Impact of Distribution Functions in Optimization under Uncertainty of the Field Management for Carbon Capture and Storage

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Abstract

The main objective of this paper is to examine the impact of probability distribution functions in optimizing a field management plan that accounts for various sources of uncertainties. The uncertainty arises due to the flow of CO_2 in the system and the various costs associated with the project. This paper addresses the cases of the known and unknown values of uncertain parameters and their probability distribution. The case for which the uncertainties are known is solved by formulating a two-stage stochastic programming problem where investment decisions (number of wells to be drilled and number of buffer tanks) are set as stage-1 variables and while other variables are set as stage-2 or recourse variables. The deterministic equivalent model is formulated in the form of mixed-integer nonlinear programming (MINLP) which is solved. For distributions with different mean values and variances, assess the impact on other distributions. In the case where the distribution of the random variables is unknown, the moment matching problem(MMP) is formulated and solved to generate a scenario tree based on the historical data, which can be used for the two-stage programming model.

Keywords - Two-stage stochastic programming, Moment matching problem, Mixed integer nonlinear programming, Scenario tree

1 Introduction

In this paper, we consider the impact of uncertainties in the MINLP model that we have recently proposed in [1] for optimizing field management for carbon capture and storage, an area that has received increased attention [2] [3] [4] [5]. The area of optimization under uncertainty has greatly expanded through, stochastic programming (SP) [6] which is among the two most widely adopted frameworks for incorporating uncertainty in optimization models, the reader can refer to [7] for a recent review of this area. Previous works have extensively explored the optimization of CCS infrastructure under uncertainty, focusing on both environmental and financial risks [8] [9].

A schematic representation of a two-stage stochastic programming problem is shown in Figure 1. Here, x is the first-stage decision variable at time $t = 1$. The uncertainty, w is realized after

$t = 1$ and the recourse variable $y(w)$ at $t = 2$ takes into account the uncertainty by taking corrective action also known as recourse action.

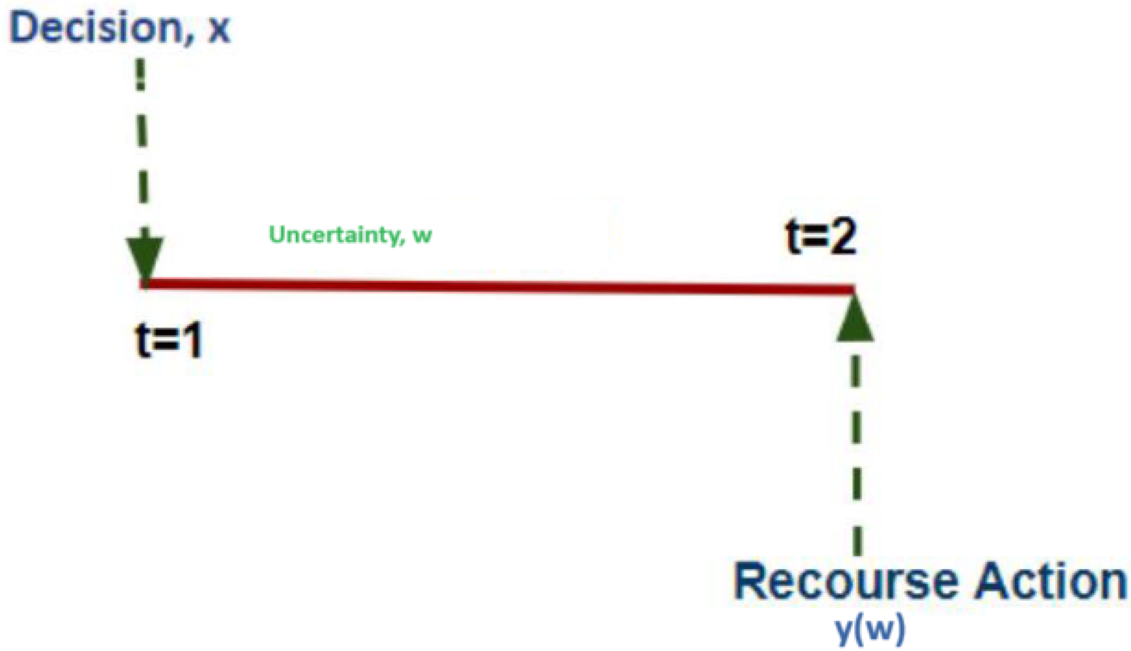

Figure 1: A schematic representation of a two-stage stochastic programming problem

The simplest approach to address stochastic Mixed-Integer Nonlinear Programming (MINLP) problems is to directly solve the deterministic equivalent problem using [6] optimization solvers like DICOPT [10], BARON [11], or SCIP [12] which is the approach that is used in this paper. For problems with a large number of scenarios for uncertain parameters, strategies such as Lagrangean decomposition and Benders decomposition are required to effectively solve these problems [7].

Since the chosen scenarios directly impact the solution to the stochastic problem, an alternative is to use sampling techniques like Monte Carlo sampling and Sample Average Approximations can be used methods to approximate the probability distribution [6].

The most common assumption made in stochastic programming is that the probability distribution is pre-defined and the uncertainty varies between a certain minimum and maximum range. In general, the highest probability is given to the average value of the uncertain parameters[13]. However, an alternative approach is to generate the scenario trees from historical data instead of assuming certain probability distributions and a range of values for a set of uncertain parameters. This data-driven approach has been reported recently by [14] who formulated the problem as an NLP.

The goal in this paper is to assess the effect of the probability distribution function in field management problems for carbon capture and storage, whether by the use of deterministic for the two-stage programming or by generating scenario trees through the moment matching problem [14].

2 Problem Statement

We consider the following problem in this paper. Given is a Carbon Capture Utilization and Sequestration (CCUS) system that comprises capturing, transporting, and sequestration of CO_2-rich fluid. There is a system of logistic supply of CO_2 capture, logistic supply, terminal storage tanks, and a pipeline network connecting injection wells to the reservoirs. The system is defined with a fixed design in terms of the number of wells, well injection potential as well as their status along with the availability of the reservoirs. A CO_2 terminal injects CO_2-rich fluid (mixture of cryogenic and gaseous) through the pipeline network. The uncertainties considered are associated with the flow rates of CO_2 in gaseous and cryogenic states as a function of time. We should clarify that these are not the only uncertainties in the system.

