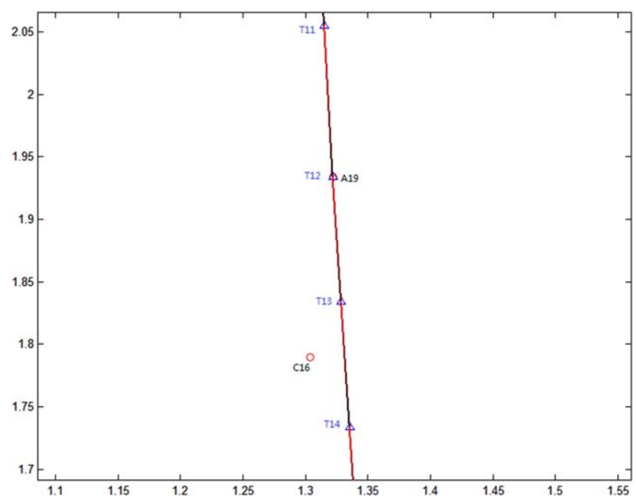

Figure 9. Design without requirement (enlarged).

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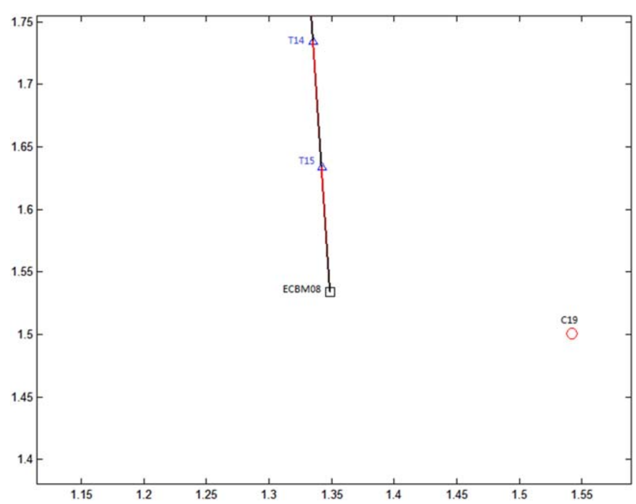

Figure 10. Design without requirement (enlarged).

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Table 3. Design Result Without Requirement of Sequestration Quantity (I)

Source/Sink	CO_2 Captured (Mton/yr)	CO_2 Sequestrated (Mton/yr)
A01	1.96	0
A04	0.78	0
A12	0.39	0
A13	0.35	0
A15	0.33	0
A19	0.26	0
A27	0.16	0
A28	0.13	0
EOR18	0	0.72
EOR27	0	1.89
ECBM08	0	1.75

submodel to be the same as the results of the second submodel, while leaving the pressure-related variables undetermined. The details of the third submodel can be found in Appendix D. This problem is nonconvex. We solve this problem with the MINLP solver BARON,[29] which guarantees the global optimal solution to the third submodel.

Case Study

To test the effectiveness of the model, we apply the model to the square region highlighted in Figure 3,[26] which is the southwest of Hebei province in China. Data of this region come from studies of Zheng[6] and Yang.[26] We assume the life span of transportation system to be 15 years. Thus, annual capability of the sinks is 1/15 of the total capability. Tables 1 and 2 are the information of the sources and the sinks of the region under consideration.

For the convenience of presenting the results, the region under consideration is further processed and shown in Figure 4. Red circles in the map represent carbon dioxide emission sources, whereas black squares represent carbon dioxide sinks. As shown in Tables 1 and 2, there are sources sharing the same geographic coordinates, these sources thus share the same symbols on the map, which are labeled by one of them. Numbers in the parenthesis show the numbers of

Table 4. Design Result without Requirement of Sequestration Quantity (II)

Pipeline	Diameter (in)	CO_2 Flow Rate (kg/s)	Pressure Rise (MPa)
A01 → T1	6	66.289	0
T1 → T2	6	66.289	5.657
T2 → T3	6	66.289	5.02
A12 → T3	4	12.419	0
T3 → T4	8	78.708	0.637
T4 → T5	8	78.708	5.043
T5 → A28	8	78.708	5.043
A28 → T6	8	82.848	0
T6 → EOR18	8	82.848	1.656
EOR18 → T7	6	60.078	0
T7 → T8	6	60.078	6.4
T8 → T9	6	60.078	3.276
T9 → EOR27	6	60.078	3.427
A01 → A10	6	47.279	0
T10 → T11	6	47.279	3.657
T11 → T12	6	47.279	5.486
T12 → A19	6	47.279	5.486
A19 → T13	6	55.559	0
T13 → T14	6	55.559	4.659
T14 → T15	6	55.559	6.259
T15 → ECBM08	6	55.559	6.117

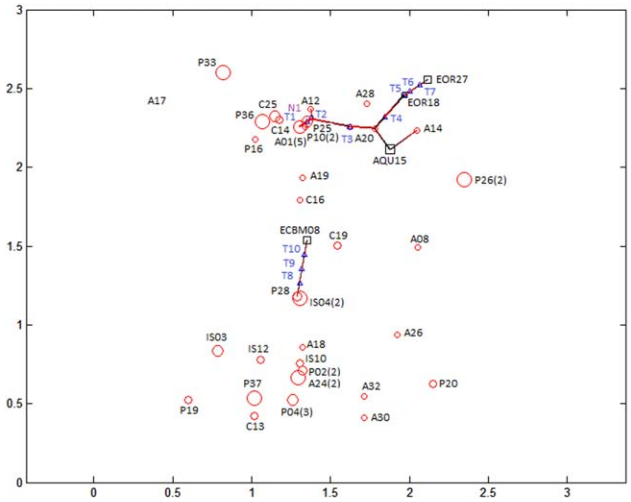

Figure 11. Design of 10% case.

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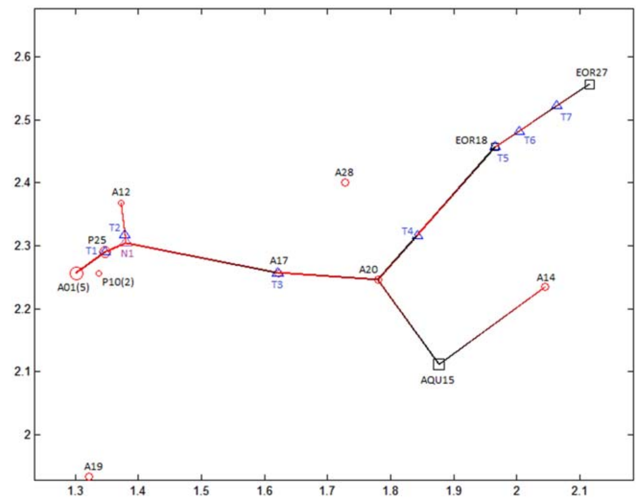

Figure 13. Design of 10% case (enlarged).

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sources the symbols represent. Sizes of the symbols are proportional to the aggregate capacities of the sources or sinks. The horizontal and vertical coordinates both have the unit of 100 km.

As is known to all, China has promised to cut its carbon emission intensity by 40–45% in 2020, comparing with that in 2005. We apply the model to design pipeline networks subject to the targets of sequestrating 10, 25, and 40% of total CO_2 emissions, as well as no requirement of target sequestration quantity, respectively. For each segment of the pipeline network, there are eight alternative types of pipelines to be selected, which are different in diameter. Their diameters are 4 in. (0.1016 m), 6 in. (0.1524 m), 8 in. (0.2032 m), 12 in. (0.3048 m), 16 in. (0.4064 m), 20 in. (0.508 m), 24 in. (0.6096 m), and 30 in. (0.762 m) respectively.

