Stochastic optimization of the geological sequestration of carbon dioxide

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Abstract. Geological sequestration has been identified as having potential to reduce increasing atmospheric concentrations of carbon dioxide (CO_2). However, a global impact will only be achieved if this technology is implemented on a massive scale. This work presents a methodology for finding optimal operational schemes for potential sequestration sites having uncertain physical parameters. This tool uses a semi-analytical algorithm to estimate leakage rather than a calibrated numerical model enabling application to potential sites having vastly different domain characteristics. A genetic algorithm is used to heuristically determine non-dominated solutions between the following competing objectives: 1) minimize project cost, 2) minimize risk, and 3) maximize mass of CO_2 sequestered. Parallel processing and archiving are employed to reduce computational cost. This framework has been developed into an application (COSMOS: CO_2 sequestration simulation and multi-objective optimization software) to visually display domain characteristics, pressure pulse and CO_2 plume propagation during simulation, and pareto-optimal tradeoff solutions. Due to the large set of assumptions made by the semi-analytical CO_2 leakage algorithm, this framework may only be used for initial site planning and characterization. Once full developed, this tool has the potential for initial screening and ranking of large sets of potential geological sequestration sites.

1. Introduction

A stochastic optimization framework has been created to aid in preliminary project planning for geological sequestration (GS) of carbon dioxide. Mass of CO_2 sequestered is maximized while project cost and risk are minimized by selecting optimal injection well locations and injection rates for potential injection sites having parameter uncertainty. This framework has been compiled into a computational tool (*COSMOS: CO_2 Sequestration Simulation and Multi-objective Optimization Software*) to display output results.

Planning operations such as site selection, optimization, and sensitivity analysis require large numbers of model simulations for multiple potential injections site domains making calibrated numerical modeling infeasible. Therefore a fast, though less accurate, semi-analytical (SA) model will be used to estimate CO_2 flux throughout the domain. After 'coarse scale' project planning has been completed using this stochastic optimization framework, more rigorous, although slower, numerical models should be used for final project development of individual potential injection sites.

2. Stochastic Optimization Framework

The general procedure followed by this algorithm is presented below in Figure 1. Once all input files are read, an initial population of injection scenarios is randomly generated. Each injection scenario is represented by a chromosome (i.e. a vector of numbers) with

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length equal to double the number of injection wells. The first half of the chromosome represents each injection well's injection location index while the second half represents injection rate.
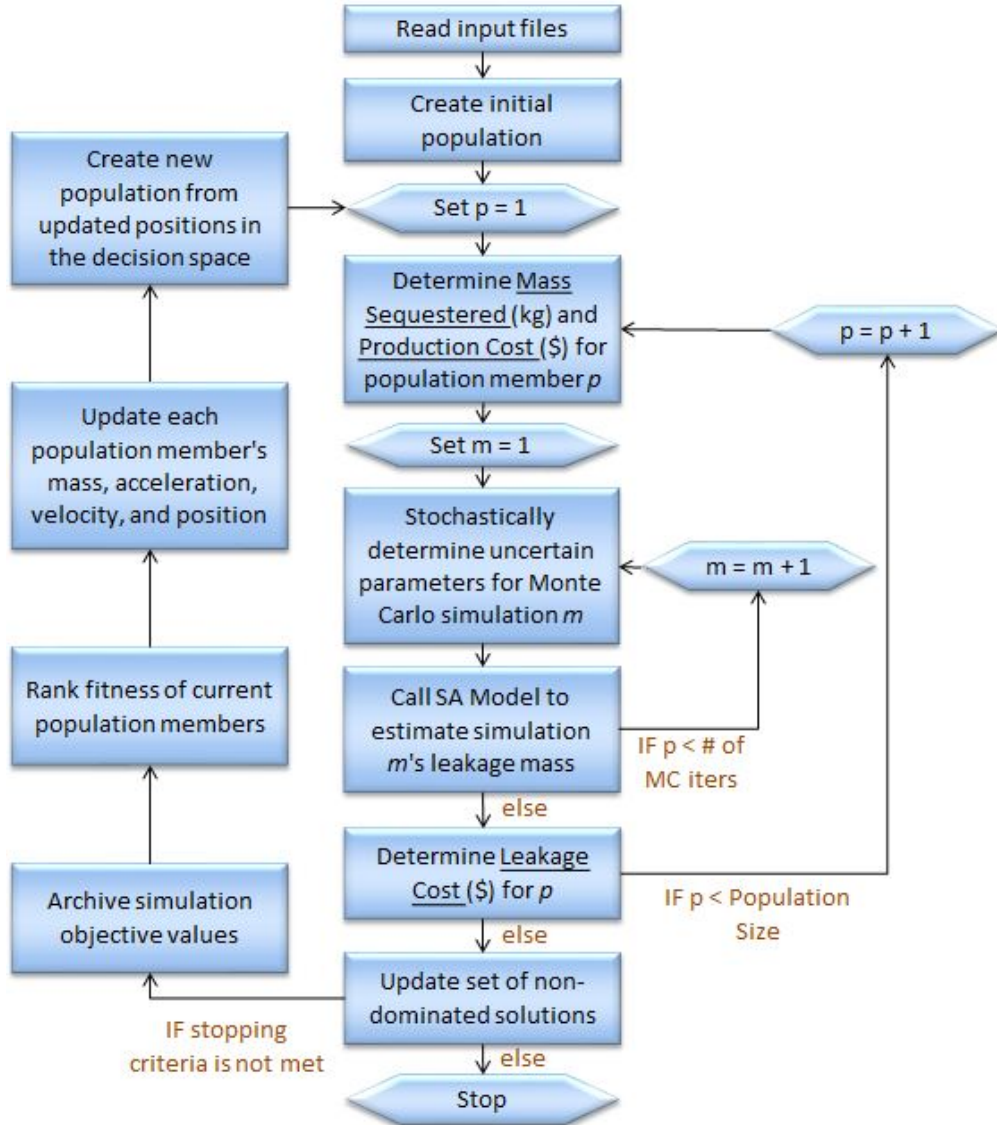
Figure 1. Schematic of the stochastic optimization algorithm