The objective of the model by [1] is to determine the following items to minimize the total cost.

1. The number of buffer tanks used for storing CO_2.
2. The number of wells to be drilled during gasfield operations.
3. The rate of CO_2 to the wells that include uncertainties in the flow of CO_2 from various industries (gaseous) in metric ton per annum, MTPA.

A schematic diagram of a CO_2 terminal is shown in Figure 2 that consists of boats that carry cryogenic CO_2, storage tanks on the terminal, and a pipeline network injecting to the wells from the terminal including transport of cryogenic carbon dioxide to the terminal and supply from varies industries in gaseous form. The CO_2 flow from the storage tank is controlled flowrate together with the gaseous flowrate supplied by various industries to reach the field injection rate R_F, that is to be injected into the injection wells.

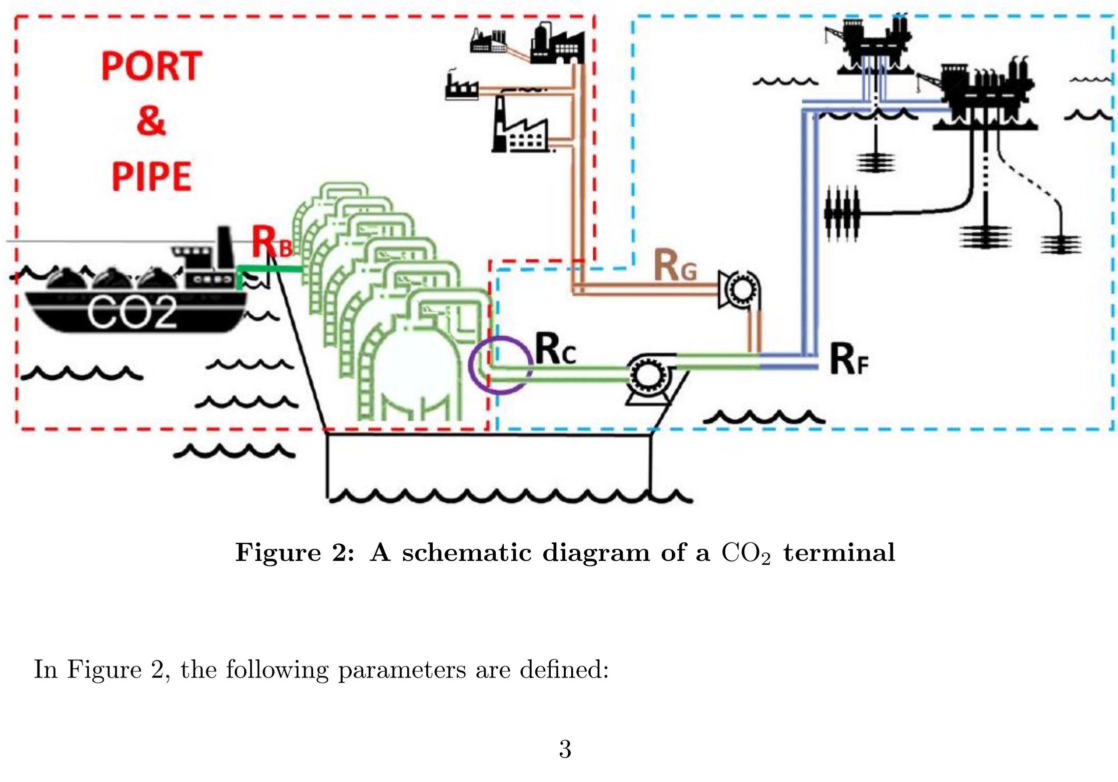

Figure 2: A schematic diagram of a CO_2 terminal

In Figure 2, the following parameters are defined:

1. R_B represents the rate of cryogenic CO_2 being supplied from the boats carrying cryogenic CO_2
2. R_G represents the gaseous rate of CO_2 from various industrial suppliers that cannot be controlled.
3. R_C represents the outlet rate from the terminal storage tanks.
4. R_F represents the rate of CO_2 supply to the fields.

R_F represents the total CO_2 supply, which is the sum of R_B, the CO_2 received from ships, and R_G, the CO_2 supplied by industry. Due to the uncertainty in R_B (the CO_2 from ships), a buffer tank is installed to ensure we can meet our commitment to the required CO_2 injection quantity. The buffer tank mitigates the risk of supply shortfalls by storing excess CO_2 when available and compensating for days when the supply from ships is insufficient.

Building on the deterministic MINLP model by [1], the primary objective of the two-stage stochastic programming model is to optimize the expected value of CAPEX (Capital Expenditure) and OPEX (Operational Expenditure) such that all the physical, as well as the operational constraints, are satisfied. The major decisions consist of determining the total number of wells to be operated, the installation cost associated with the number of buffer tanks, and the total cost associated with venting CO_2 during the operation. The uncertainty lies with the flow of CO_2 and with the investment cost associated with the construction and operations of terminals.

In this paper, we assess the impact of the uncertainty parameters for two cases.

1. Case 1: The form of the probability distribution function of the uncertain parameters is known (eg. Normal distribution) except for its mean and variance.
2. Case 2: The probability distribution and the values of uncertain parameters are unknown. The scenario tree is generated from the historical data for the uncertain parameters.

For the first case, we assume the probability distribution and the corresponding discrete values of uncertainties. For the second case, the probability distribution is unknown and we generate the scenario tree from the historical data provided for the uncertain parameters by TotalEnergies. In case-1 a two-stage stochastic programming model is formulated which assumes that the uncertainties are given in the form of scenario tree. This stochastic programming aims to minimize the overall expected CAPEX and OPEX for the problem. Case 2 focuses on the Moment Matching Problem(MMP) [14], a scenario-generation algorithm for which we compute the unknown random variables and their corresponding probabilities. Our model independently employs a two-stage stochastic programming approach, similar in concept to that discussed in [15]. However, our implementation diverges significantly by integrating advanced moment-matching techniques

2.1 Assumptions

The model proposed in this work is based on the following assumptions:

1. The uncertainties are considered with the flowrate coming from the boat and the gaseous nature of CO_2 from the various industries.
2. The injection flowrate for the field is bounded between certain values.