The MIP models were solved on the platform of GAMS Development Corporation (2008) with the solver CPLEX.[28] The MINLP models were solved on the platform of GAMS Development Corporation (2008) with the solver BARON.[29] A computer with a Core i5 CPU of 2.50 GHz and 4 GB memory was used to run the processes. Considering capabilities of the computer, the submodels aforementioned were used in this case study.

When there is no requirement for the quantity of carbon dioxide to be sequestrated, the minimum total cost of CCS is about −19.660 billion yuan. The total quantity of carbon dioxide sequestrated in this case turn out to account for 6.1% of the total emission. In this case, the first submodels have 4723 variables, with 1444 binary variables, and 4761 constraints each. The solving time scale of the first submodels is 10 s, while the iteration scale of the first submodels is 10,000.[28] The second submodel has 37,404 variables, with 6700 binary variables, and 68,424 constraints, and the corresponding solving time and iterations are 90.103s and 706,053 respectively.[28] The third submodel has 598 variables, with 192 binary variables, and 1022 constraints. The solving time and iterations of the third submodel are 566.9s

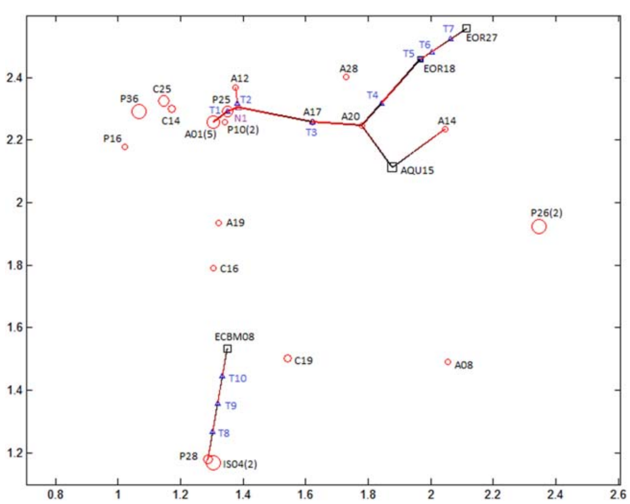

Figure 12. Design of 10% case (enlarged).

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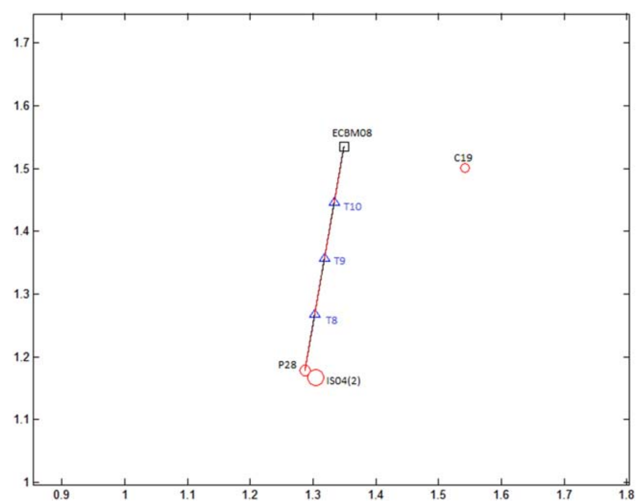

Figure 14. Design of 10% case (enlarged).

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Table 5. Design Result under Condition of Sequestrating 10% of Total Emissions (I)

Source/Sink	CO_2 Captured (Mton/yr)	CO_2 Sequestrated (Mton/yr)
A01	1.96	0
A04	0.78	0
A12	0.39	0
A13	0.35	0
A14	0.33	0
A15	0.33	0
A17	0.26	0
A20	0.23	0
A27	0.16	0
P25	0.61	0
P28	1.85	0
EOR18	0	0.72
EOR27	0	1.89
ECBM08	0	1.85
AQU15	0	2.79

and 41,344 respectively.[29] Figure 5 presents the optimal design of the pipeline network with the model under such condition. Figures 6–10 are the enlarged graphs of the pipeline network. The color of the segments changes to represent pressure distribution of CO_2 flows in pipelines. Flow with higher pressure is colored redder. The diameters of the pipelines are positively correlated with the widths of the lines. For the convenience of presentation, pipelines of 4 and 6 in. will be represented by lines of the same width. Similarly, 8 and 12 in. pipelines have lines of the same width, 16 and 20 in. pipelines have the same width, and 24 and 30 in. pipelines have the same width. The blue triangles represent pump stations (triangle sizes are not proportional to the values of pressure rise). The green triangles represent intersection sites with pumps (triangle sizes are not proportional to the values of pressure rise). The purple triangles represent intersection sites without pumps. Tables 3 and 4 present other details of the design.

Under the condition of sequestrating 10% of total CO_2 emissions, total cost is about −6.931 billion yuan. In this case, the first submodels have 4723 variables, with 1444 binary variables, and 4762 constraints each. The solving time scale of the first submodels is 10 s, while the iteration

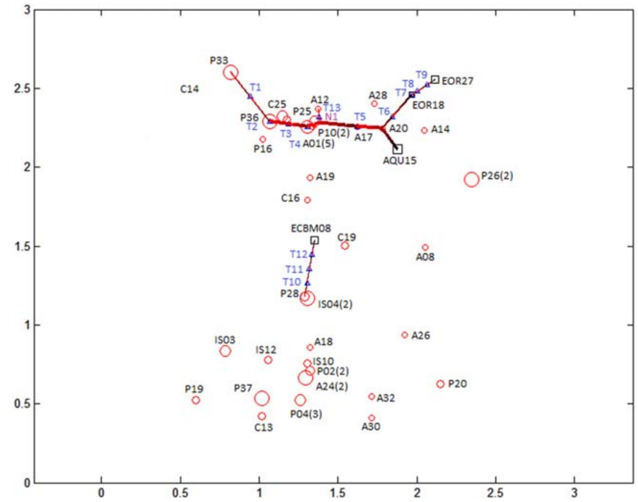

Figure 15. Design of 25% case.

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scale of the first submodels is 10,000.[28] The second submodel has 44,452 variables, with 8368 binary variables, and 81,364 constraints, and the corresponding solving time and iterations are 235.391 s and 2,126,325 respectively.[28] The third submodel has 2240 variables, with 837 binary variables, and 3673 constraints. The solving time and iterations of the third submodel are 8.87 s and 103 respectively.[29] Figure 11 shows the design of pipeline network under such condition. Figures 12–14 are the enlarged graphs of the pipeline network. Tables 5 and 6 present other details of the design.

Under the condition of sequestrating 25% of total CO_2 emissions, total cost is about 47.178 billion yuan. In this case, the first submodels have 4723 variables, with 1444 binary variables, and 4762 constraints each. The solving time scale of the first submodels is 100 s, while the iteration scale of the first submodels is 100,000.[28] The second submodel has 53,476 variables, with 10,528 binary variables, and 97,156 constraints, and the corresponding solving time and iterations are 2857.397s and 19,682,796 respectively.[28] The

Table 6. Design Result under Condition of Sequestrating 10% of Total Emissions (II)

Pipeline	Diameter (in)	CO_2 Flow Rate (kg/s)	Pressure Rise (MPa)
A01 → T1	8	113.568	0
T1 → P25	8	113.568	3.455
P25 → N1	12	132.963	0
A12 → T2	4	12.419	0
T2 → N1	4	12.419	1.117
N1 → T3	12	145.382	0
T3 → A17	12	145.382	4.085
A17 → A20	12	153.662	0
A20 → AQU15	8	78.057	0
A14 → AQU15	4	10.35	0
A20 → T4	8	82.85	0
T4 → EOR18	8	82.85	5.232
EOR18 → T5	6	60.078	0
T5 → T6	6	60.078	6.4
T6 → T7	6	60.078	3.276
T7 → EOR27	6	60.078	3.427
P28 → T8	6	58.743	0
T8 → T9	6	58.743	6.306
T9 → T10	6	58.743	6.306
T10 → ECBM08	6	58.743	6.212