Objective values are calculated for each population member. Mass sequestered is simply total mass of CO_2 injected and is calculated by multiplying the sum of injection well flow rates by the injection duration.

$$M_{Seq} = \sum_{w=1}^{nIW} Q_w^c * t_{inj} \tag{1}$$

In Equation (1), w is the injection well index, $nIWs$ is the number of injection wells, Q_w^c is the CO_2 injection rate for well w, and t_{inj} is the injection duration . The project cost ($Cost$), consisting of the capital (Cap_w), operational (OP_w), surface maintenance ($SurM_w$), subsurface maintenance ($SubM_w$), variable (V_w), and leakage (LC) costs, is defined as

$$Cost = \sum_{w=1}^{nIWs} [Cap_w + OP_w + SurM_w + SubM_w + V_w(Mseq_w)] + LC \qquad (2)$$

The cost associated with leakage (LC) is estimated as

$$LC = c_L \cdot Mleak^{r_A} \qquad (3)$$

where c_L is the coefficient representing penalty cost (\$), $Mleak$ is the mass of CO_2 leakage, and r_A is a risk adversity factor reflecting preferences of the decision maker.

Project costs at each risk probability are calculated. The following list of input variables may be represented as stochastic with this framework:

- Aquifer thicknesses for each layer
- Aquitard thicknesses for each layer
- Aquifer porosity for each layer
- Radial aquifer permeabilities for each layer
- Vertical aquifer permeabilities for each layer
- Total effective compressibility for each layer
- Aquifer specific storage for each layer
- The bottom depth of the lowest aquifer from the surface
- Leaky well radii for each horizontal location in each aquitard
- Leaky well permeabilities for each horizontal location in each aquitard

Each uncertain parameter will be assigned a discrete probability distribution function (PDF) index. This index represents a user defined PDF. As an example, data may suggest that the permeability of a given leaky well is represented by the PDF shown in Figure 2. For this well, the permeability has a 5% chance of being 0.1 mD, a 20% chance of being 1.0 mD, a 50% chance of being 10 mD, a 20% chance of being 100 mD, and a 5% chance of being 1000 mD.
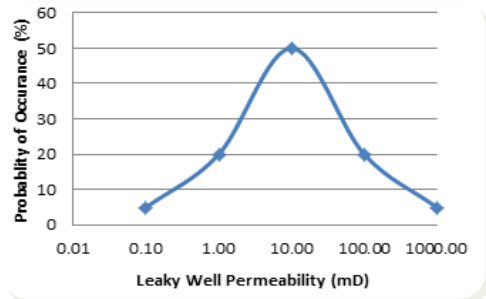

Leaky Well Permeability (mD)	Probability Of Occurance	Selection Criteria
0.1	5%	0.00 - 0.05
1	20%	>0.05 - 0.25
10	50%	>0.25 - 0.75
100	20%	>0.75 - 0.95
1000	5%	>0.95 - 1.00

Figure 2. Graphical example of a deterministic PDF

Figure 3. Uncertain variable selection criteria

A random number between 0 and 1 will be generated for each uncertain parameter in each Monte Carlo (MC) simulation. This number will determine the value of the uncertain parameter used in the simulation. In the example above, if a random number of 0.10 was generated for the leaky well in Figure 3 the algorithm would assign a permeability value of 1 mD. Once values are assigned to all stochastic variables, the simulation runs as normal and outputs a leakage mass. In this method, each Monte Carlo simulation has an equal probability of occurrence. Figures 4 and 5 show examples of stochastic input data.

