

Capturing the Effects of Oil Price Uncertainty in Carbon Integration Network Design

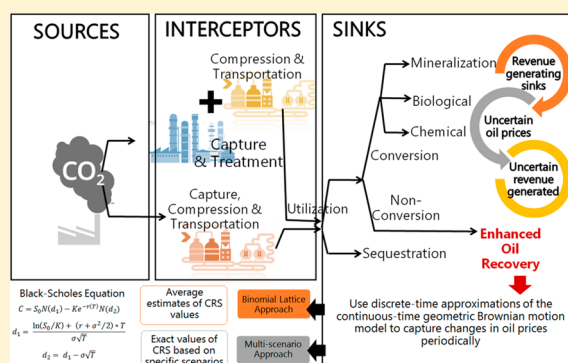
Rola Malaeb,[†] Hussein Tarhini,^{*,†,‡,ID} and Sabla Y. Alnouri[‡]

[†]Department of Industrial Engineering and Management, American University of Beirut, P.O. Box 11-0236, Riyad El-Solh, Beirut 11-0236, Lebanon

[‡]Department of Chemical and Petroleum Engineering, American University of Beirut, PO Box 11-0236, Riyad El-Solh, Beirut 11-0236, Lebanon

Supporting Information

ABSTRACT: Carbon integration is a novel concept that targets the recovery and allocation of industrially emitted CO₂ streams into CO₂-using sinks, with the goal of attaining a CO₂ allocation strategy that meets a desired carbon dioxide emission reduction target and an ultimate aim of minimizing the cost of the network while maximizing any revenue. Enhanced oil recovery (EOR) is considered one of the most attractive CO₂ sink options. CO₂ streams that are delivered and injected into EOR sites are great revenue sources for CO₂-supplying entities. Since oil pricing heavily affects the revenue generated via CO₂ streams injected into EOR sites, this paper studies the effect of oil price fluctuations onto the design of carbon integration networks. Hence, oil pricing has been selected as the main uncertainty parameter and has been fed into a linearized multiperiod carbon integration model using stochastic data. Since oil prices vary periodically, this model has been formulated over several time periods, in which the oil pricing parameters are allowed to change over time. The proposed model has been optimized using two different approaches: (1) the binomial lattice approach, which primarily utilizes average uncertainties as expected values, and (2) the multisenario approach.



1. INTRODUCTION

Most greenhouse gas (GHG) emissions in industry are primarily a result of burning fossil fuels or natural gas material for energy production in the form of either heat or power. In 2010, such activities accounted for about 65% of all global CO₂ gas emissions.¹ Several industrial processes also produce CO₂ emissions through chemical reactions that do not involve combustion activities. Many countries are realizing an imperative need for the industrial sector to manage their carbon footprints by enforcing carbon dioxide reduction targets on GHG emissions.¹ However, meeting such targets introduces numerous challenges, especially for energy-intensive industries.

Carbon integration aims to identify CO₂ capture, recovery, and allocation schemes in the form of carbon dioxide networks by employing cost-effective and revenue-generating source-to-sink allocation strategies.² Carbon dioxide can be utilized in many different ways through chemical or biological conversion to other value-added products.³ An industrial zone, which usually consists of a cluster of processing facilities within geographic proximity, could ideally incorporate many economic options for carbon dioxide converting processes which are often referred to as CO₂-using sinks. Many of those processes are very useful in converting the majority of carbon dioxide emissions that result from industrial activities into

value-added products. Introducing those conversion routes greatly facilitates industrial symbiosis, which ideally involves the reuse of a generated waste stream as useful material in other processes that could potentially exist within an industrial cluster.⁴

There exist a plethora of studies that focus on carbon dioxide allocation into geological storage, such as the work of Middleton and Bielicki⁵ and Tan and Foo.⁶ While carbon dioxide allocation into storage tanks incurs additional cost onto a given system, CO₂-using sinks allow for revenue-generating opportunities like the enhanced oil recovery, EOR, sink.⁷

It should be emphasized that revenue-generating sinks often require high-purity carbon dioxide streams, which are easily attainable by incorporating treatment units that are capable of separating CO₂ gas from the remaining gaseous emission material. According to Hasan et al.,⁸ complex and multiscale optimization needs to be performed to obtain the treatment costs which depend on material selection, process design and optimization, the quality of the CO₂ source, as well as other factors. Another main cost factor to consider in such networks

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are transmission costs, which can be accounted for based on the geographic distances between emission sources and CO₂ sinks within the city, as well as the initial pressure of a given emission source and the required pressure conditions at the sink.² Hence, assessing capture costs, pipeline costs, and compression costs, as well as any CO₂ revenue options at the sink, is vital for determining economically attractive CO₂ connectivity decisions.²

When accounting for revenue aspects, any financial returns that may be generated from CO₂ sink options can vary greatly. For instance, oil prices in the range of 15–20 US\$/barrel EOR have been able to generate revenue of 10–16 US\$/ton of CO₂ injected.⁹ When oil prices were reported to be 90 US\$/barrel in 2015, the revenue generated upon injecting one ton of CO₂ grew to 70 US\$/ton of CO₂ injected.¹⁰ With the continuous oil price fluctuations, the revenue from such sink options becomes quite uncertain.

This paper mainly aims to incorporate the effect of such uncertainty factors into carbon integration network design. Carbon integration networks were first introduced by Al-Mohannadi and Linke using a deterministic mixed integer nonlinear programming, MINLP, model.² Since oil prices have been found to directly affect the corresponding CO₂ sink price, and EOR sinks were reported to be one of the greatest revenue generating sinks by Al-Mohannadi and Linke,² this paper presents a stochastic model that captures oil pricing uncertainty in the course of identifying optimal design strategies of carbon integration networks.

2. LITERATURE REVIEW

Generally speaking, investigating uncertainty elements is crucial where they have severe impact on the model, the network configuration, and the system as a whole. Not accounting for uncertainties is like observing and dealing with the system on one specific point in time, whereas in reality, the system experiences many different cases and scenarios.

Uncertainties occur in carbon capture and utilization and storage, CCUS, systems, where they may be associated with CO₂ emission sources (e.g., source operating lifetime) or CO₂ sinks (e.g., sink storage capacity), as well as in water networks, where they may be associated with water quality levels and flow rates. In addition, uncertainties can happen in energy networks, supply chain networks, etc.

One article presents the design and optimization of a carbon capture, utilization, and sequestration (CCUS) supply chain network that addresses the issues of selecting the sources, the alternate capture technologies and materials, utilization of CO₂ sites, and sequestration in different storage sites.⁷ It is a cost model whose aim is to minimize the overall network cost where the cost includes the dehydration, capture, compression, transportation, and injection costs as well as the revenues generated from utilizing the CO₂. Hasan et al.⁷ discuss the computational methods of each of the aforementioned costs as well the revenues generated from selling high-purity CO₂ to the CO₂-EOR sites which are the enhanced oil recovery sites. In doing so, a mixed integer linear programming optimization, MILP, model is developed to select the optimum network. This work concludes that the selection of the right material and capture technology is a crucial element that directly affects the overall network cost.⁷ Furthermore, a reduction in the cost is obtained by diversifying the selected sources between both utilization and sequestration. It has been reported that the higher the flow rates from the sources are, the lower the cost is,

particularly the capture and compression costs. One important fact is that the CCUS cost is directly related to the minimum CO₂ reduction target; the higher the target, the higher the cost. Finally, and most importantly, this work concludes that it is possible to reduce more than 50% of the current CO₂ emissions from the sources in the United States at reasonable costs by implementing the CCUS networks, thus enabling the continual use of fossil fuels.⁷

He et al.¹¹ propose a mixed integer linear programming, MILP, model that accounts for the following uncertain parameters: the ending time of the operating life of each source, the upper limit of carbon dioxide storage capacity of each sink, and the carbon footprint of compensatory power to make up for carbon capture and storage, CCS, energy losses. In doing so, He et al.¹¹ assume that those uncertain parameters can be represented as uniformly distributed parameters, each having a minimum and a maximum value incorporated into their model. According to their work, this model is referred to as the worst-case model. Subsequently, He et al.¹¹ propose a robust MILP model that incorporates uncertainty parameters as probability distributions. Upon developing the deterministic MILP model, the robust MILP model, and the worst-case model, their results show that uncertainties associated with those parameters greatly affect the CCUS network configuration, as well as the corresponding operating conditions. Although the deterministic model is able to provide feasible and optimal network configurations, the solutions generated from the deterministic model may turn out to be infeasible in real life practice. Hence, capturing those uncertainty elements is able to provide more realistic solutions of CCUS systems.¹¹

King et al.¹² discuss the economics of a CCUS network in which anthropogenic CO₂ captured from a fossil power plant is processed into the enhanced oil recovery, EOR, sinks. In their study, they define producers as electricity generation plants, whereas consumers as owners of the oil reservoirs.¹² After discussing their pipeline network as well as the different costs that should be taken into account, King et al.¹² develop a cash flow model that integrates CO₂ capture at the power plants, CO₂ transport through the pipelines, and CO₂ processing into the EOR sinks. Their goal is to achieve a 20% internal rate of return for each part of the process. It is shown that there is a huge uncertainty in various parameters in their model, for example, in the capital cost of capture and EOR, oil prices, amount of CO₂ needed for each barrel of oil, etc. Monte Carlo simulations are used to conclude that EOR operations are more likely to yield more than 20% internal rate of return due to the uncertainty in the oil prices, that have been mainly expected to be higher, and uncertainty in the CO₂ prices which have been expected to be lower than the values used in their reference case.¹² Monte Carlo simulation is an iterative approach where the sample inputs vary probabilistically, and consequently the model outputs are computed. Subsequently, these results are statistically analyzed.¹³ Since a complex Monte Carlo simulation is required, this approach has not been adopted in this work.