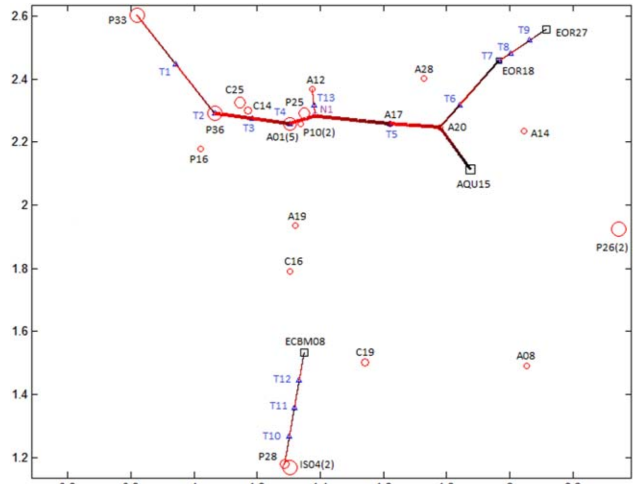

Figure 16. Design of 25% case (enlarged).

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third submodel has 2500 variables, with 1006 binary variables, and 4141 constraints. The solving time and iterations of the third submodel are 9.98 s and 124 respectively.[29] Figure 15 shows the design of pipeline network under such condition. Figures 16–19 are the enlarged graphs of the pipeline network. Tables 7 and 8 present other details of the design.

Under the condition of sequestrating 40% of total CO_2 emissions, total cost is about 104.923 billion yuan. In this case, the first submodels have 4723 variables, with 1444 binary variables, and 4762 constraints each. The solving time scale of the first submodels is 1000 s, while the iteration scale of the first submodels is 1,000,000.[28] The second submodel has 81,677 variables, with 16,830 binary variables, and 145,966 constraints, and the corresponding solving time and iterations are 128.57 s and 1,066,354 respectively.[28] The third submodel has 5327 variables, with 2100 binary variables, and 8651 constraints. The solving time and iterations of the third submodel are 193.63 s and 1733 respectively.[29] Figure 20 shows the design of the pipeline network under such condition. Figures 21–24 are the enlarged graphs of the

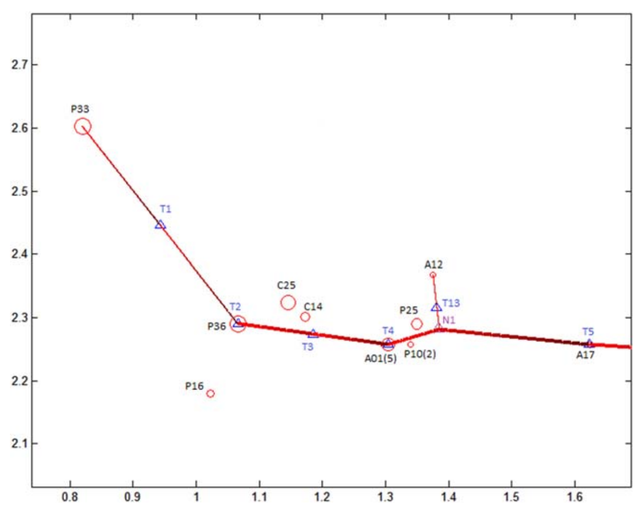

Figure 17. Design of 25% case (enlarged).

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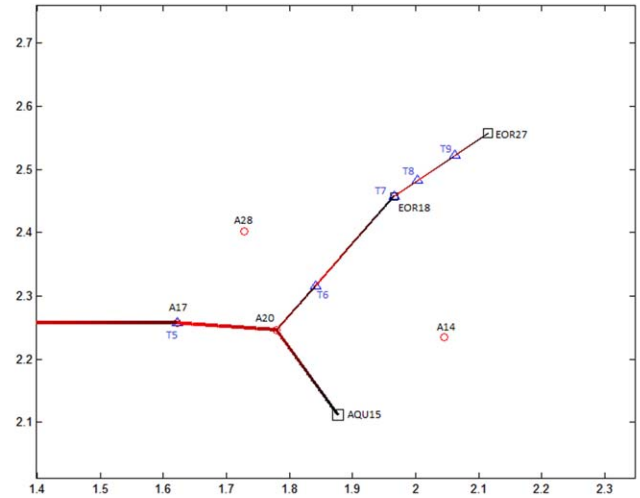

Figure 18. Design of 25% case (enlarged).

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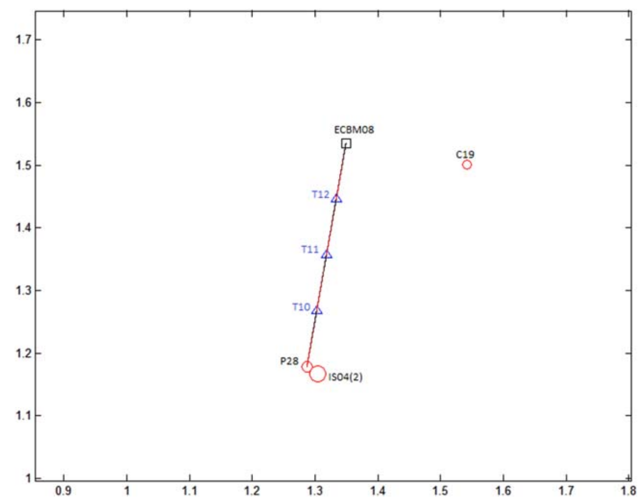

Figure 19. Design of 25% case (enlarged).

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Table 7. Design Result under Condition of Sequestrating 25% of Total Emissions (I)

Source/Sink	CO_2 Captured (Mton/yr)	CO_2 Sequestrated (Mton/yr)
A01	1.96	0
A04	0.78	0
A12	0.39	0
A13	0.35	0
A15	0.33	0
A17	0.26	0
A20	0.23	0
A27	0.16	0
P28	1.85	0
P33	5.42	0
P36	6.08	0
EOR18	0	0.72
EOR27	0	1.89
ECBM08	0	1.85
AQU15	0	13.35

Table 8. Design Result under Condition of Sequestrating 25% of Total Emissions (II)

Pipeline	Diameter (in)	CO_2 Flow Rate (kg/s)	Pressure Rise (MPa)
P33 → T1	12	171.897	0
T1 → T2	12	171.897	3.711
T2 → P36	12	171.897	3.711
P36 → T3	16	364.745	0
T3 → T4	16	364.745	1.673
T4 → A01	16	364.745	4.795
A01 → N1	20	478.313	0
A12 → T13	4	12.419	0
T13 → N1	4	12.419	1.125
N1 → T5	20	490.732	0
T5 → A17	20	490.732	3.757
A17 → A20	20	499.012	0
A20 → AQU15	16	423.407	0
A20 → T6	8	82.848	0
T6 → EOR18	8	82.848	4.807
EOR18 → T7	6	60.078	0
T7 → T8	6	60.078	6.4
T8 → T9	6	60.078	3.276
T9 → EOR27	6	60.078	3.427
P28 → T10	6	58.743	0
T10 → T11	6	58.743	6.306
T11 → T12	6	58.743	6.306
T12 → ECBM08	6	58.743	6.212

pipeline network. Tables 9 and 10 present other details of the design.