Stochastic (2) or Deterministic (1) Simulation/Optimization	2	
Number of Monte Carlo Iterations for Each Simulation	500	
Number of PDFs	2	
PDF#1: Number of Discritizations	3	
PDF#1: Disc#1: Probablity of Occurance, Variable Multiplier	0.2	0.1
PDF#1: Disc#2: Probablity of Occurance, Variable Multiplier	0.5	1
PDF#1: Disc#3: Probablity of Occurance, Variable Multiplier	0.3	10
PDF#2: Number of Discritizations	7	
PDF#2: Disc#1: Probablity of Occurance, Variable Multiplier	0.05	0.01
PDF#2: Disc#2: Probablity of Occurance, Variable Multiplier	0.1	0.1
PDF#2: Disc#3: Probablity of Occurance, Variable Multiplier	0.15	0.5
PDF#2: Disc#4: Probablity of Occurance, Variable Multiplier	0.3	1
PDF#2: Disc#5: Probablity of Occurance, Variable Multiplier	0.1	10
PDF#2: Disc#6: Probablity of Occurance, Variable Multiplier	0.25	60
PDF#2: Disc#7: Probablity of Occurance, Variable Multiplier	0.05	100

Figure 4. Input data defining a set of discrete PDFs

Probability Indicies ("0" = Deterministic, ">0" = Stochastic)	Enter Value	Auto-Calc	
Aquifer Layer Thicknesses - 1 x L matrix (m), PI_H=	0	0	0
Aquitard Layer Thicknesses - 1 x (L+1) matrix (m), PI_B=	0	0	0
Porosity - 1 x L matrix, PI_n=	0	0	0
Radial Aquifer Permeability - 1 x L matrix (mD), PI_k=	1	1	1
Vertical Aquifer Permeability - 1 x L matrix (mD),PI_ kz=	0	0	0
Aquifer Compressablity - 1 x L matrix (m^2/N), PI_c_eff=	0	0	0
Aquifer Specific Storage - 1 x L matrix, PI_Ss=	0	0	0
Bottom depth of the Lowest Aquifer from the Surface (m), PI_dbot =	0		

Figure 5. Input data assigning PDF indexes to uncertain variables

Leakage mass is then calculated for each Monte Carlo simulation using a semi-analytical multi-phase flow model. Cumulative distribution functions (CDFs) are compiled and used to define risk for each injection scenario. Injection scenarios are ranked based upon expected value of project cost.

A new population of injection scenarios is then created using rankings of current population members. First, an operation referred to as *elitism* is performed. A percentage of the best injection scenarios is selected to participate in the next generation. Next, a selection process is used to choose parents for the next generation. Population members with higher ranking are more likely to be chosen as parents. Once parents have been

selected, *crossover*, a method of taking some of the traits of each parent, is used to finish creating the new generation of injection schemes. Finally, there is a small chance, quantified as the *mutation* rate, in which chromosome elements of this new population will be randomly altered.

This process is repeated until the convergence criterion is met. Injection schemes providing the best combinations of expected project cost and sequestered mass are selected as optimal injection scenario. Risk values are calculated using each optimal injection scenario's cumulative distribution function of leakage.

3. CO2 Leakage Estimation

This framework will ultimately be used to optimize and compare large quantities of potential injection sites having vastly different domain characteristics. For this reason, leakage of CO_2 is estimated using a semi-analytical algorithm as opposed to numerical response surface technics. Creating and calibrating each potential injection site's numerical model, as well as training the resulting response surface requires user expertise and large investments of computational time. The semi-analytical leakage algorithm is very general and is able to be applied to simplified computational models of the vast majority of potential injection sites.