Ahmed and Sahinidis¹⁴ utilize a two-stage approach in which their variables have been categorized into two different sets. First stage variables, known as the design variables, are identified as variables that should be decided before the realization of the uncertain parameters. Second-stage variables, known as the control or operating variables, are identified as variables that can be decided after the uncertain parameters have been embedded into the scenario. The objective, in such

a case, is to minimize both first stage costs, and the expected value of the random second stage recourse costs. The only limitation of this approach is the fact that it only accounts for the expected value of second stage costs while ignoring any other variations that might occur due to the realization of the uncertainties.¹⁴ Thus, in an attempt to resolve this issue, a deviation term, referred to as the “robustness measure”, has later been incorporated into their model. In their paper, an alternative formulation that handles all nonlinearities which result from the use of this robustness measure term, has been then proposed.¹⁴

Ahmed and Sahinidis¹⁴ also present a motivating example to illustrate the effects of the real values of the uncertain parameters that in turn can lead to huge variations in the real cost value. To account for this variability, a goal programming approach is utilized, which in turn aims to minimize the total cost, both first stage and recourse costs, in addition to a weighted variability contribution. Their study also discusses two different frameworks: (1) a robust optimization framework which accounts for a risk measure in the objective function and (2) a restricted recourse framework that accounts for the same risk measure in the constraints. Many different applications are presented in their study, but their main difficulty is the nonlinearity involved.¹⁴ Due to the nonlinearity introduced into the model as a result of using variance as a robustness measure, and due to the fact that the variance is a symmetric risk measure which penalizes both costs, higher and lower than the expected recourse cost, Ahmed and Sahinidis¹⁴ use an upper partial mean, UPM, that is an asymmetric measure of recourse costs variability. Their work continues to illustrate the optimization robustness of their approach, using the restricted recourse framework explained earlier, for a chemical process planning problem under uncertainty. In this problem, a new variable is added, so as to account for the positive deviation in a linearized fashion. Additionally, they develop a heuristic for the restricted recourse formulation and finalize the discussion of their study using several scenarios.¹⁴

Liu and Sahinidis¹⁵ introduce a two-stage stochastic programming approach for a chemical process planning problem under uncertainty. Due to the large size of the model, Liu and Sahinidis¹⁵ develop a Benders-based decomposition approach. This decomposition algorithm divides the mixed-integer linear model into two: an integer and a continuous component. Another feature of the Benders decomposition model is its ability to break the problem into small components. Liu and Sahinidis¹⁵ explain the approach with using both discrete parameters as well as continuous random parameters.¹⁵

Bidhandi and Yusuff¹⁶ present a two-stage stochastic programming model for a supply chain network design problem under uncertainty. First-stage decisions are configuration decisions, while second-stage decisions are those associated with processing and transporting products and materials from suppliers to customers, under uncertainty. The uncertain parameters are considered to be operational costs, customer demand, and facility capacities. Each of those parameters are associated with a log-normal distribution. Due to the large number of scenarios and due to the difficulty in evaluating the expected values in the objective function, Bidhandi and Yusuff¹⁶ utilize a Sample Average Approximation, SAA, technique in their study, together with a Monte Carlo simulation, to determine approximations of expected values in place of finding real values. The objective function in

this case is to minimize the total cost while satisfying the customer demands.¹⁶ Furthermore, to improve the computational time, the accelerated Benders’ decomposition approach is used in which the integer master problems are replaced by linear problems. This modified algorithm along with the surrogate constraints leads to much better and improved results compared to the original SAA approach.¹⁶

Another paper that discusses a two-stage approach to plan for a carbon capture and storage, CCS, network under uncertainty which includes CO₂ capture, transportation, storage, sequestration, and utilization is presented by Han and Lee.¹⁷ In their study, Han and Lee¹⁷ account for uncertainties such as CO₂ emissions, operating costs, and product prices. While their model accounts for an objective function that can either maximize profit or minimize cost, their paper addresses the case of maximizing the profit while meeting a certain carbon dioxide reduction target. Furthermore, their study experiments the effect of different sizes and scales of all facilities used in the network as utilization facilities, capture facilities, etc., as well as the effect of several CO₂ reduction targets over a long-term horizon. Their MILP model is capable of deciding where, how much, and how to capture, transport, utilize, store, and sequester carbon dioxide.¹⁷ Following their multiperiod deterministic model, Han and Lee¹⁷ formulate a multiperiod stochastic model, combined with an inexact two-stage stochastic programming. Subsequently, they compare it to other approaches like multiscenario stochastic programming, and a two-stage stochastic programming.¹⁷ The uncertainties in operating costs and product prices, which are the coefficients of the objective function, have been modeled using a multiscenario stochastic programming approach, where each uncertain parameter is associated with a finite set of scenarios, each with a given probability of occurrence. Nevertheless, the uncertainties in CO₂ emissions have been formulated using a two-stage stochastic model using the expected scenario approach. This defines the inexact two-stage stochastic programming approach that combines both the multiscenario and the two-stage stochastic programming approaches.¹⁷

An alternative approach is presented by Wang et al.¹⁸ which utilizes the concept of a birandom variable and adopts an equilibrium chance-constrained programming, ECCP, to model a CCUS system under uncertainty. A “birandom” variable is a parameter that has dual random characteristics. In other words, any random variable will follow a probabilistic distribution whose characteristic values also follow a random distribution. The equilibrium chance concept is used to compare the degree of occurrence of two birandom events. In their study, it is selected over the other chance measures, like the primitive chance and average chance, because it is presented as a real number that facilitates the comparison and decision making process.¹⁸ Wang et al.¹⁸ assume that every birandom variable has a normal distribution, with characteristic values (the mean) being random as well. First, the uncertain optimization model whose objective function is to minimize the total cost while satisfying different constraints, such as those related to environmental and capacity limits, must be formulated. Following this, the random constraints that consist of the birandom variables must be converted into their deterministic equivalents using the equilibrium chance-constrained algorithm. After solving the deterministic model, various optimal solutions can be generated, each based on a specific value of the probability-violation level. The results of

the case study presented by Wang et al.¹⁸ show that for a low constraint violation level, the model is more restricted, leading to a higher system cost, and a larger amount of treated CO₂.¹⁸ Decision makers can then select the best solution while taking into account the trade-off between the profitability and reliability of the system.¹⁸

Tan et al.¹⁹ present a continuous time mixed integer nonlinear programming model for a carbon capture and storage, CCS, network whose objective is to maximize the reduction of CO₂ emissions by matching *m*-CO₂ sources to *n*-CO₂ sinks.¹⁹ The nonlinearity in the model is due to the presence of some bilinear terms. Due to its computational difficulties, this model is linearized into a mixed integer linear programming model, MILP, by eliminating these terms. An important assumption in their model is that the sources have fixed flow rates and operating lives, and the sinks have an earliest time of availability and a maximum CO₂ storage capacity.¹⁹ The result of these assumptions is the primary focus of the model on physical and temporal aspects of CCS systems.

Compernelle et al.²⁰ apply continuous time real-options models coupled with dynamic programming concepts so as to define the investment threshold levels. The real-options models are split into two: one that focuses on the investment in a CO₂ capture unit, while the other focuses on the investment in EOR.²⁰ From the first model, the critical price level of CO₂ for which the CO₂ producer becomes willing to invest in a CO₂ capture unit is determined. Similarly, from the second model, the critical price level of oil for which the oil producer becomes willing to invest in EOR is also determined, for a given CO₂ cost.²⁰ According to Compernelle et al.,²⁰ CCUS is not economically feasible due to the high investment cost required. However, one way that allows pursuing this technology is to effectively use the CO₂, for instance, in Enhanced Oil Recovery.²⁰ Assuming that CO₂ exchange will take place from a CO₂ producer to an oil producer, attractive price ranges for such transactions can be identified.²⁰ Uncertainties in oil and CO₂ prices are also addressed using a sensitivity analysis approach. In their paper, the minimum oil price needed to process the trade in CO₂ depends on several factors, such as the CO₂ permit price, the lifetime of the oil field, the rate of oil extraction per ton of CO₂ injected, and the discount rate.²⁰ The sensitivity analysis shows that a longer oil field lifetime results in a lower minimum oil price. For high CO₂ permit prices, electricity producers that invest in the capture unit must be willing to pay a fee to oil producers to store the CO₂; thus CO₂ input could also become revenue to oil producers according to Compernelle et al.²⁰

The impact of various other uncertainty elements on carbon capture, utilization and storage, CCUS, problems are profound. Many previous work investigated the impact of those effects, using a variety of different techniques. For instance, Tan et al.¹³ propose a two-stage approach that relies on the P-graph framework in the first stage to specify the *n*-best networks that are optimal and suboptimal solutions. Such alternative solutions are then considered in the second stage, in which a Monte Carlo simulation is utilized to test for the system's sensitivity to changes in the parameters. Two different case studies are considered by Tan et al.:¹³ (1) a carbon-constrained energy planning problem and (2) a carbon dioxide capture and storage planning problem between sources and sinks. After arbitrary optimal and near-optimal solutions have been obtained from both stages, the P-graph framework has then been used to test the robustness of such attained

alternatives to parameter variations using Monte Carlo simulations. Subsequently, the best network for implementation can then be selected. In the second case study, Tan et al.¹³ assume a normal distribution for both the amount of carbon dioxide that can be captured from the sources and the total capacity of the sinks. Optimizing the model using the P-graph resulted in 71 networks. Some of those solutions are optimal and the others are suboptimal networks. These networks fail if the excess storage capacity of at least one sink is negative. The Monte Carlo simulation shown in this specific case shows that there is a high probability of failure of two networks, one of which is optimal and the other is suboptimal. Thus, it has been found that the use of Monte Carlo simulations are beneficial to study the system sensitivity to perturbations of such parameters.¹³ Their work addresses two case studies, one of which is the carbon integration network with uncertainty in the availability of carbon dioxide in the sources and in the storage capacity of the sinks.¹³ In contrast to the work presented by Tan et al.,¹³ and all other previous contributions that were discussed above, this work studies a different uncertainty variable, in the form of oil pricing, and investigates its effect on carbon integration network design problems.