As the design results under different conditions clearly show, with the increase of the required capabilities of the pipeline network, the complexity of the system also increases, with more sources and sinks involved, more pipelines and pump stations constructed, and larger total cost spent on the system. Moreover, we can also easily conclude that the optimal designs of pipeline networks with larger capabilities are not compatible with the optimal designs of pipeline networks with smaller capabilities. Put differently, the former ones cannot be achieved by adding extra pipelines and pump stations to the latter ones. Thus, the conditions in the far future should be considered before designing and realizing the pipeline networks. It is also worth mentioning that our model and decomposition algorithm use grid nodes as potential locations of the intermediate sites, so the number and the locations of the intermediate sites are limited by the number and the locations of the grid nodes, which may cause differences between our design results and the global optimal ones. In future studies, the model can be developed so that the number and the locations of the intermediate sites can be decided by the model freely in the region under consideration, and better design results should thus be achieved.

Compared with Source-Sink Match Model

In this part, we apply the source-sink match optimization model to the case shown above, and compare the performance of this model and our model put forward above. For the convenience of comparison, all the pipelines used in the source-sink matching model are of 8 in. in diameter.

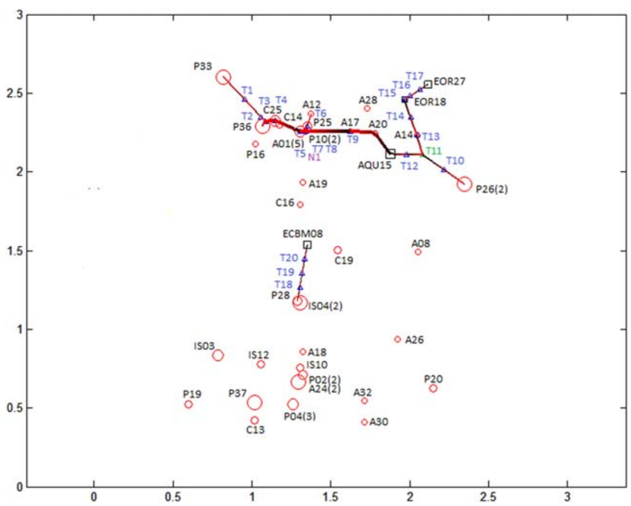

Figure 20. Design of 40% case.

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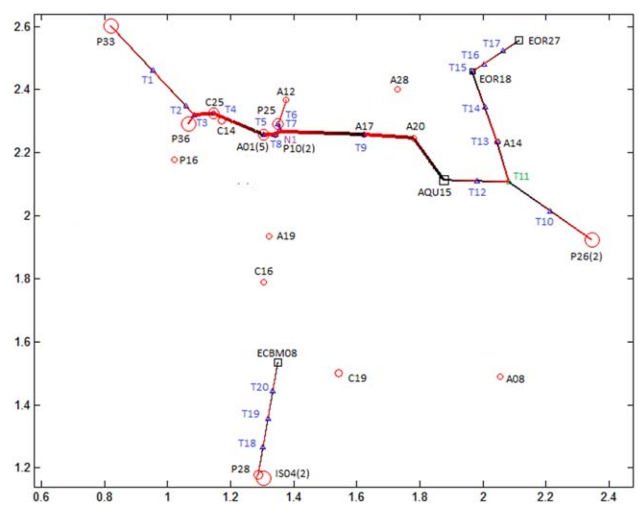

Figure 21. Design of 40% case (enlarged).

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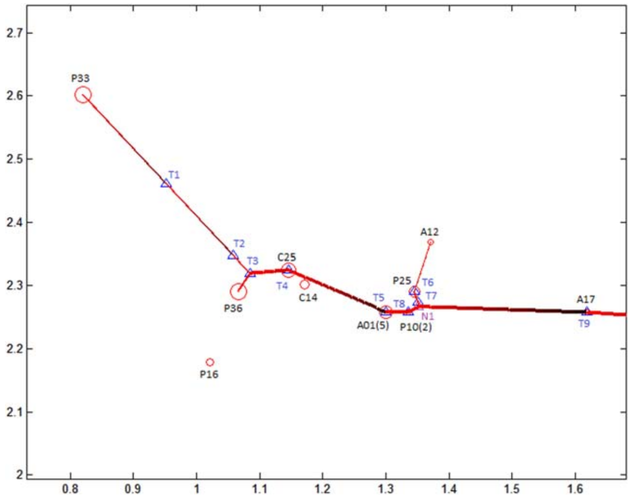

Figure 22. Design of 40% case (enlarged).

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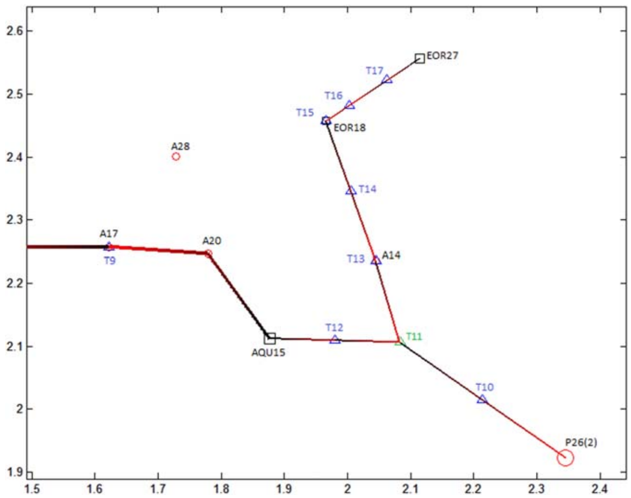

Figure 23. Design of 40% case (enlarged).

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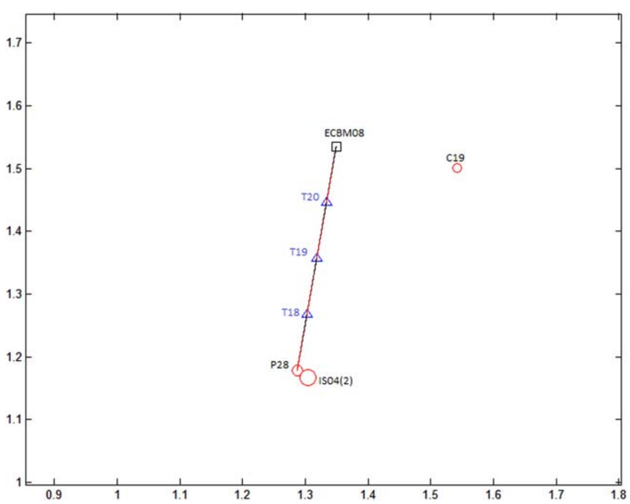

Figure 24. Design of 40% case (enlarged).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 9. Design Result under Condition of Sequestrating 40% of Total Emissions (I)

Source/Sink	CO_2 Captured (Mton/yr)	CO_2 Sequestrated (Mton/yr)
A01	1.96	0
A04	0.78	0
A12	0.39	0
A13	0.35	0
A14	0.33	0
A15	0.33	0
A17	0.26	0
A20	0.23	0
A27	0.16	0
C25	1.81	0
P10	0.37	0
P25	2.34	0
P26	2.81	0
P28	1.85	0
P29	2.81	0
P33	5.61	0
P36	6.08	0
EOR18	0	0.72
EOR27	0	1.89
ECBM08	0	1.85
AQU15	0	24.01

Figures 25–28 are the pipeline network designs of no requirement, 10, 25, and 40% cases respectively, which are all results of source-sink match optimization model.