3. At the end of a month's operations the buffer tanks are emptied.
4. The superstructure is well-defined for a network consisting of wells, buffer tanks, pipelines, and reservoirs.
5. Model-specific costs like well opening cost, cost of venting CO_2, the installation cost of buffer tanks, the injection cost, and other data are assumed to be known.
6. The time step of the operation is at least 10 days.

3 Two-stage Stochastic Programming Model

The previous work by [1] proposed an optimization model to determine the field management plan for injecting rate of CO_2-rich fluid into the wells for several years of operations. The formulation of the model was decomposed by dividing it into three levels: (a) years, (b) months, and (c) periods of injection and buffering expressed in days to reduce the complexity of the model. This work considers uncertainties through the scenarios for the values of the flowrate for different streams and the cost of installation and operation of the project. We formulate a deterministic equivalent model by optimizing across multiple scenarios of the uncertain parameters, using this as the foundation for the deterministic MINLP model. [1].

$$
\begin{aligned}
&\min f_0(x) + \sum_{\omega \in \Omega} \tau_\omega f_1\left(x, y_\omega; \theta_\omega\right) \\
\text{s.t. }\ & g_0(x) \leq 0 \\
& g_1\left(x, y_\omega; \theta_\omega\right) \leq 0 \quad \forall \omega \in \Omega \\
& x \in X, \quad X = \left\{x : x_i \in \{0,1\}, \forall i \in I_1, 0 \leq x \leq x^{ub}\right\} \\
y_\omega \in Y_\omega, \forall \omega \in \Omega, \quad & Y_\omega = \left\{y_\omega : y_{\omega j} \in \{0,1\}, \forall j \in J_1, 0 \leq y_\omega \leq y_\omega^{ub}\right\}
\end{aligned}
\tag{1}
$$

The formulation in (1) has a nonlinear objective and nonlinear constraints in terms of 0-1 and continuous variables. The functions f_0, f_1, g_0 and g_1 are nonlinear functions. The functions f_1 and g_1 are functions of the first-stage decisions x, the second-stage decisions y_w, and the uncertain parameters ω_w for the scenarios w. Although the above model is difficult to solve due to the non-linear objective and constraints present in the problem in terms of 0-1 and continuous variables, in this work it is greatly separated by the fact that we consider only three scenarios and low, medium, and high values simultaneously for all the uncertain parameters.

4 Moment Matching Problem

4.1 Introduction

The Moment Matching Problem (MMP) is a useful method for generating scenario trees that accurately reflect historical data, providing a robust basis for stochastic programming models. This section explores the MMP approach, detailing its formulation, implementation, and practical applications.

In stochastic programming, accurately modeling uncertainties is paramount for making robust decisions. Traditional methods often assume pre-defined probability distributions for uncertain parameters. However, this can lead to inaccuracies. The MMP offers a data-driven approach by generating scenario trees from historical data, ensuring a more accurate representation of uncertainties.

4.2 Problem Formulation

The MMP aims to minimize the weighted square error between the statistical properties (moments) of the generated scenario tree and those of the historical data [13]. Its main goal is to find the values at the uncertain parameters $(i \in j)$ x_{ij} with corresponding probabilities p_j in the scenario tree shown in Fig 3. This ensures that the scenario tree accurately represents the uncertainties inherent in the data.

The MMP can be formulated as a nonlinear programming (NLP) problem [14] in which the objective function of the MMP is given by:

$$\begin{aligned} \min_{x,p} \quad & Z_{MMP} = \sum_{i \in I} \sum_{k \in K} w_{i,k} \left(m_{i,k} - M_{i,k}\right)^2 + \sum_{(i,ii) \in I} w_{i,ii} \left(c_{i,ii} - C_{i,ii}\right)^2 \\ i < ii & \end{aligned} \tag{2}$$

Here $m_{i,k}$ and $M_{i,k}$ represent the k-th moments of the scenario tree and historical data, respectively, while $c_{i,ii}$ and $C_{i,ii}$ denote the covariances. The weights $w_{i,k}$ and $w_{i,ii}$ adjust the importance of each moment and covariance.

The constraints ensure that the probabilities sum to one and define the moments and covariances:

$$\begin{aligned} \sum_{j=1}^{n} p_j &= 1 \\ m_{i,1}^{i} &= \sum_{j=1}^{n} x_{i,j} p_j, \quad \forall i \in I \\ m_{i,k} &= \sum_{j=1}^{n} \left(x_{i,j} - m_{i,1}\right)^k p_j, \quad \forall i \in I, k > 1 \\ c_{i,ii} &= \sum_{j=1}^{n} \left(x_{i,j} - m_{i,1}\right) \left(x_{ii,j} - m_{ii,1}\right) p_j, \quad \forall (i,ii) \in I, i > ii \end{aligned} \tag{3}$$

The values of the parameters are bounded as follows:

$$\begin{aligned} & x_{i,j} \in \left[x_{i,j}^{UB}, x_{i,j}^{LB}\right], \quad \forall i \in I, j = 1, 2 \ldots n \longrightarrow \\ & p_j \in [0,1], \quad \forall i \in I, j = 1, 2 \ldots . x \end{aligned} \tag{4}$$

The structure of the scenario tree is illustrated in Figure 3. Each node x_j represents a possible outcome with an associated probability p_j.