3. BACKGROUND

Based on the literature review discussion presented above, it has been realized that only certain mathematical techniques can be utilized to model oil price uncertainty. For instance, Ross²¹ concludes that the continuous-time geometric Brownian motion model, which is an extensively used approach that is often utilized for modeling stock prices of real assets, cannot be used to model stochastic oil prices. This is due to a key assumption that is required by this model, which states that the future pricings are independent of past prices and past price movements. Therefore, having a general understanding of such appropriate methods that can accurately capture and model oil pricing uncertainty is crucial.

3.1. Risk-Neutral Uncertainty Model or Models That Use Data. Ross²¹ discusses many methods for modeling the oil price uncertainties, such as the risk-neutral model. This method can help identify whether a certain option is underpriced or overpriced with respect to a current price of the security itself.²¹ This model assumes, being at any state *i*, the log ratio of the next state will be a random variable with a normal distribution with a mean μ_i , and a standard deviation s_i , that are related according to eq 1, where *r* is the interest rate and *N* is the number of trading days in a year (taken to be equal to 252 days).

$$\mu_i = \frac{r}{n} - \frac{s_i^2}{2} \quad (1)$$

If this type of model is to be adopted, a separate simulation would be required to find the expected worth of an option. Hence, to avoid simulation models, oil prices will not be modeled using the Risk-Neutral model in this paper. On the other hand, if the aim is to value an option, one could use a model that assumes that the future will tend to follow the past. In such a case, the model would then assume that currently being at any state *i*, the logarithm of the ratio of tomorrow's price to today's price is a random variable that is normally distributed using a mean \bar{x}_i value and a standard deviation s_i value, which in turn would require a certain computation process so as to obtain those values based on given data.

Table 1. Nonlinear vs Linear Correlation Comparison

cost element	MINLP ²	MILP
capital cost of compression	$CC^{\text{capital}} = 158902 \left(\frac{P^{\text{comp}}(T_{s,k,t} + U_{s,k})}{224} \right)^{0.84} \text{CRF}$	$CC^{\text{capital}} = 158902 \left(\frac{P^{\text{comp}}(T_{s,k,t} + U_{s,k})}{224} \right)^{0.84} \text{CRF}$
cost of piping	$D_{s,k} = \sqrt{\frac{4(8.314)T_s[\sum_S \sum_T TF_{s,k,t} + \sum_S U_s]}{\pi v_{s,k} M_s [\Delta P_{s,k} + \Delta P_{s,k}^{\text{pipe}}]}}$	$P_{s,k} = 4 \times \frac{\text{del}_{s,k}}{2}$ $QQP_{s,k,\text{Pd}} \leq \text{ratio}_{s,k} \times 2 \times P_{s,k}$ $\text{del}_{s,k} \leq 10000D_{s,k}$ $C_{s,k}^{\text{pipe}} = \text{CRF} \times [96904D_{s,k} + 952302 \times \text{del}_{s,k}]$
capital cost of pumping	IF $\text{PPUMP}_{s,k} \geq 7.39 \text{ MPa}$ THEN $\text{PCAP}_{s,k} = \text{CRF} \times \left[\frac{1.11 \times 10^6 \times \text{PPUMP}_{s,k}}{1000} + 0.07 \times 10^6 \right]$	$\text{PCAP}_{s,k} = \text{CRF} \times \left[\frac{1.11 \times 10^6 \times \text{PPUMP}_{s,k}}{1000} + z_{p_{s,k}} \times 0.07 \times 10^6 \right]$ $\text{PPUMP}_{s,k} \leq 10000000 \times z_{p_{s,k}}$

Other methods also exist, which mainly rely on a bootstrap approach instead of a normality assumption, for which the future is dependent on the past.²¹ This latter approach assumes that the best approximation for the log distribution ratio of a certain state is to randomly choose one of the data values. In both cases, a separate simulation is required to be able to determine the expected value of a future price.

3.2. Chance Constrained Programming. In addition to all aforementioned approaches, the Chance Constrained Programming is also an alternative modeling method, which in turn combines a mathematical programming model with chance constraints in the form of probability levels of attainment.²² A typical mathematical programming model often follows the following structure:

$$\max f(x) \tag{2}$$

$$\text{s. t. } Ax \leq b \tag{3}$$

Chance constrained models can be utilized in many applications.²² The objective function $f(x)$ can be a profit function that needs to be maximized. It consists of n variables x and includes the profit contribution rate constants. There are m constraints in Ax , each of which is limited by constant b .²² Charnes and Cooper presented three formulations of the chance constraint models:²²

3.2.1. Maximize the Expected Value of a Probabilistic Function.

$$\max E[Y] \quad (\text{where } Y = f(x)) \tag{4}$$

$$\text{s. t. } \Pr(Ax \leq b) \geq \alpha \tag{5}$$

This formulation renders the maximization (or minimization) of a function and guarantees that a constraint is met with a probability α (where α is user defined). This formulation is recommended when the target is to optimize the objective function while staying within the limits of the resources at a certain probability level.²²

3.2.2. Minimize the Variance.

$$\min \text{Var}[Y] \tag{6}$$

$$\text{s. t. } \Pr(Ax \leq b) \geq \alpha \tag{7}$$

This formulation is usually applied to identify portfolio investments with the minimum variance while satisfying the set of chance constraints. It is often used to measure the risk

associated with a certain activity, which is not the case in this paper. Variance was not considered a major issue in this work. Instead, the effect of uncertain parameters was investigated.

3.2.3. Maximize the Probability To Satisfy a Chance Constraint Set.

$$\max \Pr(Y \geq \text{target}) \tag{8}$$

$$\text{s. t. } \Pr(Ax \leq b) \geq \alpha \tag{9}$$

This formulation is generally much more difficult to accomplish.²² The structure of the chance constraints in the form of probability levels renders it a nonlinear set which requires a nonlinear programming solution. This nonlinearity limits the size of the model; as such, it can no longer yield a solution in case a large number of constraints or variables is involved.²² As a result, this approach was not adopted in this work.

3.3. Black–Scholes Equation. The Black–Scholes equation is used to find the price of a financial security after certain time and is mainly used to determine the price of European call options. However, for the security being oil, the European call option must be used.²³ The Black–Scholes equation assumes that the price of a security follows a geometric Brownian motion with a drift parameter μ , and volatility parameter σ , and gives a no-arbitrage cost of a call option on this security.²¹ The Black–Scholes equation for a call option is

$$C = S_0 N(d_1) - Ke^{-r(T)} N(d_2) \tag{10}$$

$$d_1 = \frac{\ln(S_0/K) + (r + \sigma^2/2)*T}{\sigma\sqrt{T}} \tag{11}$$

$$d_2 = d_1 - \sigma\sqrt{T} \tag{12}$$

The no-arbitrage option cost, C , depends on the security's current price S_0 , the expiration time T of the option, the strike price K , the volatility of the security σ , and the interest rate r . Here, N represents a normal random variable. It is important to note that Black–Scholes equation assumes continuous compounding for interest.²¹

In this paper, the Black–Scholes equation has been utilized to obtain the volatility of the oil price, and a more detailed description of the procedure has been provided together with the binomial lattice approach description.

4. METHODOLOGY

The deterministic model presented by Al-Mohannadi and Linke² that represents the carbon integration network has been utilized as the base model in this study. The base model combines a set of equations that mathematically describe the capture process of carbon dioxide sources, in both treated or untreated forms, followed by a series of pressurization stages (compression and pumping), and then transportation of CO₂ streams to the various sinks into which they are allocated.² The same model has also been extended in later studies so as to account for multiperiod considerations²⁴ and natural gas monetization strategies.²⁵

The objective function of the base model aims to minimize the total cost of the network, which is a combination of the following individual costs: the treatment cost to treat the captured CO₂ streams, the capital and operating costs of the compressors and pumps needed in each source-sink connection, the transportation cost to transport the treated and untreated flows from the sources to the sinks, and the processing cost of these streams into the sinks.² The deterministic model includes a set of constraints that must be satisfied, for instance, the capacity's limit of each sink, the available amount of CO₂ in each source, etc. Since the model involves several integer and binary variables, it is classified as a mixed integer nonlinear programming, MINLP, model according to Al-Mohannadi and Linke.² Since most parts of the model are already linear to begin with, the modifications which have been implemented onto the MINLP model adopted from Al-Mohannadi and Linke^{2,24} are summarized in Table 1.

According to Table 1, the MINLP model has been linearized into an MILP, mixed integer linear programming, model by implementing an alternative linear equation that describes both the compression and pumping costs. In addition, the highly nonlinear diameter computations which were previously utilized in the transportation cost using if statements, have all been replaced with a linear alternative. Following this, the linearized deterministic model has then been converted into a stochastic one to model uncertain parameters taking into account multiple time periods instead of only one period. The MILP model was very convenient for extracting optimum network configurations using a standard CPLEX solver, for all the different scenarios which have been investigated, using the two different approaches (binomial lattice, and multiscenario). Hence, a nonlinear solver with multistart features, which was adopted in Al-Mohannadi and Linke,² was not utilized in this work. Moreover, the MILP model required very few CPU seconds to converge, and global optimality of all extracted solutions can be guaranteed.