Table 10. Design Result under Condition of Sequestrating 40% of Total Emissions (II)

Pipeline	Diameter (in)	CO_2 Flow Rate (kg/s)	Pressure Rise (MPa)
P33 → T1	12	178.014	0
T1 → T2	12	178.014	3.476
T2 → T3	12	178.014	3.476
P36 → T3	12	192.848	0
T3 → T4	16	370.862	0.815
T4 → C25	16	370.862	1.263
C25 → T5	16	428.341	0
T5 → A01	16	428.341	4.724
A01 → T8	20	541.909	0
T8 → P10	20	541.909	0.52
P10 → N1	20	553.777	0
A12 → T6	4	12.419	0
T6 → P25	4	12.419	1.498
P25 → T7	8	86.591	0
T7 → N1	8	86.591	0.62
N1 → T9	20	640.368	0
T9 → A17	20	640.368	5.684
A17 → A20	20	648.648	0
A20 → AQU15	20	655.893	0
P26 → T10	12	178.014	0
T10 → T11	12	178.014	0.02
T11 → T12	8	105.516	6.4
T12 → AQU15	8	105.516	4.614
T11 → T13	8	72.498	6.4
T13 → A14	8	72.498	4.614
A14 → T14	8	82.848	0
T14 → EOR18	8	82.848	1.364
EOR18 → T15	6	60.078	0
T15 → T16	6	60.078	6.4
T16 → T17	6	60.078	3.276
T17 → EOR27	6	60.078	3.427
P28 → T18	6	58.743	0
T18 → T19	6	58.743	6.306
T19 → T20	6	58.743	6.306
T20 → ECBM08	6	58.743	6.212

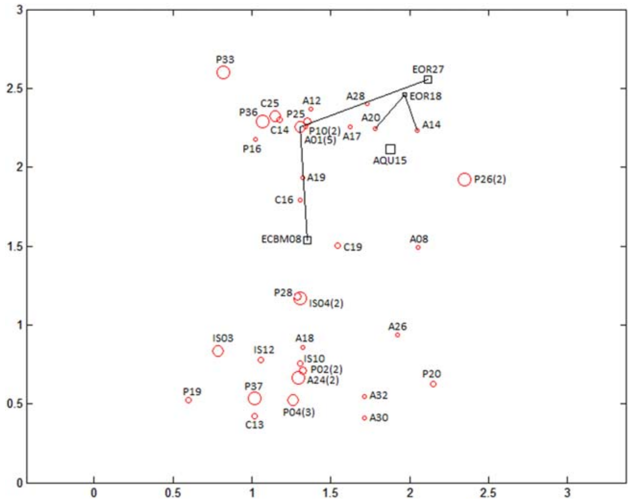

Figure 25. Design without requirement (source-sink matching model).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

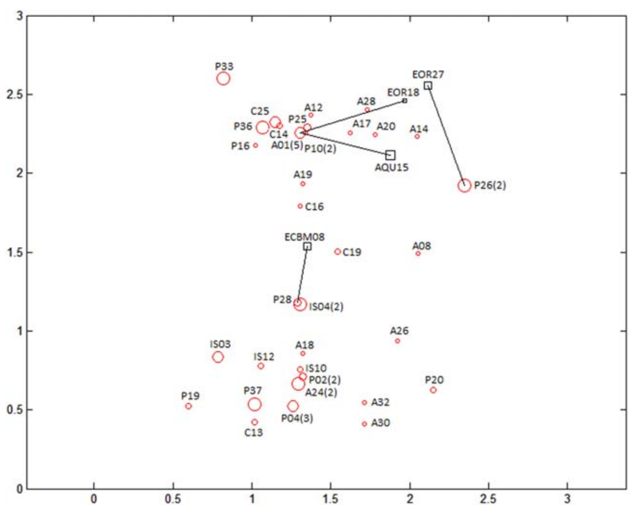

Figure 26. Design of 10% case (source-sink matching model).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 11 shows the comparison of the results between the two models. As can be seen in the table, although our new model has many more constraints and add pump cost and extra carbon emission cost into its objective function, it still performs much better than the source-sink match model. Moreover, it seems that the results worked out by our model can save more money as more carbon dioxide is required to be sequestrated.

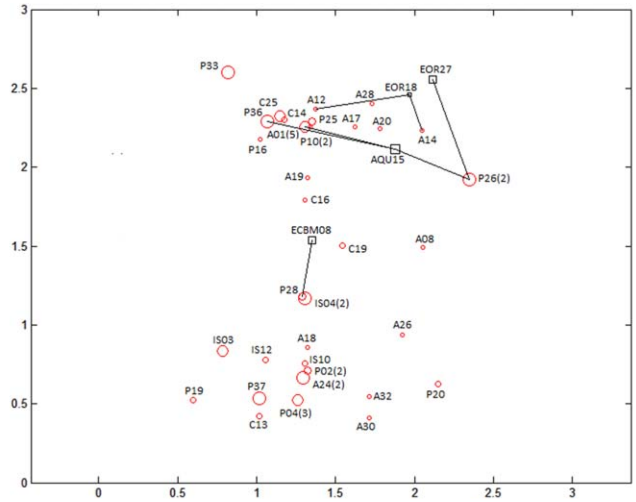

Figure 27. Design of 25% case (source-sink matching model).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

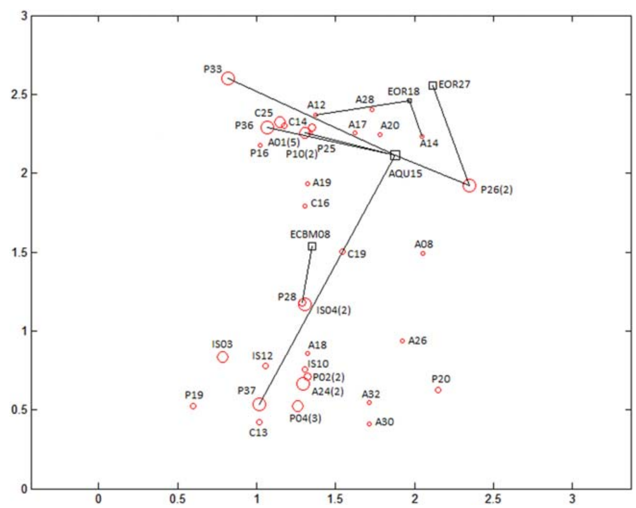

Figure 28. Design of 40% case (source-sink matching model).

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Conclusions

In this article, we provide a superstructure-based mathematical model to work out the optimal design of pipeline networks, targeting on minimizing the integrated costs of CCS, including capture cost, storage cost, and transportation cost, which subject to the constraints of transportation capability requirements and pressure requirements. Then, the model is disassembled into three submodels in order that it

Table 11. Compare of Costs Calculated by Two Models

Case	New Model Cost (billion yuan)	Source-Sink Match Model Cost (billion yuan)	Source-Sink Match Model Cost-New Model Cost (billion yuan)
Unrestricted	−19.660	−14.690	4.970
10%	−6.931	0.309	7.240
25%	47.178	54.584	7.406
40%	104.923	120.119	15.196

can be solved efficiently. The case study which applies the model to design the pipeline networks in North China under different conditions confirms the applicability of the model. At last, the advantages of the model are revealed by comparing it with the traditional source-sink matching model.