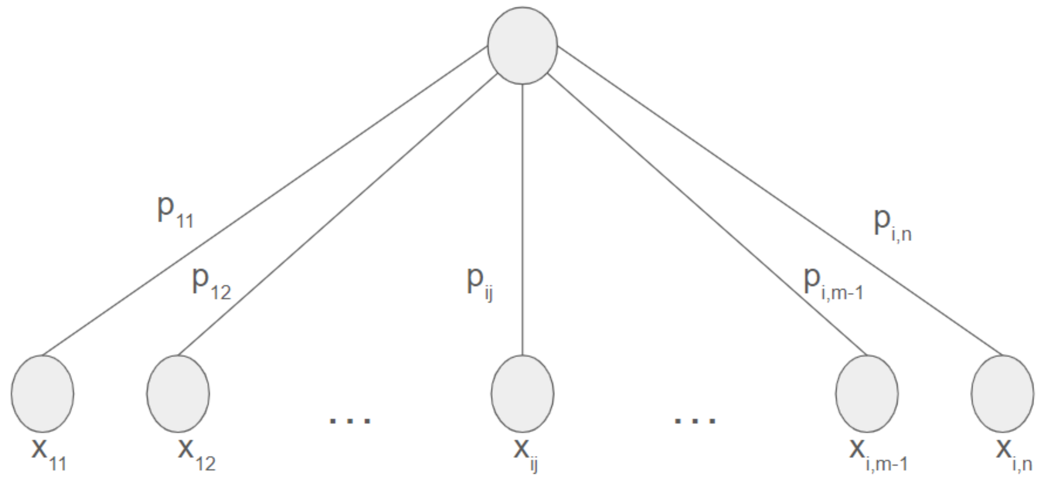

Figure 3: Scenario Tree Structure

The Moment Matching Problem builds on the idea that by matching the statistical moments of a scenario tree with those of the historical data, one can generate a tree that accurately reflects the underlying uncertainties. This method, originally proposed by [13], has been further developed by [14] to include matching cumulative distribution functions (CDFs) and empirical CDFs (ECDFs).

The weights $w_{i,k}$ and $w_{i,ii}$ are optimized through parameter hypertuning over a range from 0.1 to 1.0, with increments of 0.1 i.e (0.1, 0.2, 0.3,...., 1.0). The optimal weights are calculated as follows:

$$w_{i,k} = \frac{w'_{i,k}}{M^2_{i,k}} \quad w_{i,ii} = \frac{w'_{i,ii}}{C^2_{i,ii}} \tag{5}$$

4.3 Data-Driven Scenario Generation

A significant advantage of the MMP is its data-driven nature. By using historical data for example like Figure 4 (his figure is provided for reference only and is not directly related to the problem at hand), to generate scenario trees, the method avoids the need to assume pre-defined probability distributions. This approach is particularly beneficial in fields with abundant data and complex uncertainties.

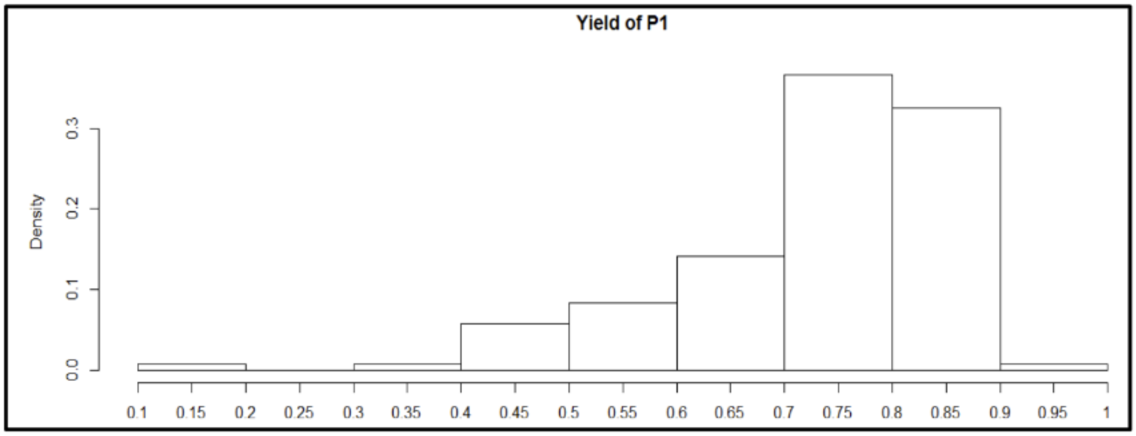

Figure 4: Example of Historical data

As indicated before solving the MMP involves a nonconvex NLP problem, which can be computationally challenging., especially for large-scale problems. Advanced solvers like BARON or multi-start strategies can be employed to find global optima. Additionally, parallel computing techniques can be utilized to speed up the computation, making the MMP feasible for real-time applications.

5 Results and Discussion

5.1 Data, Bounds and Initial Values

It is assumed that the parameters for the investment and the operational costs along with the coefficients are uncertain. The injection rate to the gasfield is bounded between the maximum and the minimum injection capacity, which is determined by fitting a degree-3 polynomial curve to the data provided by TotalEnergies [1]. The NLP model which includes OPEX in the objective function as opposed to the model described by [1] has been executed on an Intel 8^{th} generation $i7$ processor with 16 GB of RAM.

5.2 Case 1: Two-Stage Stochastic Programming Problem

Two approaches are analyzed in detail to guide investment decisions, considering different sources of uncertainty in the system. The first approach addresses the uncertainty in the target flow, which remains unaffected by external factors such as the costs associated with well installation and operational expenses. On the other hand, the second approach considers a broader spectrum of uncertainties that affect the system both from investment and operational perspectives. This includes variables like the target flow rate, and the costs associated with investment and operations, examined across three scenarios.

5.2.1 Uncertainty in Target flowrate, R_F

The approach for considering the uncertainty in the target flow rate consists of three realizations R_F representing optimistic, average, and pessimistic conditions. As shown in Figure 5, the buffer tank is not needed during the first 420 days when R_B is consistent. However, after this period, as the supply from ships becomes irregular, the buffer tank is used to maintain the required injection rate. The injection from the buffer tank varies depending on the supply deficit, ensuring only the necessary amount of CO_2 is drawn to match the injection commitment.