As explained earlier, the oil prices are never certain, directly affect the processing cost into the EOR sink, which in turn affects the total cost. This is why it is crucial to capture the uncertainty and fluctuations of the oil prices by which the goal of this paper is achieved which is to find the optimal carbon integration network under the uncertain oil prices that vary randomly with the objective to minimize the total cost. Dealing with uncertain parameters is more realistic because uncertainty is with no doubt one of the most controlling phenomena. The model's main target is to investigate the effect of having stochastic parameters, particularly the oil price, on the design of the carbon integration network as well as on the total cost/

revenue of the network. This uncertain parameter is modeled using two approaches.

In this paper, the variability, uncertainty, and oil price fluctuations are first modeled using a binomial lattice model, which was developed by Luenberger.²³ This model is classified as a discrete-time approximation of the continuous-time geometric Brownian motion model.²⁶ This approach overcomes the independence assumption of the continuous-time geometric Brownian motion model; this is why it is the first chosen approach in this paper. Second, the uncertain oil prices are modeled using a multiscenario approach which considers real scenarios that may occur and averages the result over a subset of scenarios. This approach is heavily used since it takes into account realistic scenarios that might take place.

The base model which was utilized for this work has already been presented by Al-Mohannadi and Linke,² this work primarily investigates how uncertainty impacts carbon integration solutions by accounting for oil price fluctuations. Since two different approaches have been utilized to account for this uncertainty dimension, this paper presents how the base model would need to be modified and implemented accordingly. Hence, the implementation aspect was crucial, since many additional aspects need to be considered, the most important of which is the selection of a number of suitable techniques that could accurately model uncertainty in oil pricing for such systems. Following this, the incorporation of those aspects into the base model was highly dependent on the technique being utilized for modeling this uncertainty parameter. As a result, a thorough description of the implementation procedure was provided for each of the two proposed methods in the sections that follow.

4.1. Binomial Lattice Approach. The binomial lattice model is derived from the continuous-time geometric Brownian motion model that is widely used to model the stock price behavior. This model takes into consideration the quality of the oil being extracted and sold; the oil might be treated, liquefied, or both before being sent to the consumers.²⁶ These mentioned factors explicitly affect the selling price of the oil, which in turn will affect the revenue generated from carbon dioxide streams injected into these EOR sites. Melki²⁶ states that to model this uncertainty and fluctuations of the oil price, the respective data must be collected and the volatility and the expected growth rate of the oil price must be estimated. These data and estimates will then be used to model the oil prices using a binomial lattice model. Furthermore, oil treatment issues will not be accounted for. Instead, it is assumed that consumers are held responsible for treating the oil received, based on its respective use at the sink.²⁶

Generally speaking, the binomial lattice, which is a discrete-time model, is capable of capturing oil prices periodically. This means that if the price at the beginning of the period is S , then the price at the beginning of the next period will have one of two values. It will either go up by a factor $u > 1$ with a probability $0 < p < 1$ to be equal to uS , or it will go down by a factor $d < 1$, with a probability $1 - p$ to be equal to dS . Having S , u and d all positive then the price can never have a negative value which allows the consideration of the logarithm of the price as a variable.²³ Luenberger²³ defines the parameters of the Binomial Lattice model as follows:

The expected yearly growth rate

$$gr = E[\ln(S_T/S_0)] \quad (13)$$

Table 2. U.S Daily Treasury Yield Curve Rates of October 2017^{27a}

date	1 mo	3 mo	6 mo	1 yr	2 yr	3 yr	5 yr	7 yr	10 yr
10/02/17	0.95	1.01	1.22	1.31	1.49	1.63	1.94	2.17	2.34
10/03/17	1.01	1.07	1.21	1.32	1.47	1.62	1.92	2.15	2.33
10/04/17	1.00	1.08	1.21	1.33	1.47	1.62	1.92	2.15	2.33
10/05/17	1.02	1.07	1.21	1.35	1.49	1.63	1.94	2.17	2.35
10/06/17	1.03	1.07 ^b	1.22	1.35	1.54	1.66	1.97	2.20	2.37

^aSource: www.ustreas.gov. ^bThe treasury yield interest rate at 3 months maturity.

where S_T is the price at the end of the whole period (1 year) and S_s is the initial stock price;

The yearly variance

$$\sigma^2 = \text{var}[\ln(S_T/S_s)] \quad (14)$$

The probability

$$p = \frac{1}{2} + \frac{1}{2} \left(\frac{gr}{\sigma} \right) \sqrt{\Delta t} \quad (15)$$

where σ is the yearly standard deviation and Δt is the period length that is very small.

The factor associated with price increase

$$u = e^{\sigma\sqrt{\Delta t}} \quad (16)$$

The factor associated with price decrease

$$d = e^{-\sigma\sqrt{\Delta t}} \quad (17)$$

An option is defined as the right to buy (a call option) or to sell (a put option) an asset under specified price and specified period of time. The option premium is defined as the price of the option itself which may be only a fraction of the price of the asset. This premium cannot be returned in case the option holder does not want to exercise the option. The term exercise the option is usually used when the holder actually buys or sells the asset by obeying the terms of the option.²³

It is required to specify the details of the option, which are often description of the asset, stating whether it is a call or a put option, the exercise price or the strike price, the expiration date stating if it is an American or European option, and the premium price. The strike price is the price at which the asset will be bought or sold when the option is exercised. The expiration date is the period of time during which the option is valid. There are two styles of the expiration date; the American option states that the option can be exercised anytime during this period until the last day, whereas the European option states that the option can only be exercised on the last day which is exactly the expiration date.²³

The procedure to find the parameters of the binomial lattice model requires collecting several data such as the risk-free interest rate, the current oil price, the oil futures prices and the oil futures options prices on a specific date. The data refers to three months maturity for the European option. The daily treasury yield curve rates for October 2017 have been obtained from the U.S Department of the Treasury.²⁷ Table 2 summarizes the relevant information. Assuming a maturity of 3 months for future options prices, the U.S. Treasury interest rate at 3 months becomes $r = 1.07\%$. The market price of crude oil has been considered as a spot market which has then been used to obtain the future oil prices. The corresponding data presented in Table 3 provide two important values: (1) the current oil price and (2) the oil price value after one time period, which in turn corresponds to the same duration of the

Table 3. Crude Oil Futures Prices^{29a}

month	last
crude oil – electronic Nov 2017	49.25 ^b
crude oil – electronic Dec 2017	49.60
crude oil – electronic Jan 2018	49.84
crude oil – electronic Feb 2018	50.09
crude oil – electronic Mar 2018	50.22
crude oil – electronic Apr 2018	50.38
crude oil – electronic May 2018	50.37
crude oil – electronic Jun 2018	50.39
crude oil – electronic Jul 2018	50.34
crude oil – electronic Aug 2018	50.31
crude oil – electronic Sep 2018	50.27
crude oil – electronic Oct 2018	50.28
crude oil – electronic Nov 2018	52.31 ^c

^aSource: *Wall Street Journal*, Aug 10, 2017. ^bThe current crude oil future price on November 2017. ^cThe crude oil future price 1 year from now, on November 2018.

time period studied in this work. The current price is taken to be the price of the hydrocarbon that will be delivered the next month due to the delay that occurs in delivering the oil which is almost a month. Thus, the current crude oil price according to October 2017, as shown in Table 3, is \$49.25/barrel.

In addition to the above information, future crude oil prices are needed to estimate the volatility of the oil price. In order to be able to use the Black–Scholes equation, the data collected must correspond to a European call option with an expiration date on January 2018 (3 months maturity). The strike price taken from Chicago Mercantile Exchange²⁸ which was found to satisfy the aforementioned criteria is \$50/barrel, and the value of the option is \$6.82/barrel.

Following the above data collection process, the Black–Scholes equation has then been used with parameters referring to 3 months maturity in order to calculate the implied volatility of the oil price. The call option Black–Scholes formula is stated in eq 18, where C is the price of the option, S_0 is the current future price, $N(x)$ is the standard cumulative normal probability distribution, K is the strike price, r is the risk-free interest rate, T is the expiration time, and σ is the volatility of oil price:²³

$$C = S_0 N(d_1) - Ke^{-r(T)} N(d_2) \quad (18)$$

$$d_1 = \frac{\ln(S_0/K) + (r + \sigma^2/2) \times T}{\sigma\sqrt{T}} \quad (19)$$

$$d_2 = d_1 - \sigma\sqrt{T} \quad (20)$$

It should be noted that the Black–Scholes equation was found to yield a volatility $\sigma = 72.46\%$.

Now, using this value of the volatility of oil prices, the two factors representing the increase and the decrease of the oil

price per each time period have been calculated using Equations 21 and (22) respectively. This time period can be changed, and the two factors can be calculated similarly and accordingly.

$$u = e^{\sigma\sqrt{\Delta t}} = 2.064 \quad (21)$$

$$d = e^{-\sigma\sqrt{\Delta t}} = 0.485 \quad (22)$$

In this work, the length of each time period was taken as 1 year, since oil prices were found to vary a little over a couple of months. However, a much more significant oil price variation was reported to take place on a yearly basis. As a result, all corresponding increase/decrease factors in this work have been calculated on a yearly basis. It should be noted that the time period duration can be set to a different value, if the required volatility factors can be obtained on a similar basis according to the process described above, in case the necessary data is available.