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Appendix A: Nomenclature of the Model

Set

$I,\ J=\{\text{Source 1, Source 2, Source 3},\cdots,\text{Sink 1, Sink 2, Sink 3},\ \cdots,\text{Node 1, Node 2, Node 3},\cdots\}$ Sites

N = {Node 1, Node 2, Node 3, ⋯} Grid Nodes, a sub set of Sites

SO = {Source 1, Source 2, Source 3, ⋯} Sources, a sub set of Sites

SI = {Sink 1, Sink 2, Sink 3, ⋯} Sinks, a sub set of Sites

D = {Diameter 1, Diameter 2, Diameter 3, ⋯} Types of pipelines with different diameters

Continuous variables

$\text{rise}_{i,j}$ = pressure rise of CO_2 flow from site i to site j at site i, $\text{rise}_{i,j} \in [0,\ 6.4)$, MPa

$F_{i,j}$ = mass flow rate of CO_2 from site i to site j, positive variable, kg/s

c_i = CO_2 captured at site i, positive variable, kg/s

k_i = CO_2 sequestrated at site i, positive variable, kg/s

$pd_{i,j}$ = pressure drop of CO_2 flow from site i to site j, caused by friction of the pipe, $pd_{i,j} \in [0,\ 6.4)$, MPa

$po_{i,j}$ = pressure of outflow from site i to site j, $po_{i,j} \in [8.6,\ 15)$, MPa

pi_j = pressure of inflow at site j, $pi_j \in [8.6,\ 15)$, MPa

capture cost = capture cost of the CCS project, yuan

storage cost = storage cost of the CCS project, yuan

pipe cost = pipeline construction cost of the CCS project, yuan

pump cost = pump O&M cost of the CCS project, yuan

carbon cost = CO_2 emission permit cost of the CCS project, yuan

total cost = total cost of the CCS project, yuan

Discrete variables

$y_{i,j,d}$ = binary variable, if there is a pipeline of type d connecting i and j, it equals 1. Otherwise, it equals 0.

Parameters

θ_k^{LB} = the lower bound of the kth subinterval of the domain of $\text{rise}_{i,j}$, MPa

θ_k^{UB} = the upper bound of the kth subinterval of the domain of $rise_{i,j}$, MPa
δ_p^{LB} = the lower bound of the pth subinterval of the domain of $F_{i,j}$, kg/s
δ_p^{UB} = the upper bound of the pth subinterval of the domain of $F_{i,j}$, kg/s
α_p = the slope of the piecewise linear function in the pth subinterval of the domain of $F_{i,j}$, kg/s
β_p = the intercept of the piecewise linear function in the pth subinterval of the domain of $F_{i,j}$, kg^2/s^2
L_d = diameter of the pipeline of type d, m
S_d = cross-sectional area of the pipeline of type d, m^2
$dis_{i,j}$ = distance between site i and site j, km
ep = electricity price factor, used to calculate for expenditure on a certain quantity of electricity, yuan/(MPa kg)
tm = time factor, represent the life span of the system, s
cp = carbon price factor, used to calculate the expenditure on carbon dioxide emission permits for carbon dioxide emission caused by a certain quantity of electricity consumption, unit: yuan/(MPa kg)
T = target of CO_2 to be sequestrated, kg/s
f = friction factor of the pipe
ρ = density of CO_2 flow, kg/m^3
e_i = CO_2 emitted at site i, kg/s
u_i = Maximum CO_2 sequestration capacity at site i, kg/s
cap_i = CO_2 capture cost at site i, yuan/kg
$sink_i$ = CO_2 sequestration cost at site i, yuan/kg

Appendix B: illustrations of the First Submodel

The first submodel, which is developed from the source-sink matching model, can be summarized as follows
Outline:

Minimize U obj = capture + storage + pipe

s.t.

$$h(x,y)=0, g(x,y)\leq 0\begin{cases}\text{CCS target (optional)}\\ \text{Mass flow equations}\\ \text{Capabilities of sources and sinks}\\ \text{single pipe constraint}\end{cases}$$

$$\boldsymbol{x}\in R^n, y\in \boldsymbol{Y}=\{0,1\}^m$$

Tasks (outputs):

1. Select the sources to capture carbon dioxide from, and decide on the quantity of carbon dioxide to be captured at each selected source.
2. Select the sinks to sequestrate carbon dioxide in, and decide on the quantity of carbon dioxide to be sequestrated at each selected sink.
3. Decide on whether to construct a pipeline between any pair of sites.
4. Decide on the mass flow rates in the pipelines.

Assumptions:

1. The pipe cost is a function of pipe length. The expression is as shown in formula (B2) below. We try all the diameter alternatives in this sub model to find out all sinks and sources possibly involved in the CCS project.
2. The region under consideration is homogenous in geography. This assumption allows us to neglect differences in costs of constructing pipelines in regions with different geographies.

Inputs:

1. Geographic coordinates of the sources and the sinks.
2. The capacities of the sources and the sinks.
3. Capture/storage costs of the sources/sinks.
4. The diameter of the pipelines.
5. Life span of the system.
6. Target quantity of carbon dioxide to be sequestrated. (optional)

Set

$I,\ J=\{\text{Source 1, Source 2, Source 3},\cdots\}$ Sites
$SO=\{\text{Source 1, Source 2, Source 3},\cdots\}$ Sources, a sub set of Sites
$SI=\{\text{Sink 1, Sink 2, Sink 3},\cdots\}$ Sinks, a sub set of Sites

Continuous variables

$F_{i,j}$ = mass flow rate of CO_2 from site i to site j, positive variable, kg/s
c_i = CO_2 captured at site i, positive variable, kg/s
k_i = CO_2 sequestrated at site i, positive variable, kg/s
capture cost = capture cost of the CCS project, yuan
storage cost = storage cost of the CCS project, yuan
pipe cost = pipeline construction cost of the CCS project, yuan
total cost = total cost of the CCS project, yuan

Discrete variables

$y_{i,j}$ = binary variable, if there is a pipeline connecting i and j, it equals 1. Otherwise, it equals 0.

Parameters

L = the diameter of pipelines used in the submodel, m
$dis_{i,j}$ = distance between site i and site j, km
tm = time factor, represent the life span of the system, s
T = target of CO_2 to be sequestrated, kg/s
e_i = CO_2 emitted at site i, kg/s
u_i = maximum CO_2 sequestration capacity at site i, kg/s
cap_i = CO_2 capture cost at site i, yuan/kg
$sink_i$ = CO_2 sequestration cost at site i, yuan/kg

Objective function

$$\text{total cost}=\text{pipe cost}+\text{capture cost}+\text{storage cost} \tag{B1}$$

$$\text{pipe cost}=\sum_{i,j}[(73.2\cdot L^2+28.67\cdot L+23.79)\cdot dis_{i,j}+1.22]\cdot y_{i,j}\cdot 10^5,\ \ i\neq j \tag{B2}$$

$$\text{capture cost}=tm\cdot\sum_i cap_i\cdot c_i \tag{B3}$$

$$\text{storage cost}=tm\cdot\sum_i sink_i\cdot k_i \tag{B4}$$

Constraints

1. CCS Target (optional)

$$\sum_i c_i\geq T \tag{B5}$$

2. Mass flow equations

$$\sum_{j\neq i}F_{j,i}+c_i=\sum_{j\neq i}F_{i,j}+k_i \tag{B6}$$

3. Capabilities of sources and sinks

$$c_i \le e_i \quad \text{(B7)}$$

$$k_i \le u_i \quad \text{(B8)}$$

4. Single pipe constraint

$$y_{i,j}=\begin{cases} 1 & \text{if } F_{i,j}>0 \\ 0 & \text{otherwise} \end{cases}, \quad i \ne j \quad \text{(B9)}$$

Appendix C: Illustrations of the Second Submodel

The second submodel can be summarized as follows.