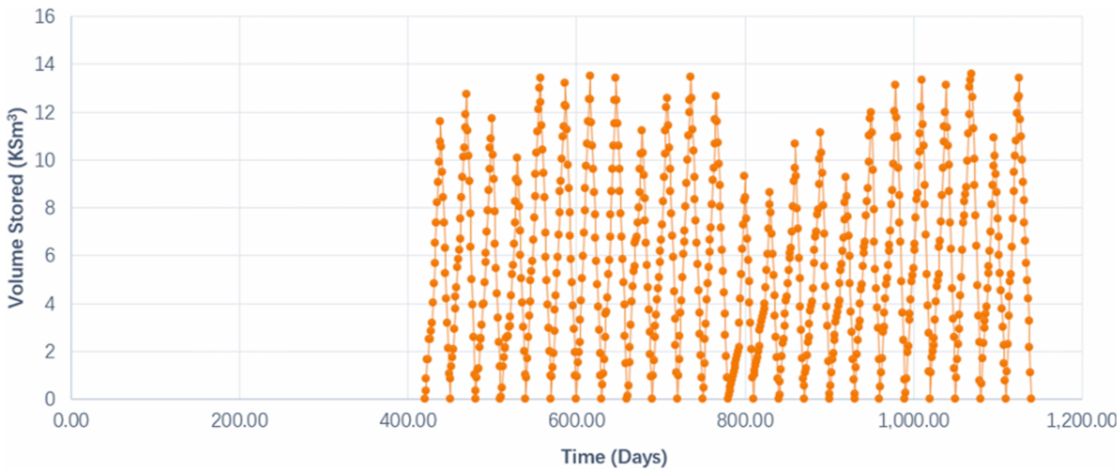

Figure 5: Cryogenic CO_2 stored volume profile of a buffer tank generated by solving the MINLP problem for 36 months of operation.

The probability distribution is varied to account for different instances. The results are recorded for 5 different probability distributions shown in Table 1. For the first instance, the probability is distributed evenly among the three realizations. The computational time and the objective values are recorded for all 5 test cases on different distributions. The longest computational time of 957.90 seconds is reported for the distribution of $25\% - 50\% - 25\%$. The objective value of 188.39 is achieved by including an additional operational cost: the injection cost. This cost is \$15 per ton for the injection rate and is accounted for with a high probability of 95%.

The deterministic equivalent model in the form of MINLP-SP has 25,584 constraints with 10,572 continuous variables and 1,289 discrete variables solved for one month of operational time. The model is solved by BARON in GAMS, a state-of-the-art solver that ensures global minima which cannot be ensured by other solvers like DICOPT or SBB. The model for all the instances selects wells 1,2 and 3. The results for the five sets of probability distributions are recorded in Table 1.

Q_{tgt} : Low: 4,900kSm^3 /day Average : 5000kSm^3/day High: 5,100kSm^3/day				
Probability Distributions			Objective Value (in million $)	Computational Time (sec)
0.333	0.333	0.333	190.95	773.38
0.250	0.500	0.250	190.72	959.9
0.200	0.600	0.200	190.05	941.0
0.100	0.800	0.100	189.27	796.0
0.025	0.950	0.025	188.39	773.31

Table 1: Objective values and computational time for different distributions in target flowrate

5.2.2 Uncertainty in Target flow rate and the Investment costs

The uncertainty in the target rate is related to flowrate, investment costs, and operational costs associated with the project. Numerous factors like delays in the project, and availability of resources have an impact on the investment costs like the possibilities of opening a well, the cost of installing a buffer tank, and operational costs like penalty cost for venting CO_2 and also the cost of injection of CO_2.

In this section, the values for different costs and flowrates are assumed as per the historical data issued by TotalEnergies. The probability distribution was 25% for the pessimistic value, 50% for the average, and the 25% belong to the optimistic value for the costs and the flowrates. For this specific case, we redefined the range of target flowrate for the low and high values. The average value for the target injection rate remains unchanged. The new low value utilized for the target injection rate is $4,700\frac{KSm^3}{day}$. Similarly, the target injection rate for a much higher value of $5,300\frac{\mathrm{KSm}^3}{\mathrm{day}^3}$ is considered to record the difference in the investment strategies made by the stochastic model as compared to that from the deterministic equivalent. The model is solved first using DICOPT which does not guarantee global optimality yielding an objective value of 190.72 for 3,8544 constraints and 20,373 variables out of which 3,809 are discrete variables. The CPU time recorded for the problem is 396.66 seconds. Fig 5 represents the wells and reservoirs connection that are operated to meet the demand for the target injection rate. There are 5 wells and 4 reservoirs to store the CO_2-rich fluid, however, the model selects 2 reservoirs and 3 wells as shown in figure 5. The same optimization model is solved by BARON, to determine the global minima of 190.72. BARON guarantees a global optimal as it applies the Spatial Branch and Bound algorithm. However, the CPU time recorded for the problem was 1,196.47 seconds. After solving the SP MINLP by BARON, a change in the process decision is observed. Well 3,4 and 5 are selected. However, different sets of combinations for the wells and reservoirs are selected as shown in the Figure 6 .