The probabilities associated with an increase (u) or decrease (d) in the oil price have been defined as q_u and q_d , respectively. Those two values have been determined by setting the current value of futures price to zero, as shown in eqs 23–25 below.

$$q_u S[u - (1 + r')] + q_d S[d - (1 + r')] = 0 \quad (23)$$

$$q_u = \frac{(1 + r') - d}{u - d} = 0.365 \quad (24)$$

$$q_d = 1 - q_u = 0.635 \quad (25)$$

In the above equations, r' is defined as the rate of increase of the different oil futures prices, which is not the same as the risk-free interest rate, r .²³ Using the future oil prices highlighted in Table 3, r' has been calculated to be 6.2%, according to eq 26:

$$r' = \frac{\text{crude oil future price}_{\text{Nov 2018}}}{\text{crude oil future price}_{\text{Nov 2017}}} - 1 = \frac{52.31}{49.25} - 1 \quad (26)$$

Upon collecting all the necessary data which is required to execute the multiperiod binomial lattice model, it is essential to note the following:

1. Due to the limited information available, it has been assumed that the same values for the parameters (u , d , q_u , q_d) hold on for all the time periods
2. Starting by the current price $S_0 = \$49.25$ at the end of the zeroth period, the oil price has a probability q_u to increase and become $u \times S_0$ and a probability q_d to decrease and become $d \times S_0$. Similarly, the binomial lattice tree goes on with each node giving two new nodes.
3. At the end of every time period, the expected value of the oil price is calculated using eq 27 and is considered to be the value for the processing cost parameter, CRS, into the EOR sink in the model.

$$\text{CRS}_{\text{period}} = \sum_{i \in I} (p_i \times \text{op}_i) \quad (27)$$

Here, $\text{CRS}_{\text{period}}$ stands for the processing cost parameter value at the end of every time period, p_i is the probability of oil price increase/decrease in time period i , and op_i is the oil price relative to this probability at the specific node in time period i . The summation must be carried out over all the nodes at each time period separately. It should be noted that the main

multiperiod binomial lattice model has been implemented using AMPL. However, since the expected value of the CRS parameter that is associated with the EOR sink must first be calculated, a separate MATLAB code has been used to perform those calculations. The AMPL model file that has been used to implement the multiperiod binomial lattice approach is provided in the Supporting Information file (section A). It should be noted that this model has been implemented using "MATLAB version R2017, and optimized using the CPLEX solver via AMPL, on a laptop with Intel Core i5-2410M, 2.30 GHz, 4.00 GB RAM, 64-bit Operating System". A flowchart that summarizes the main steps involved in the MATLAB code which has been utilized to iteratively calculate the expected CRS value for each time period is illustrated in Figure 1. The

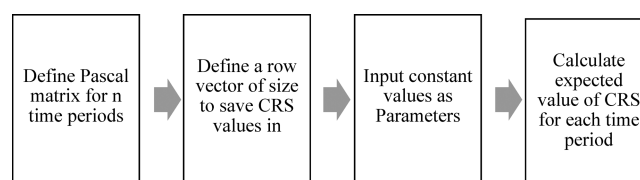


Figure 1. Steps in MATLAB code to calculate expected values of CRS for each time period for the binomial lattice approach.

code starts by defining a Pascal matrix for n time periods, as well as a row vector to have the CRS values in after calculating these values using the for loops. The detailed MATLAB code is provided in the Supporting Information file (section B). All MATLAB codes have been implemented using "MATLAB version R2017 on a laptop with Intel Core i5-2410M, 2.30 GHz, 4.00 GB RAM, 64-bit Operating System". Following the execution of the MATLAB code, the eight expected CRS values attained have been exported into AMPL and have been used as input data for the EOR sink in each of the eight time periods in the carbon integration multiperiod Binomial Lattice model.

In summary, Figure 2 outlines the main sequence of steps that have been utilized to execute the binomial lattice

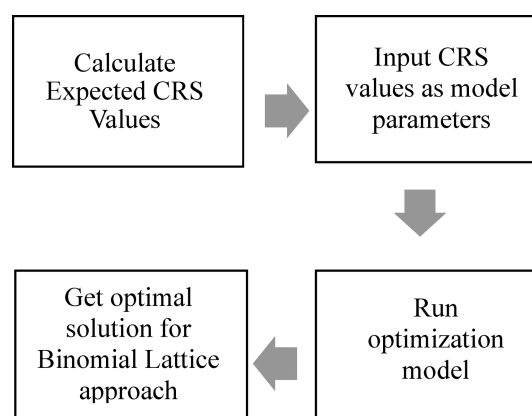


Figure 2. Sequence of steps utilized for the multiperiod binomial lattice.

approach. As has been discussed above, the MATLAB code is first used to calculate the expected values of CRS parameters for each time period, and then these values are used as input data into the optimization model to obtain the optimal solution for the binomial lattice multiperiod approach.

4.2. The Multiscenario Approach. The second approach is the multiscenario approach where each scenario consists of several time periods. This approach relies on oil prices either increasing or decreasing by the end of each time period, in each scenario. First, a subset of random and unique scenarios are to be selected for uncertain oil prices that might occur over the time periods under study (eight different time periods have been utilized in this study). This subset of scenarios, represented by binary numbers for either an increase (one) or a decrease (zero) in the oil price in each time period, is to be converted into another matrix to calculate the processing cost parameter, CRS, into the enhanced oil recovery sink for each time period in every scenario to be used as data in the optimization model. Then, the model is run to get the optimal solution for the multiscenario multiperiod approach. This procedure is summarized in Figure 3. Moreover, the model,

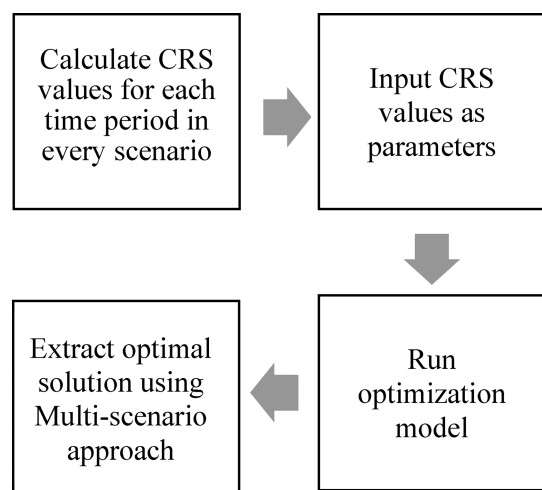


Figure 3. Sequence of steps utilized for the multiperiod Multiscenario approach. In order to run the formulated multiperiod Multiscenario model for a subset of random and unique scenarios as previously explained, the CRS values associated with the EOR sink must be calculated for each time period of these scenarios. The MATLAB code that is utilized to perform those calculations is summarized in the [Supporting Information](#) (section D).

detailed in the [Supporting Information](#) file (section C), is a modified version that incorporates the multiperiod multiscenario approach, which in turn relies on averaging the objective function (total cost) over all scenarios considered in the subset. This model has also been implemented using AMPL, and the optimal solution was found using the “CPLEX solver, on a laptop with Intel Core i5-2410M, 2.30 GHz, 4.00 GB RAM, 64-bit Operating System”.

It is important to shed light on the difference between the two approaches and how each approach handles the uncertain oil price parameters. The binomial lattice approach mainly generates average estimates for CRS, the processing cost parameter that is associated with the EOR sink in every time period, using the binomial lattice MATLAB code provided. On the other hand, the multiscenario approach renders a subset of random and unique scenarios that might take place, using the multiscenario MATLAB code provided. Each scenario is then associated with an exact value of the processing cost parameter that is associated with the EOR sink in every time period. Thus, the binomial lattice AMPL model imports 8 expected CRS values for the EOR sink over eight time periods, while the

multiscenario model imports 800 exact CRS values for the EOR sink covering 100 scenarios of eight time periods each. This difference between the input parameters is the main reason behind the significant difference in the system costs.

It is imperative to point out that in addition to uncertain oil pricing, other parameters that involve an uncertainty element could also be studied in a similar manner, such as the capacity of carbon dioxide sinks, the available carbon dioxide source flows, and the cost of electricity. For instance, the uncertainty of the CO₂ emissions from the sources can be modeled using two-stage stochastic programming approach.¹⁷ As for the uncertainty in the capacity of the sinks, they can be modeled as intervals or by probabilistic distributions using a robust two-stage stochastic approach.¹¹ The cost of electricity on the other hand, is very similar to the oil pricing where this cost depends mainly on the fuel price which in turn vary randomly. Thus, the future oil and electricity prices do not follow a smooth transition curve. One method to model these uncertain prices is to account for three levels of the price: low, medium, and high.³⁰ In this case, the solution might not be optimal but rather flexible.³⁰

5. SCENARIO EVALUATION

The presented optimization-based model is primarily useful for determining which CO₂ sources are the best to capture and to which sinks they should be allocated, under uncertain sink revenue conditions. The model takes into account the treatment, compression and pumping of the streams needed to satisfy the sinks requirements. In order to illustrate the benefits of the proposed model, the same case study which was presented by Al-Mohannadi and Linke,² has been revisited, for the purpose of illustrating the two different approaches which have been detailed above (1) the multiperiod binomial lattice approach and (2) the multiperiod multiscenario approach, for estimating the total cost of an optimum carbon integration network. The case study involves five different plants within an industrial cluster: namely an ammonia plant, an iron and steel plant, a refinery, a power plant, and a fuel additive plant. In total, there are four carbon dioxide source streams which have been considered: one stream from the ammonia plant, one stream from the steel plant, one stream from the power plant, and one stream from the refinery. Moreover, a total of six carbon dioxide utilizing sinks have been considered: (1) an algae sink, (2) a greenhouse sink, (3) a methanol sink, (4) a urea sink, (5) an EOR sink, and (6) a storage sink. All details pertaining to flow rate and composition data associated with the outlined source and sink streams are outlined in Al-Mohannadi and Linke.²

The purpose of this section is to analyze and compare the accuracy of each described approach. Eight different time periods (assuming 1 year each) have been considered when conducting this analysis, and the net carbon reduction target, NCRT, has been set to 3%, over eight time periods. Depending on which specific scenario will be occurring, the actual total network cost can be calculated and compared to the estimated optimal total network cost, which was attained using the AMPL model. Hence, a MATLAB code is initially used to generate a subset of 100 random scenarios. The case study assumes eight different time periods. In each time period, the oil price was allowed to either increase or decrease, which in turn results in a total of 256 (2⁸) scenarios. Only 100 scenarios were randomly selected to be further investigated, since the amount of information that could be extracted out of 100

scenarios was found enough to conduct a fair comparison between the accuracy of the two different approaches that have been presented.