Outline

Minimize U obj = capture + storage + pipe + pump + carbon

$s.t.$

$$h^{mc}(x,y)=0, g^{mc}(x,y) \le 0 \begin{cases} \text{CCS target (optional)} \\ \text{Conservation of mass} \\ \text{Capabilities of sources and sinks} \\ \text{Single pipe constraint} \end{cases}$$

$$h^{sc}(x,y)=0, g^{sc}(x,y) \le 0 \begin{cases} \text{Pressure drop of carbon dioxide flow} \\ \text{Pressure drop constraints} \\ \text{Pressure rise constraints} \end{cases}$$

$$\boldsymbol{x} \in R^n, y \in \boldsymbol{Y}=\{0,1\}^m$$

Tasks (outputs)

1. Select the sources to capture carbon dioxide from, and decide on the quantity of carbon dioxide to be captured at each selected source.
2. Select the sinks to sequestrate carbon dioxide in, and decide on the quantity of carbon dioxide to be sequestrated at each selected sink.
3. Decide on the number of intermediate sites, with their positions and values of pressure rise.
4. Decide on whether to construct pipeline between any two sites, with the diameter of the pipeline.
5. Decide on the mass flow rates in the pipelines.
6. Guarantee that the pressure of the carbon dioxide is above 8.6 MPa throughout the pipeline network system.

Assumptions

1. Carbon dioxide newly captured at sources has the pressure of 15 MPa.
2. The cost of pumps is mainly electricity cost, and other costs are negligible in magnitude. The electricity price is 0.6 yuan/(kWh). The cost of extra carbon dioxide emission caused by electricity consumption by the pumps is measured by the price of permit for carbon dioxide emission, which is 17 euros/ton (137.7 yuan/ton). The carbon dioxide intensity of electricity is 0.977kg/kWh.
3. The pipe cost is a function of pipe length and pipe diameter. The expression is as shown in formula (C2) below.
4. The pressures of different inlet flows of a certain site must be a constant. This assumption requires the inlet flow with pressure higher than the constant to depressurize before flowing into the node, through throttles valves or other devices. On the other hand, the pressures of outlet flows of a certain site can be different because they can be pressurized separately.
5. The region under consideration is homogenous in geography. This assumption allows us to neglect differences in costs of constructing pipelines and intermediate sites in regions with different geographies.
6. The density of CO_2 in our model is regarded to be 731kg/m^3 as a constant. Our model neglects the density variance of carbon dioxide in the pipeline network due to the temperature changes and pressure changes.

Inputs

1. Geographic coordinates of the sources and the sinks.
2. Geographic coordinates of the nodes of the grids.
3. The capacities of the sources and the sinks.
4. Capture/storage costs of the sources/sinks.
5. Alternative diameters of the pipelines.
6. Electricity price and carbon emission permit price.
7. Life span of the system.
8. Target quantity of carbon dioxide to be sequestrated. (optional)

Set

$I, J=\{\text{Source 1, Source 2, Source 3}, \cdots, \text{Sink 1, Sink 2, Sink 3}, \cdots, \text{Node 1, Node 2, Node 3}, \cdots\}$ Sites

$N=\{\text{Node 1, Node 2, Node 3}, \cdots\}$ Grid Nodes, a sub set of Sites

$SO=\{\text{Source 1, Source 2, Source 3}, \cdots\}$ Sources, a sub set of Sites

$SI=\{\text{Sink 1, Sink 2, Sink 3}, \cdots\}$ Sinks, a sub set of Sites

$D=\{\text{Diameter 1, Diameter 2, Diameter 3}, \cdots\}$ Types of pipelines with different diameters

Continuous variables

$\text{rise}_{i,j}$ = pressure rise of CO_2 flow from site i to site j at site i, $\text{rise}_{i,j} \in [0,+\infty)$, MPa
$F_{i,j}$ = mass flow rate of CO_2 from site i to site j, positive variable, kg/s
c_i = CO_2 captured at site i, positive variable, kg/s
k_i = CO_2 sequestrated at site i, positive variable, kg/s
$pd_{i,j}$ = pressure drop of CO_2 flow from site i to site j, caused by friction of the pipe, $pd_{i,j} \in [0,+\infty)$, MPa
$po_{i,j}$ = pressure of outflow from site i to site j, $po_{i,j} \in [8.6,+\infty)$, MPa
pi_j = pressure of inflow at site j, $pi_j \in [8.6,+\infty)$, MPa
capture cost = capture cost of the CCS project, yuan
storage cost = storage cost of the CCS project, yuan
pipe cost = pipeline construction cost of the CCS project, yuan
pump cost = pump O&M cost of the CCS project, yuan
carbon cost = CO_2 emission permit cost of the CCS project, yuan
total cost = total cost of the CCS project, yuan

Discrete variables

$y_{i,j,d}$ = binary variable, if there is a pipeline of type d connecting i and j, it equals 1. Otherwise, it equals 0

Parameters

θ_k^{LB} = the lower bound of the kth subinterval of the domain of $\text{rise}_{i,j}$, MPa
θ_k^{UB} = the upper bound of the kth subinterval of the domain of $\text{rise}_{i,j}$, MPa
δ_p^{LB} = the lower bound of the pth subinterval of the domain of $F_{i,j}$, kg/s
δ_p^{UB} = the upper bound of the pth subinterval of the domain of $F_{i,j}$, kg/s
α_p = the slope of the piecewise linear function in the pth subinterval of the domain of $F_{i,j}$, kg/s

β_p = The intercept of the piecewise linear function in the pth subinterval of the domain of $F_{i,j}$, kg^2/s^2
L_d = diameter of the pipeline of type d, m
S_d = cross-sectional area of the pipeline of type d, m^2
$dis_{i,j}$ = distance between site i and site j, km
ep = electricity price factor, used to calculate for expenditure on a certain quantity of electricity, yuan/(MPa kg)
tm = time factor, represent the life span of the system, s
cp = carbon price factor, used to calculate the expenditure on carbon dioxide emission permits for carbon dioxide emission caused by a certain quantity of electricity consumption, yuan/(MPa kg)
T = target of CO_2 to be sequestrated, kg/s
f = friction factor of the pipe
ρ = density of CO_2 flow, kg/m^3
e_i = CO_2 emitted at site i, kg/s
u_i = maximum CO_2 sequestration capacity at site i, kg/s
cap_i = CO_2 capture cost at site i, yuan/kg
$sink_i$ = CO_2 sequestration cost at site i, yuan/kg

Objective function

$$\text{total cost} = \text{capture cost} + \text{storage cost} + \text{pipe cost} + \text{pump cost} + \text{carbon cost} \tag{C1}$$

$$\text{pipe cost} = \sum_{i,j,d}[(73.2 \cdot {L_d}^2 + 28.67 \cdot L_d + 23.79) \cdot \text{dis}_{i,j} + 1.22] \cdot y_{i,j,d} \cdot 10^5, \; i \neq j \tag{C2}$$

$$\text{pump cost} = tm \cdot ep \cdot \sum_{i,j}(\theta_k^{UB} \cdot F_{i,j}), \; i \neq j \quad \text{if } \text{rise}_{i,j} \in \left[\theta_k^{LB}, \; \theta_k^{UB}\right) \tag{C3}$$

$$\text{capture cost} = tm \cdot \sum_i \text{cap}_i \cdot c_i \tag{C4}$$

$$\text{storage cost} = tm \cdot \sum_i \text{sink}_i \cdot k_i \tag{C5}$$

$$\text{carbon cost} = tm \cdot cp \cdot \sum_{i,j}(\theta_k^{UB} \cdot F_{i,j}), \; i \neq j \quad \text{if } \text{rise}_{i,j} \in \left[\theta_k^{LB}, \; \theta_k^{UB}\right) \tag{C6}$$

Constraints

1. CCS Target (optional)

$$\sum_i c_i \geq T \tag{C7}$$

2. Conservation of mass

$$\sum_{j \neq i} F_{j,i} + c_i = \sum_{j \neq i} F_{i,j} + k_i \tag{C8}$$

3. Single pipe constraint

$$\sum_d y_{i,j,d} = \begin{cases} 1 & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases} \quad i \neq j \tag{C9}$$