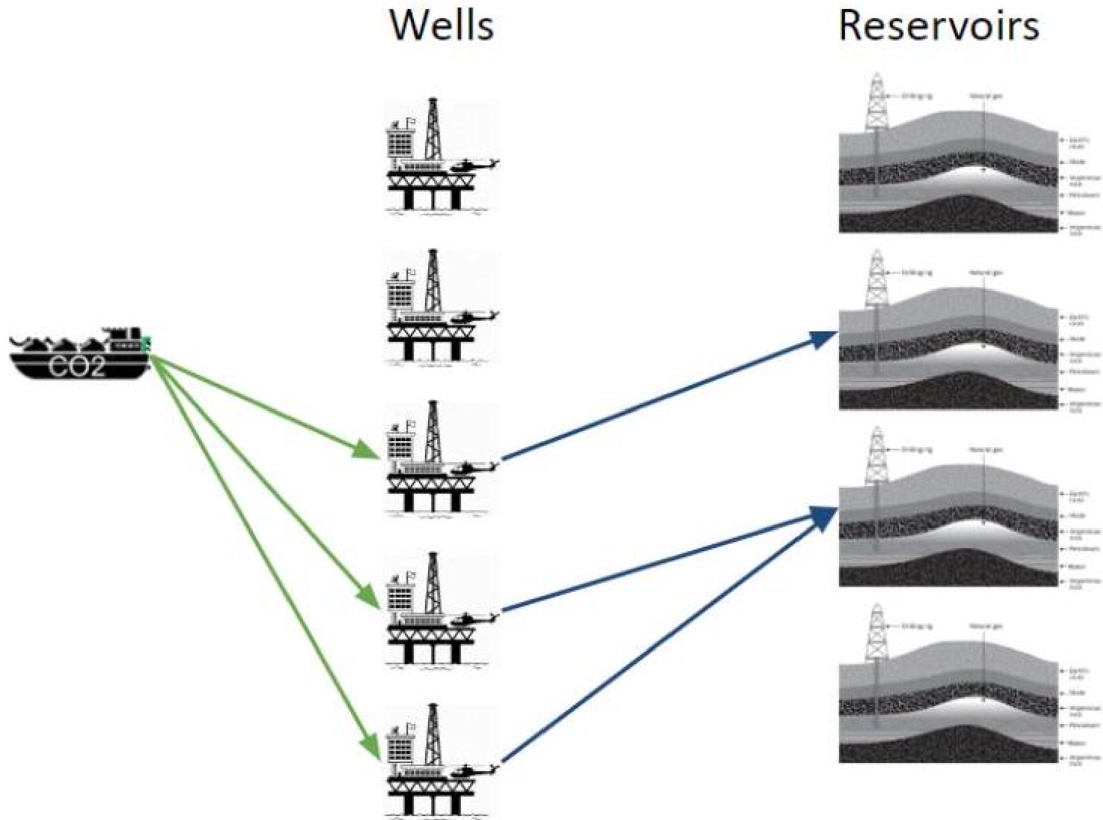

Figure 6: The selected choices of wells and reservoirs for Approach 2 using DICOPT

Figures 7 and 8 show that the cumulative reservoir volume for reservoir 3 and the actual flowrate to the fields are plotted against a 1 month time horizon. It is inferred that in the first two scenarios (s1 and s2) which are lower than an equivalent to the deterministic value, we observe a constant target flowrate, R_f is achieved by the model. However, in the case of the third scenario where R_f is high, the actual flowrate to the field Q_{act}, changes with respect to time to meet the higher demand.