Once all the above steps have been completed, a total of 100 simulations have been executed, one at a time using each MATLAB code separately, and the actual total costs attained from each simulation have been extracted and reported. The cost information was found imperative at this stage to be able to compare it with the estimated total network cost attained using each approach, respectively. Finally, the two approaches are compared. To provide a better understanding of the procedure followed, the sequence of steps outlined above is demonstrated in Figure 4 using an illustrative flowchart.

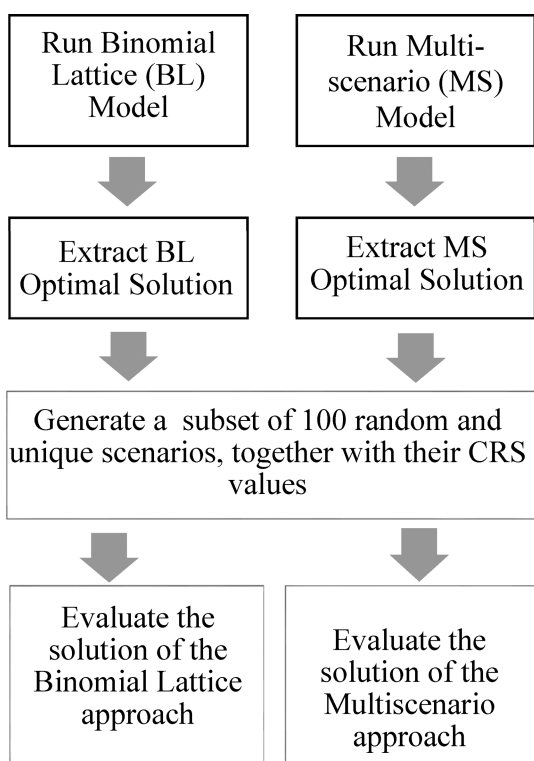


Figure 4. Summary flowchart.

First, an optimal network solution is attained independently for each of the two approaches, using an AMPL model that calls the CPLEX solver. Then, 100 specific scenarios are generated using a MATLAB code along with their CRS values. Following the generation of those specific scenarios, each scenario is implemented separately using two independent MATLAB codes that calculate the actual total network cost based on the respective CRS values of this scenario (which is provided in the Supporting Information file); the first code follows the binomial lattice approach, while the second follows the multiscenario approach.

5.1. Evaluating a Scenario by a Generated Solution.

Since the ILP understudy contains stochastic parameters, the solution performance will depend on the realized scenario. To evaluate the solution, the total cost needs to be calculated.

To calculate the total cost for a realized scenario, the following costs will be the same irrespective of the scenario: the treatment cost, $C_{\text{treatment}}$, the compressor capital and operating costs, CCAP and COP, the pump operating cost, POP, and the transportation cost, $C_{\text{transportation}}$. The pump

capital cost PCAP, for all source-sink connections over the n time periods can be also taken for the generated solution.

Next, to calculate the processing cost into the sink, C_{sink} , the following is used:

$$C_{\text{sink}} = \sum_{Pd=1..n} 365 \times \text{FCO}_2(k, Pd) \text{CRS}(Pd) \quad (28)$$

where CRS is dependent on the realized scenario.

$$\begin{aligned} \text{Tot}_{\text{cost}} = & C_{\text{treatment}} + \text{CCAP} + \text{COP} + \text{POP} \\ & + C_{\text{transportation}} + \text{PCAP} + C_{\text{sink}} \end{aligned} \quad (29)$$

The results of optimizing both approaches with a net carbon reduction target of 3% are presented in Table 4. Moreover, the

Table 4. Optimal Solution of Both Approaches

	binomial lattice	multiscenario
objective function	-372266106	-943331624
net capture over all periods	21850	15627

resulting values of the flow of CO_2 coming from all sources to each sink in every period in the Binomial approach are presented in Tables 5 and 6, while those of the Multiscenario approach are presented in Tables 7 and 8.

Table 5. Flow of CO_2 Coming from All Sources to Each Sink in Every Period, ton CO_2/day (Periods 1–4) (Binomial)

	period 1	period 2	period 3	period 4
algae	0	0	0	0
EOR	2914	2914	2914	2914
greenhouse	0	0	0	0
methanol	0	0	0	0
storage	0	0	0	0
urea	0	0	0	0

Table 6. Flow of CO_2 Coming from All Sources to Each Sink in Every Period, ton CO_2/day (Periods 5–8) (Binomial)

	period 5	period 6	period 7	period 8
algae	0	0	0	0
EOR	2914	2914	2914	2914
greenhouse	0	0	0	0
methanol	0	0	0	0
storage	0	0	0	0
urea	0	0	0	0

Table 7. Flow of CO_2 Coming from All Sources to Each Sink in Every Period, ton CO_2/day (Periods 1–4) (Multiscenario)

	period 1	period 2	period 3	period 4
algae	0	0	0	0
EOR	2082	2232	1829	1889
greenhouse	0	0	0	0
methanol	5	198	102	324
storage	0	0	0	0
urea	0	0	0	0

Table 8. Flow of CO₂ Coming from All Sources to Each Sink in Every Period, ton CO₂/day (Periods 5–8) (Multiscenario)

	period 5	period 6	period 7	period 8
algae	0	0	0	0
EOR	1683	1884	1696	1732
greenhouse	0	0	0	0
methanol	169	324	247	382
storage	0	0	0	0
urea	0	0	0	0

The last step involved performing 100 simulations on both MATLAB codes, one scenario at a time, and the total actual cost is reported. All terms of the objective function take the optimal values obtained by AMPL model, except for the processing cost into the sinks which depends on the scenario chosen because it is based on the uncertain oil prices. First, 100 simulations of the binomial lattice approach have been documented, followed by the results obtained using the multiscenario approach. The respective network total cost together with the standard deviation for each scenario, are provided by Tables S.1 and S.2, respectively, in the [Supporting Information](#).

It should be emphasized that the individual scenarios reported in [Tables S.1 and S.2](#) represent specific cases that might occur and are not solutions of the network problem itself. The AMPL model has been primarily utilized to extract the optimal network solution upfront, but then a single scenario will actually occur in reality, which would ultimately yield a different network cost compared to that attained from the AMPL model. In other words, the decision maker is capable of modeling uncertain oil prices, then formulating the problem using one of the two proposed approaches according to the steps that have been detailed in this paper. Optimized solutions together with an estimated total network cost may be extracted using the AMPL code implementation, based on the selected approach. In this case, the respective solution that is reported as the optimal network would suggest the amount of flow to be sent from each source to each sink, in every time period. In real life, a single random scenario of oil pricing takes place, in which the oil price either increases or decreases at the end of every time period. At this stage, the costs associated with all other system components of the carbon integration network have been identified, based on the optimal network configuration obtained, except for the processing cost into the EOR sink, since it is directly correlated to the uncertain oil price parameter. Therefore, when one scenario is realized, this cost can be computed, which will lead to an actual network cost that differs from the estimated optimal cost that was obtained previously via AMPL. Moreover, when one specific scenario of the oil price change is realized, the total network cost is reported to change from an estimated case to an actual case. Therefore, the decision maker is then able to select an appropriate approach that could model this uncertain element, as desired..

The oil prices change very similarly in both approaches, and because a specific scenario is carried out individually each time, the exact oil price is associated with the respective scenario being carried out. The two different approaches have been compared in order to identify which of the two provides a better and a closer estimate of the network cost with that of the optimal case obtained from AMPL model.

From the results attained, it has been observed that both approaches can be effective for decision-making, however, while both capture uncertainty using a multiperiod base model, the two approaches differ in several aspects, especially in terms of the amount of random data it utilizes in the execution process. Hence, any decision maker should be aware of those differences. First, it has been observed that the binomial lattice approach is able to provide an optimal multiperiod carbon network solution that is based on average estimates of the CRS values, without taking into account the differences in network connectivity that could probably occur over the different time periods. On the other hand, the Multiscenario approach can provide multiperiod carbon network solutions that is based on exact CRS values using a subset of possible scenarios, while accounting for network connectivity differences that may result due to the uncertain oil prices (which can either increase or decrease in each time period).

When comparing the CRS execution procedure of both methods, the binomial model involves a MATLAB code that calculates expected CRS values for every time period; thus, only eight CRS values have been utilized in this study as input values into the AMPL model for extracting optimal network solutions. On the other hand, the MATLAB code that was used to calculate the CRS values for the Multiscenario approach results in 100 different scenarios, each of which consisting of eight time periods; thus, in total 800 CRS values have been imported into the AMPL model for extracting optimal network solutions, averaged over all 100 scenarios. Thus, the binomial approach uses expected CRS values that are calculated using the probabilities of the uncertain oil prices going up or down together with the new price predictions in each case. On the contrary, the multiscenario approach utilizes a more rigorous approach for calculating CRS values, using data from various scenarios that might occur. Hence, the multiscenario approach calculates more exact CRS values given the current state of the oil price (i.e., whether it increased or decreased in this specific period of this specific scenario under study) and then uses all attained CRS values to obtain the optimal network solution.