4. Pressure drop of CO_2 flow

$$pd_{i,j} \geq f \cdot \frac{(\alpha_p \cdot F_{i,j} + \beta_p) \cdot \text{dis}_{i,j}}{2\rho \cdot L_d \cdot {S_d}^2}, \; i \neq j \quad \text{if } \; y_{i,j,d} = 1, F_{i,j} \in \left[\delta_p^{LB}, \; \delta_p^{UB}\right) \tag{C10}$$

5. Pressure drop constraint

$$pd_{i,j} = \begin{cases} (po_{i,j} - pi_j) & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases}, \; i \neq j \tag{C11}$$

6. Pressure rise constraint

$$\text{rise}_{i,j} = \begin{cases} po_{i,j} - pi_i & \textit{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases}, \; i \neq j \tag{C12}$$

7. Capabilities of sources and sinks

$$c_i \leq e_i \tag{C13}$$

$$k_i \leq u_i \tag{C14}$$

Appendix D: Illustrations of the Third Submodel

The outline of the third submodel is listed below

Minimize U obj=pipe + pump + carbon

s.t.

$$h(x,y)=0, g(x,y) \leq 0 \begin{cases} \text{Single pipe constraint} \\ \text{Distance equations} \\ \text{Pressure drop of carbon dioxide flow} \\ \text{Pressure drop constraints} \\ \text{Pressure rise constraints} \end{cases}$$

$$\boldsymbol{x} \in R^n, y \in \boldsymbol{Y} = \{0,1\}^m$$

Tasks (outputs)

1. Decide on the positions of the intersection sites.
2. Guarantee that the pressure of the carbon dioxide is above 8.6 MPa throughout the pipeline network system.

As prerequisites of our model, some assumptions have to be held, which are

1. Carbon dioxide newly captured at sources has the pressure of 15 MPa.
2. The cost of pumps is mainly electricity cost, and other costs are negligible in magnitude. The electricity price is 0.6 yuan/(kWh). The cost of extra carbon dioxide emission caused by electricity consumption by the pumps is measured by the price of permit for carbon dioxide emission, which is 17 euros/ton (137.7 yuan/ton). The carbon dioxide intensity of electricity is 0.977kg/kWh.
3. The pipe cost is a function of pipe length and pipe diameter. The expression is as shown in formula (D2) below.
4. The pressures of different inlet flows of a certain site must be a constant. This assumption requires the inlet flow with pressure higher than the constant to depressurize before flowing into the node, through throttles valves or other devices. Similarly, the pressure of outlet flows of a certain site also must be a constant.
5. The region under consideration is homogenous in geography. This assumption allows us to neglect differences in costs of constructing pipelines and intermediate sites in regions with different geographies.

Besides, inputs of the model are as listed below

1. Geographic coordinates of the sources, sinks, intermediate sites of the second submodel.
2. The configuration of carbon dioxide mass flows.

3. Alternative diameters of the pipelines.
4. Electricity price and carbon emission permit price.
5. Life span of the system.

Set

$I,\ J=\{\text{Source 1, Source 2, Source 3}, \cdots, \text{Sink 1, Sink 2, Sink 3}, \cdots, \text{Node 1, Node 2, Node 3}, \cdots\}$ Sites

$N=\{\text{Node 1, Node 2, Node 3}, \cdots\}$ Intersection sites, a sub set of Sites

SO, SOO $=\{\text{Source 1, Source 2, Source 3}, \cdots\}$ Sources, a sub set of Sites

SI, SII $=\{\text{Sink 1, Sink 2, Sink 3}, \cdots\}$ Sinks, a sub set of Sites

D $=\{\text{Diameter 1, Diameter 2, Diameter 3}, \cdots\}$ Types of pipelines with different diameters

Continuous variables

$\text{rise}_{i,j}$ = pressure rise of CO_2 flow from site i to site j at site i, $\text{rise}_{i,j} \in [0, +\infty]$, MPa
x_n = the horizontal coordinate of node n, km
y_n = the vertical coordinate of node n, km
$\text{dis}_{n,i}$, $\text{dis}_{i,n}$ = distance between site i and node n, km
$pd_{i,j}$ = pressure drop of CO_2 flow from site i to site j, caused by friction of the pipe, $pd_{i,j} \in [0, +\infty]$, MPa
$po_{i,j}$ = pressure of outflow from site i to site j, $po_{i,j} \in [8.6+\infty]$, MPa
pi_j = pressure of inflow at site j, $pi_j \in [8.6, +\infty]$, MPa
pipe cost = pipeline construction cost of the CCS project, yuan
pump cost = pump O&M cost of the CCS project, yuan
carbon cost = CO_2 emission permit cost of the CCS project, yuan
total cost = total cost of the CCS project, yuan

Parameters

$F_{i,j}$ = mass flow rate of CO_2 from site i to site j, kg/s
x_{so} = the horizontal coordinate of so, km
y_{so} = the vertical coordinate of so, km
x_{si} = the horizontal coordinate of si, km
y_{si} = the vertical coordinate of si, km
$\text{dis}_{so,soo}$, $\text{dis}_{so,si}$, $\text{dis}_{si,sii}$, $\text{dis}_{si,so}$ = distance between so (si) and soo (sii), km
L_d = diameter of the pipeline of type d, m
S_d = cross-sectional area of the pipeline of type d, m^2
ep = electricity price factor, used to calculate for expenditure on a certain quantity of electricity, yuan/(MPa kg)
tm = time factor, represent the life span of the system, s
cp = carbon price factor, used to calculate the expenditure on carbon dioxide emission permits for carbon dioxide emission caused by a certain quantity of electricity consumption, unit: yuan/(MPa kg)
T = target of CO_2 to be sequestrated, kg/s
f = friction factor of the pipe
ρ = density of CO_2 flow, kg/m^3

Objective function

$$\text{total cost} = \text{pipe cost} + \text{pump cost} + \text{carbon cost} \tag{D1}$$

$$\text{pipe cost} = \sum_{i,j,d} [(73.2 \cdot L_d{}^2 + 28.67 \cdot L_d + 23.79) \cdot \text{dis}_{i,j} + 1.22] \cdot y_{i,j,d} \cdot 10^5,\ \ i \neq j \tag{D2}$$

$$\text{pump cost} = tm \cdot ep \cdot \sum_{i,j} \left(\text{rise}_{i,j} \cdot F_{i,j}\right),\ \ i \neq j \tag{D3}$$

$$\text{carbon cost} = tm \cdot cp \cdot \sum_{i,j} \left(\text{rise}_{i,j} \cdot F_{i,j}\right),\ \ i \neq j \tag{D4}$$

Constraints

1. Single pipe constraint

$$\sum_d y_{i,j,d} = \begin{cases} 1 & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases},\ \ i \neq j \tag{D5}$$

2. Distance equations

$$\text{dis}_{i,j} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2},\ \ i \neq j \tag{D6}$$

3. Pressure drop of CO_2 flow

$$pd_{i,j} \geq f \cdot \frac{F_{i,j}{}^2 \cdot \text{dis}_{i,j}}{2\rho \cdot L_d \cdot S_d{}^2},\ \ i \neq j \quad \text{if} \ \ y_{i,j,d} = 1 \tag{D7}$$

4. Pressure drop constraint

$$pd_{i,j} = \begin{cases} (po_{i,j} - pi_j) & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases},\ \ i \neq j \tag{D8}$$

5. Pressure rise constraint

$$\text{rise}_{i,j} = \begin{cases} po_{i,j} - pi_i & \text{if } F_{i,j} > 0 \\ 0 & \text{otherwise} \end{cases},\ \ i \neq j \tag{D9}$$

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