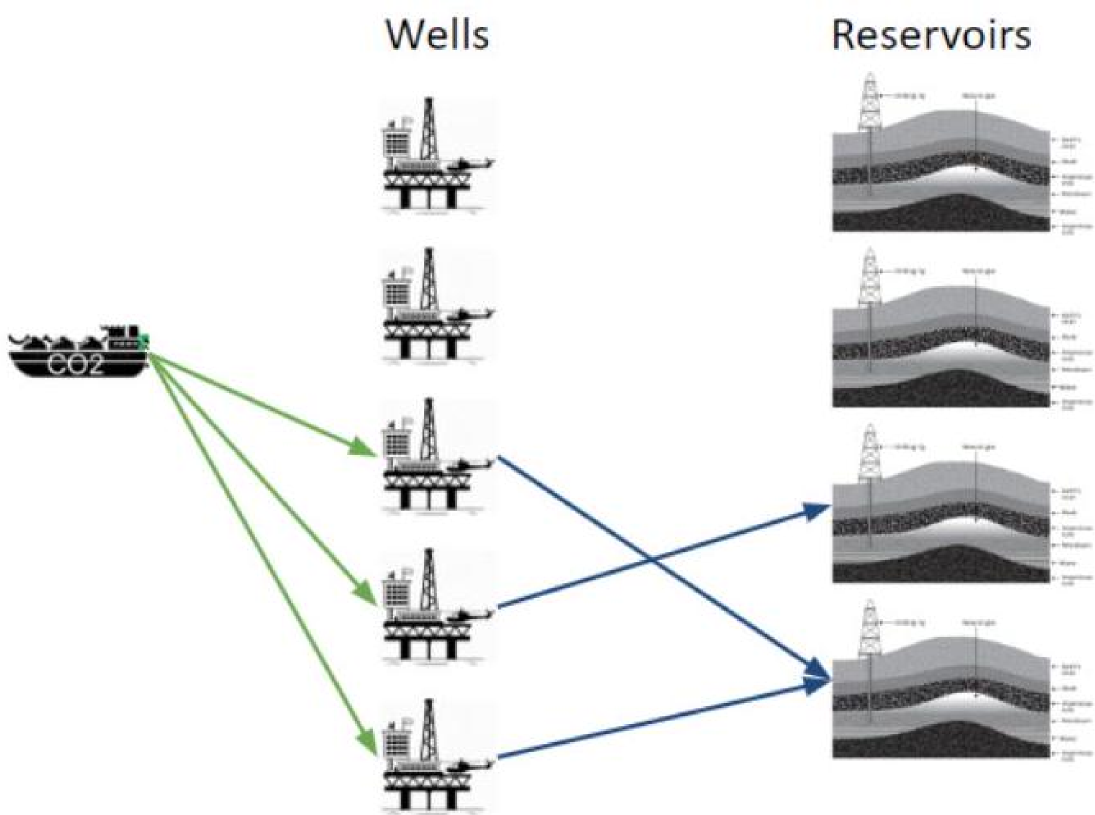

Figure 7: The selected choices of wells and reservoirs for global minima

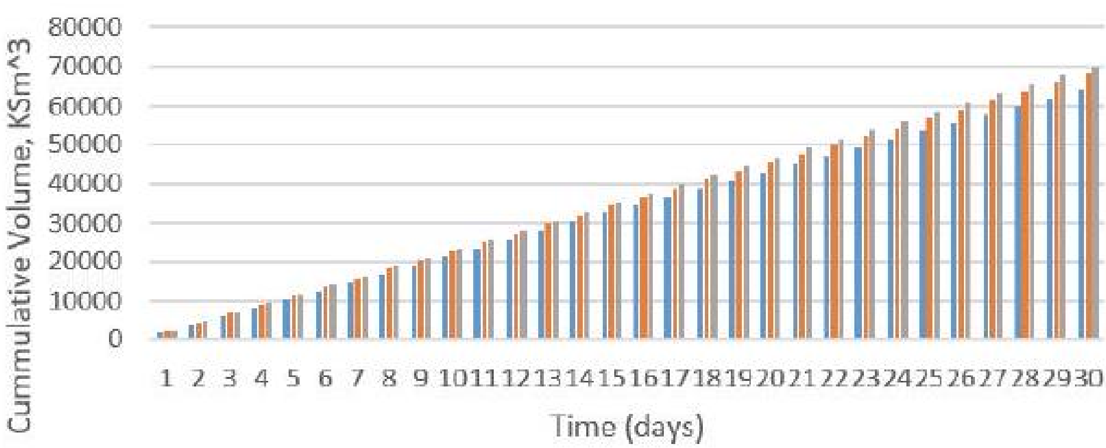

Figure 8: Cumulative reservoir volume for reservoir-3

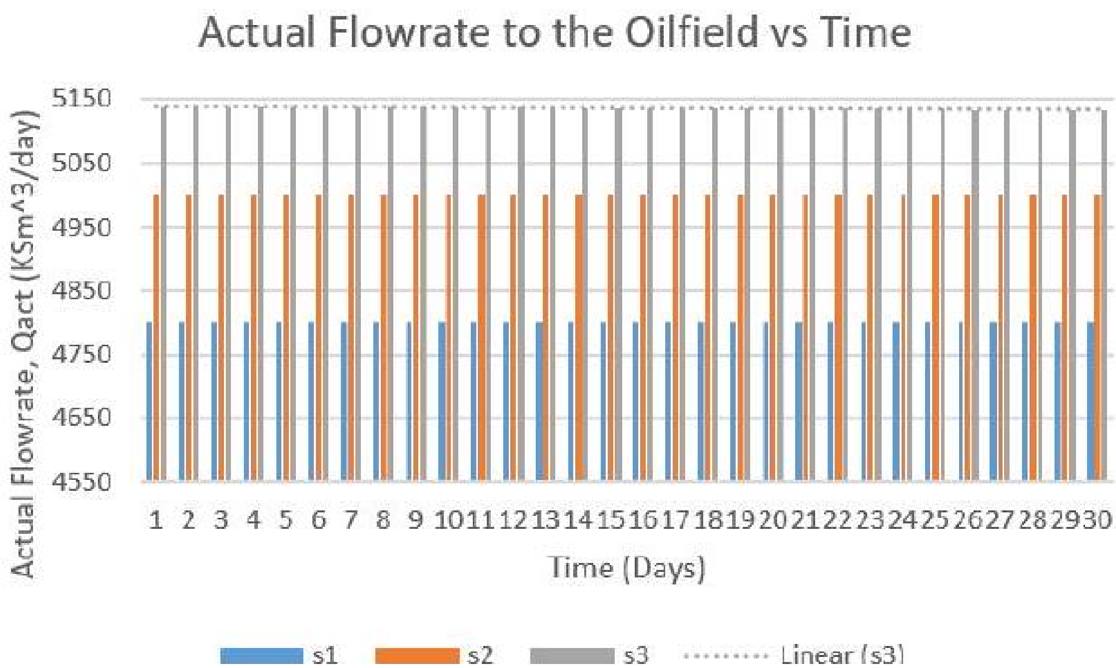

Figure 9: The actual injection flowrate to reservoir-3

5.3 Value of Stochastic Solution (VSS)

To provide further insight into the impact of the mean and variance of the distribution function we determine the value of the stochastic solution for the 5 cases in Table 2.

The Value of the Stochastic Solution [6] is determined by comparing the solution of the stochastic problem with the solution of a stochastic version in which the investment (decisions like the number of wells, nw, and the number of buffer tanks n required for the problem) are fixed to the values of the deterministic solution. If the investment strategy devised by the stochastic version is the same as that of the deterministic model, VSS is 0 for that case as shown in Figure 8. The Value of the Stochastic Solution (VSS) tends to 0 as the probability of the nominal value of the distribution increases as shown by point 5 in Fig 9. On the other hand, as the distribution widens (e.g., point 1 in Fig. 9), the VSS reaches its highest value.

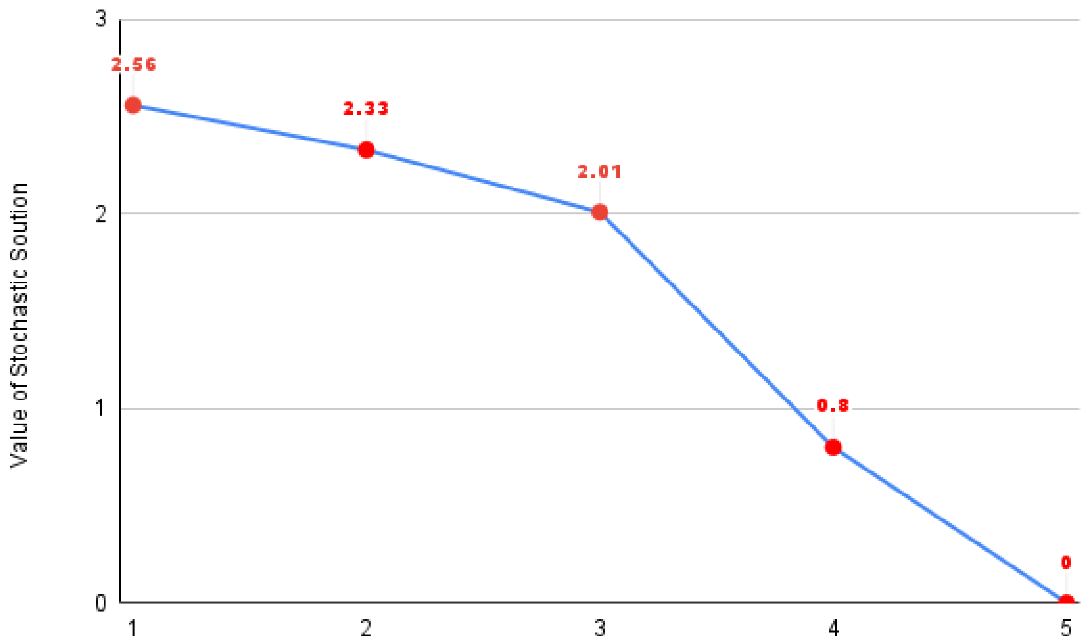

Figure 10: The VSS calculated for five probability distributions

5.4 Case 2: Moment Matching Problem

In this section, we implement the formulation in (2) of the moment matching problem, which is a non-convex nonlinear programming problem. In this section, we consider the source of uncertainty coming from the downloading rate from the boat, R_B which carries CO_2 in the cryogenic state. The objective of this case study is twofold, first, to determine the decision variable, $x_{i,j}$, and second, to determine the probability distributions. The NLP model is solved for a global minimum by Branch-And-Reduce Optimization Navigator (BARON) [11] solver. The computation time recorded for the model is 93 seconds to obtain the global minima over 50 iterations. An objective value of 0.78334 is obtained. In addition, it consists of 14 constraints and 25 variables.