Analyzing the different results that are outlined in [Tables S.1 and S.2](#) associated with every scenario, one can realize several differences. The AMPL model of the binomial lattice approach estimates a revenue of \$ 372,266,106 as an optimal solution. Going through the individual scenarios, one can spot a case that generates a revenue of \$10491000000, differing by almost \$10 billion, compared to the optimal solution that was extracted through AMPL. Moreover, another odd case is reported, where the network is predicted to be highly unprofitable, with a total reported cost of around \$131 million. When analyzing the scenarios generated using the multiscenario approach, more realistic network cost estimates have been reported. The AMPL model reports an optimal solution with a suggested revenue of \$943331624, which is obviously higher than the revenue suggested by the optimal AMPL solution obtained using the binomial lattice approach. This is most likely due to the fact that the multiscenario approach is able to generate different scenarios that might occur not only average values as it is the case with the Binomial approach. The most profitable scenario is reported to result in a revenue of \$6523400000 which differs by almost \$5.5 billion when compared to the estimated multiscenario solution generated by AMPL. Hence, almost half of the difference is reported using the multiscenario approach, compared to the binomial lattice

case (with the binomial it differs by almost \$10 billion, whereas with the Multiscenario approach, it differs by around \$5.5 billion). Moreover, the most expensive scenario is reported at a total actual cost of \$56052000, which is much more realistic than the most expensive case reported by the binomial lattice solutions.

Since all the scenarios that were investigated in this case study involve a net carbon reduction target of 3%, the optimal network configuration obtained for each of those scenarios investigated, using the two different proposed strategies, were found to be similar to the multiperiod network design that was presented by Al-Mohannadi et al.²⁴ at a 3% net carbon reduction target. A multiperiod carbon integration approach was thoroughly presented, together with a detailed discussion of the various system components in Al-Mohannadi et al.²⁴ Moreover, several figures that describe the evolution of the network design over time has also been discussed and presented by Al-Mohannadi et al.,²⁴ for different net carbon capture reduction targets. On the other hand, since this paper mainly investigates the effects of oil price uncertainty on such networks, the main differences observed for the various scenarios investigated in this paper lie in the total cost of the network. The major contributor of such differences was mainly attributed to the variation of the revenue generated by the EOR sink, as a result of the oil price fluctuations taking place in every time period. In some scenarios, the source-to-sink allocation from ammonia-to-EOR sink would suffice to attain a 3% net capture reduction, while in other cases, especially those that were associated with a low oil price situation, an additional source-to-sink allocation from steel-to-methanol was observed. Very little structural variation has been perceived in the carbon integration network configuration at a 3% net reduction target.

Regarding the variation in system cost attained for the different scenarios, Figures 5 and 6 demonstrate the number of scenarios that were able to attain a certain % of EOR revenue, with respect to the total network cost, across different time periods using the multiscenario approach, as an example. For instance, a total of 34 (out of 100) scenarios reported a network with an EOR revenue between 5 and 10% of the total network cost, in time period 1, while this number increased to 36 (out of 100) in time period 2. Similarly, a total of 19 (out of 100) scenarios reported a network with an EOR revenue between 10 and 15% of the total network cost, in time period 1, while this number increased to 18 (out of 100) in time period 2. Similar information can be extracted for the remainder of the % revenue brackets that are indicated in Figures 5 and 6. To summarize, Figure 7 provides a comparison between the binomial lattice and multiscenario results, by indicating the frequency of scenarios associated with a certain % EOR revenue attained by the network across all time periods altogether, with respect to the total network cost. It is evident that most of the scenarios were able to achieve somewhere between 95 and 99% of sink revenue (i.e., the costs associated with those systems were found to lie between 1 and 5%). The revenue side was much more dominating compared to the required network expenditures (primarily piping, compression, and pumping costs) for most of the scenarios that have been reported, since only 1 structural connection was depicted, mainly the ammonia to EOR allocation, to achieve a 3% net carbon reduction.

Definitely, incorporating more than one uncertain parameter will yield very different results to those presented in this work. The optimal network behavior will drastically change,

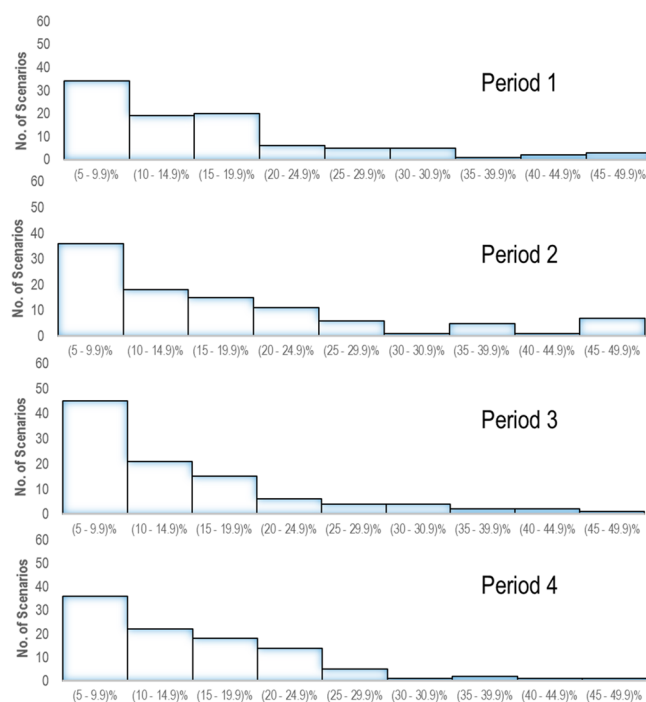


Figure 5. Histogram illustrations that demonstrate the frequency of scenarios that are associated with a certain % EOR revenue attained by the network, with respect to the total network cost, across time periods 1–4 using the multiscenario approach.

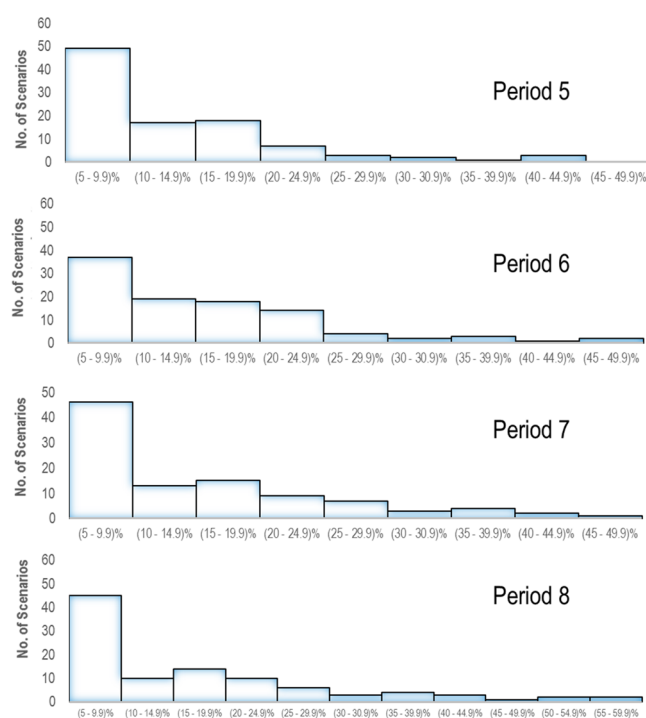


Figure 6. Histogram illustrations that demonstrate the frequency of scenarios that are associated with a certain % EOR revenue attained by the network, with respect to the total network cost, across time periods 5–8 using the multiscenario approach.

especially the optimal structures attainable, in case the capacity of carbon dioxide sinks as well as available carbon dioxide source flows were allowed to vary, unlike the cases that were reported in this work, which have been observed to be