The optimized weights across the four moments and the covariance have been obtained from tuning weights, as a hyperparameter. The values for the optimized weights for the moments are reported in Table 2 and the weights across the covariances are reported in Table 3, respectively.

Table 2: Weights across the four moments

Weights for moments, w_1	$w_{i,k}$
Data	Tree
0.0982318	0.13624
1.343	0.10541
0.01	0.693289
0.0172331	0.01

Table 3: Weights of the covariance

Weights for covariance, w_2	$w_{i,ii}$
Data	Tree
0.00295396	-0.149839
-0.149839	0.0892857

In this way, applying the moment matching problem, the scenario tree is generated. The two-stage scenario tree involves 3 realizations and associated probability distribution. The red node represents the root node followed by three blue nodes for stage- 2 branches of the tree. The probability distribution of $97.4\%, 1.14\%$, and 1.4% is recorded for the corresponding values of the random parameter R_B that represent the download rate of the boats at the CO_2 logistic terminal.

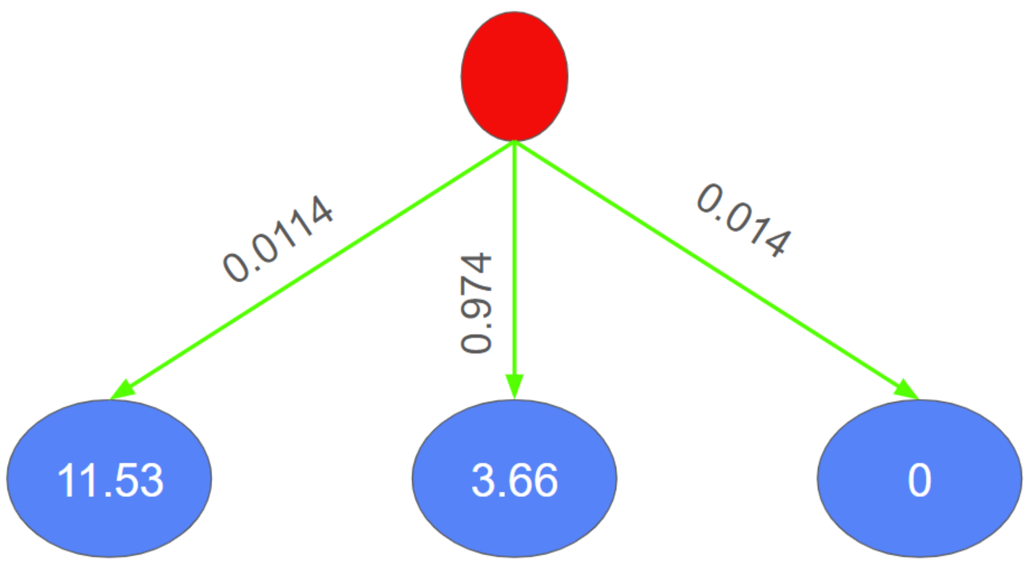

Figure 11: A two-stage generated scenario tree

5.4.1 Comparative Study

We have implemented the solutions of the deterministic equivalent problem for the proposed two-stage stochastic MINLP model. The Moment Matching Problem (MMP) is described in section 4.2.2, the uncertainties are accounted for by the target injection flowrate. The proposed deterministic equivalent MINLP optimization model was solved by DICOPT. The MINLPSP model consists of 10,572 variables, 25,584 constraints along with 1,289 discrete variables. The objective value of \$190.72 million was determined for the probability distribution of 25%, 50%, and 25%. The probability distribution is based on low, average, and high values of the target injection flowrate.

The probability distribution and the values recorded for the random parameters obtained from the Moment Matching problem (MMP) are applied to the MINP-SP model. An objective value of \$190.24 million was obtained compared to \$190.72 million in the case of the solution obtained from the MINLP-SP problem. The optimal well-reservoir configuration of well-03 to reservoir-03, well-04 to reservoir-3, and well- 05 to reservoir- 04 is determined by the optimization model based on the initial condition. In the case of the high scenario for the target injection rate of 5100Ksm^3/ day, there was the venting of CO2 to the atmosphere.

6 Conclusion and Future Work

This paper has examined the impact of distribution functions in two strategies to anticipate uncertainties in the optimal field management problem. The goal is to examine two different mathematical formulations to tackle uncertain parameters in the model. We first consider the case for which the probability distribution and the uncertain values are known, and next the case for which the probability distribution and values for the uncertain parameters are unknown.

For the first case, a two-stage stochastic programming problem is formulated for the fields with various sources of uncertainties. In addition, the value of the stochastic solution was calculated for different probability distributions. A small deviation from the expected objective value of the deterministic equivalent of the problem and the stochastic version of the problem was found. For cases with a higher probability of the average value, the value of the stochastic solution tends to 0. However, a larger deviation can be observed when there is an equal distribution of probability over the three scenarios of the uncertain parameters which in turn lead to different investment strategies.

For the second case, the scenario tree is generated by employing the Moment Matching Problem. The first four moments are calculated across the mean of the historical data. The hyperparameters that include weights for the moments and covariance are optimized and reported. A scenario tree was generated by solving the corresponding non-convex NLP problem. The weighted squared error for statistical properties determined for the tree and the data is minimized. This method can determine the unknown parameters and their probability distribution, given the historical data for the uncertain parameters.

This paper has greatly simplified the stochastic programming problem by simply considering three scenarios, high, average, and low. For more realistic cases in which the number of scenarios can be much larger, the high computational time required to solve the model remains a challenge. With the increase in the number of scenarios, the computational time increases exponentially. Decomposition techniques like Benders Decomposition technique can be applied to decrease the model's computational time.

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