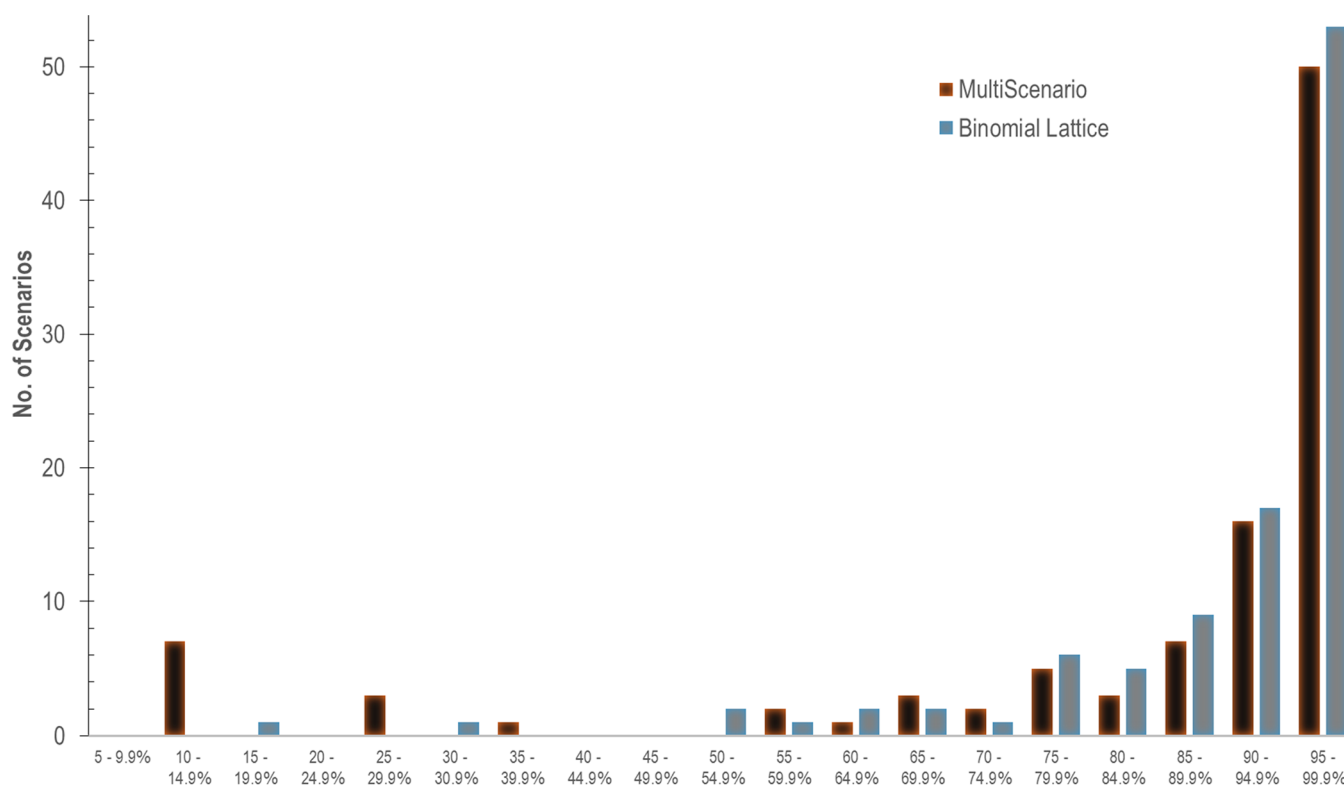


Figure 7. Comparison between the binomial lattice and multisenario approach, demonstrating the frequency of scenarios associated with a certain % EOR revenue attained by the network across all time periods, with respect to the total network cost.

associated with very little structural variation. This is because the network structure would then be highly dependent on which of the available carbon dioxide sources could be captured, and to which sinks would the captured CO₂ be allocated to, based on the available capacity of each. However, there will definitely be more concerns with regards to the extraction of optimal solutions, more than just uncertain oil price concerns. Even if more than one uncertain parameter were to be investigated, the binomial lattice approach would always generate average estimates, while the multisenario approach will take into account the different possible scenarios with all possible uncertainties and solves the model over these scenarios. Thus, even though the optimal results extracted would certainly be different, the overall behavior of the two different approaches would remain the same.

6. CONCLUSION

Two different stochastic linearized multiperiod models that can be utilized to generate optimal carbon integration networks have been proposed in this paper: (1) the binomial lattice model and (2) the multisenario model. Ultimately, the goal was to be able to determine the best CO₂ source-to-sink allocations, under uncertain oil price conditions. Both approaches have been reported to be effective and easy to implement. However, several differences between the two methods have been reported. As for which approach to recommend, it has been found that it completely depends on the desired quality of information that could help achieve a viable and informed decision. In some cases, the use of average estimates provided by binomial lattice approach, may prove to be enough, while in other cases when a more detailed analysis is required, the multisenario approach might prove to be more rigorous in terms of the quality of network solutions that can

be extracted under uncertain conditions. When it comes to decision-making activities, having a specified list of criteria before making any real decisions would certainly be useful, and it should be emphasized that exact same solutions may or may not be attainable in real situations, depending on the circumstances.

■ ASSOCIATED CONTENT

📄 Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.8b05185.

Linearized optimization-based model for the binomial lattice approach; MATLAB code for obtaining the CRS values for the binomial lattice; linearized optimization-based model for the multisenario approach; MATLAB code for obtaining the CRS values for the multisenario approach; total network cost and standard deviation results attained for 100 scenarios implemented for the binomial lattice; and multisenario approach (PDF)

■ AUTHOR INFORMATION

Corresponding Author

*E-mail: ht27@aub.edu.lb.

ORCID

Hussein Tarhini: 0000-0002-8512-2925

Notes

The authors declare no competing financial interest.

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NOMENCLATURE

Acronyms List

EOR = enhanced oil recovery
 GHG = greenhouse gas
 MINLP = mixed integer nonlinear programming
 CCUS = carbon capture and utilization and storage
 MILP = mixed integer linear programming
 CCS = carbon capture and storage
 UPM = upper partial mean
 SAA = sample average approximation
 ECCP = equilibrium chance-constrained programming
 CRS = processing cost parameter
 AMPL = A Mathematical Programming Language (software)
 MATLAB = MATrix LABoratory (software)
 CPLEX = IBM ILOG CPLEX optimization studio (solver)
 NCRT = net carbon reduction target
 BL = binomial Lattice
 MS = multiscenario

Variable List:

μ_i = the mean of a normally distributed random variable which is the log ratio of the next state i
 σ_i = standard deviation of the normally distributed log ratio of the next state i
 r = interest rate (%)
 N = number of trading days in a year (taken to be equal to 252 days)
 \bar{x}_i = the mean of a normally distributed random variable (logarithm of the ratio of tomorrow's price to today's price), where i stands for the current state
 α = confidence level (dimensionless)
 $f(x)$ = objective function in chance constrained programming model
 x = the decision variables in chance constrained programming model
 A = coefficients of the decision variables in chance constrained programming model
 b = constants in chance constrained programming model
 $E[Y]$ = expected value of a probabilistic function
 $f(x)$ = objective function
 Pr = probability (%)
 $Var(Y)$ = variance of Y
 u = actor for the price increase (dimensionless)
 p = probability
 d = factor for the price decrease (dimensionless)
 gr = expected yearly growth rate
 S_T = price at the end of the whole period T , starting from now (\$)
 S_s = initial stock price, where s stands for the beginning of the period (\$)
 Δt = period length (years)
 C = price of the option (\$)
 S_0 = current future price at time 0 (\$/barrel)
 $N(x)$ = standard cumulative normal probability distribution
 K = strike price (\$)
 T = expiration time (years)
 σ = volatility of the oil price (\$/barrel)
 q_u = probability to have an increase by "u" factor in the oil price
 q_d = probability to have a decrease by "d" factor in the oil price
 r' = rate of increase of the different oil futures prices

p_i = probability of oil price increase/decrease in time period i
 op_i = oil price at a specific node in time period i (\$/barrel)
 Pd = time period
 $C_{treatment}$ = positive, treatment and separation cost of CO₂ from source s to satisfy sink k 's requirement over all periods (\$)
 $CCAP$ = positive, total capital cost of the compressors for all $s-k$ connections over all periods (\$)
 COP = positive, total operating cost of the compressors over all periods (\$)
 POP = positive, total operating cost of the pump over all periods (\$)
 $C_{transportation}$ = positive, total transportation cost over all periods (\$)
 $PCAP$ = total pumping capital cost (\$)
 CS = matrix that has CRS values
 FCO_2 = flow of CO₂ coming from all sources to each sink k in every time period ton CO₂/day
 CRS = processing costs of CO₂ streams into the sinks (\$)
 CSC = summation of CS elements along the columns
 CSR = summation of CSC elements along the rows
 Tot_{cost} = total cost (\$)
 C_{treat} = positive, average treatment and separation cost of CO₂ from source s to satisfy sink k 's requirement, over all periods and scenarios (\$)
 $CCAPT$ = positive, average capital cost of the compressors, for all periods, all scenarios (\$)
 $COPT$ = positive, average operating cost of the compressors, over all periods and scenarios (\$)
 $PCAPT$ = positive, average capital cost of the pumps used in all periods and scenarios (\$)
 $POPT$ = positive, average operating cost of the pumps over all periods and scenarios (\$)
 $FCO_2T[k,Pd]$ = positive, average flow of CO₂ to sink k coming from all sources and treatment units in every time period, over all scenarios (ton CO₂/day)
 e_{ij} = inputs for the FCO₂ matrix for each sink i and period j
 s_{ij} = inputs for the FCO₂T matrix for each sink i and period j
 r_{ij} = inputs for the CRS matrix for each sink i and period j
 $CC^{capital}$ = capital cost of compressors (\$)
 P^{comp} = power parameter for the compressor (bar)
 CRF = capital recovery factor (dimensionless)
 $T_{s,k,t}$ = flow from treated source s to sink k (ton CO₂/day)
 $U_{s,k}$ = flow from untreated source s to sink k (ton CO₂/day)
 T_s = temperature of source s stream outlet (K)
 $U_{s,k}$ = flow from untreated source s to sink k (ton CO₂/day)
 $F_{s,k,t}$ = treated flow from source s to sink k (ton CO₂/day)
 $\Delta P_{s,k}$ = pressure difference between source s and sink k (bar)
 $\Delta P_{s,k}^{pipe}$ = pressure drop between source s and sink k (bar)
 $C_{s,k}^{pipe}$ = pipe cost per unit length of connection between source s and sink k (\$/m)
 $PPUMP_{s,k}$ = power required for pumping source s to sink k (bar)
 $PCAP_{s,k}$ = capital cost of pump required from source s to sink k (\$)
 $D_{s,k}$ = diameter of pipe between source s and sink k (m)
 $ratio_{s,k}$ = ratio parameter for the diameter (dimensionless)
 $P_{s,k}$ = positive integer variable that approximates the diameter needed for every $s-k$ connection (dimensionless)
 $QQP_{s,k,Pd}$ = positive, the total of treated and untreated flows from s to k , in every period Pd (ton CO₂/day)

$del_{s,k}$ = positive variable to find the diameter needed for the flow from s to k
 $zp_{s,k}$ = binary, for if else pumping cost, in every period Pd and scenario i

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