A semi-analytical algorithm, developed by Celia et al. (2011) and Nordbotten et al. (2009), estimates both brine and CO_2 flux through permeable caprock locations caused by GS. Originally conceptualized as segments of abandoned wells, permeable caprock locations represent cylindrical portions of the aquitard layers having permeability values greater than or equal to zero. Referred to as 'leaky wells', these are the only pathways for fluid flux between aquifer layers. Users of this algorithm are able to specify the number and spatial location of injection wells (M), leaky wells (N), and aquifer/aquitard layers (L).
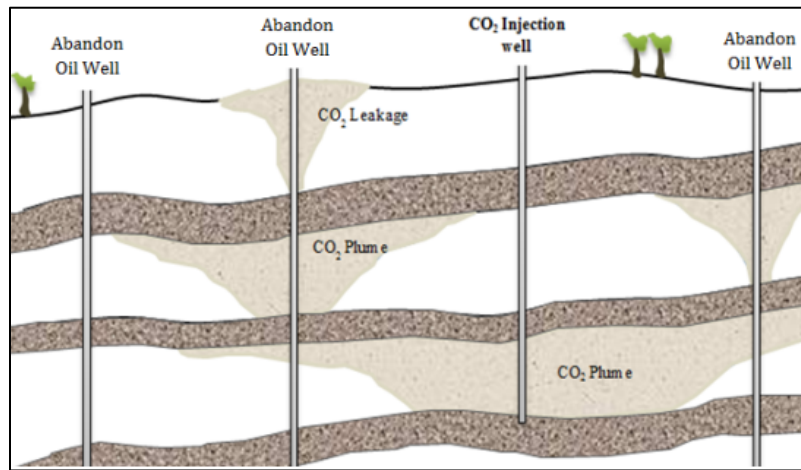

Figure 6. Subsurface domain layout

The domain is structured as a horizontal stack of aquifer/aquitard layers perforated by injection and leaky wells. Injection wells are able to inject CO_2 into any layer. There are several assumptions made by this algorithm:

1. Aquifers are initially saturated with brine at hydrostatic pressure.
2. Aquifers are horizontally level, homogenous, and isotropic.

3. Aquitards are impermeable, except where there is a leaky well.
4. Aquifers typically exhibit horizontal flow.
5. Capillary pressure is negligible resulting sharp fluid interface.
6. CO_2 plume thickness at any given location is assumed to be the maximum plume thickness from any given source or sink in the aquifer.
7. Pressure response from sources and sinks are superimposed in each aquifer.

Initially, fluid is not flowing through any of the leaky wells because the entire domain is assumed to be saturated with brine at hydrostatic pressure. At the start of fluid injection the pressure throughout the domain begins to change resulting in fluid flux through leaky well locations in the aquitards.

4. Visual Simulation and Optimization

CO_2 sequestration simulation and multi-objective optimization software (COSMOS) has been created to provide visualization of output data. Domain characteristics such as plan views of leaky will locations with map overlays and profile views of subsurface layer profiles (both seen in Figure 6) are displayed as well as simulation data regarding CO_2 plume and pressure propagation and injection well information (Figure 7).
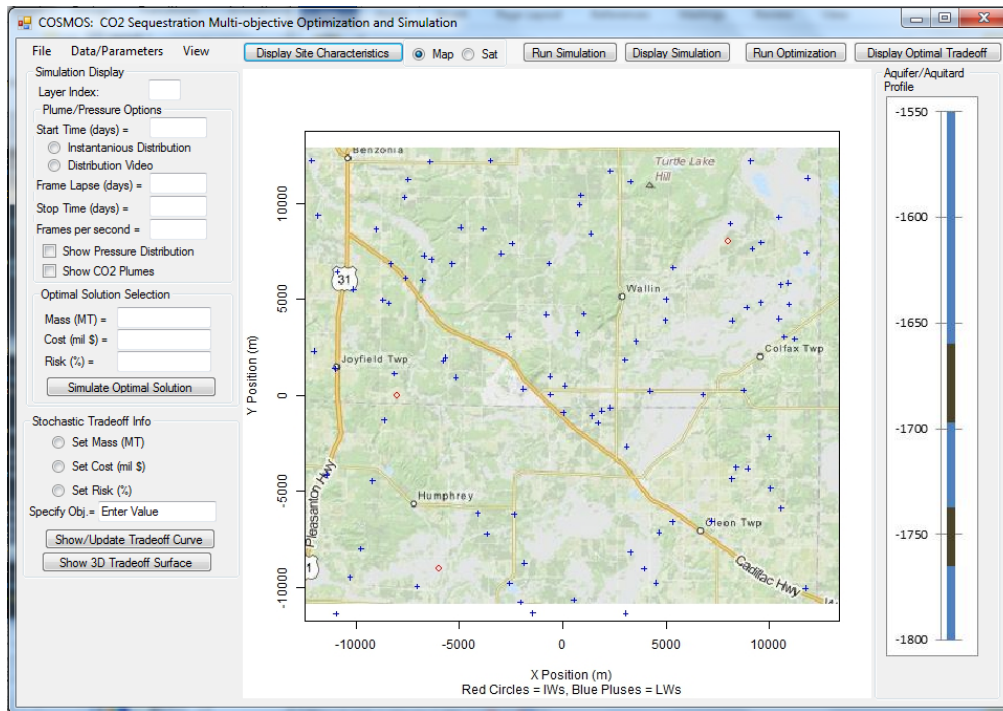
Figure 6. Plan view showing injection and leaky well locations superimposed over a map of an example potential injection well location
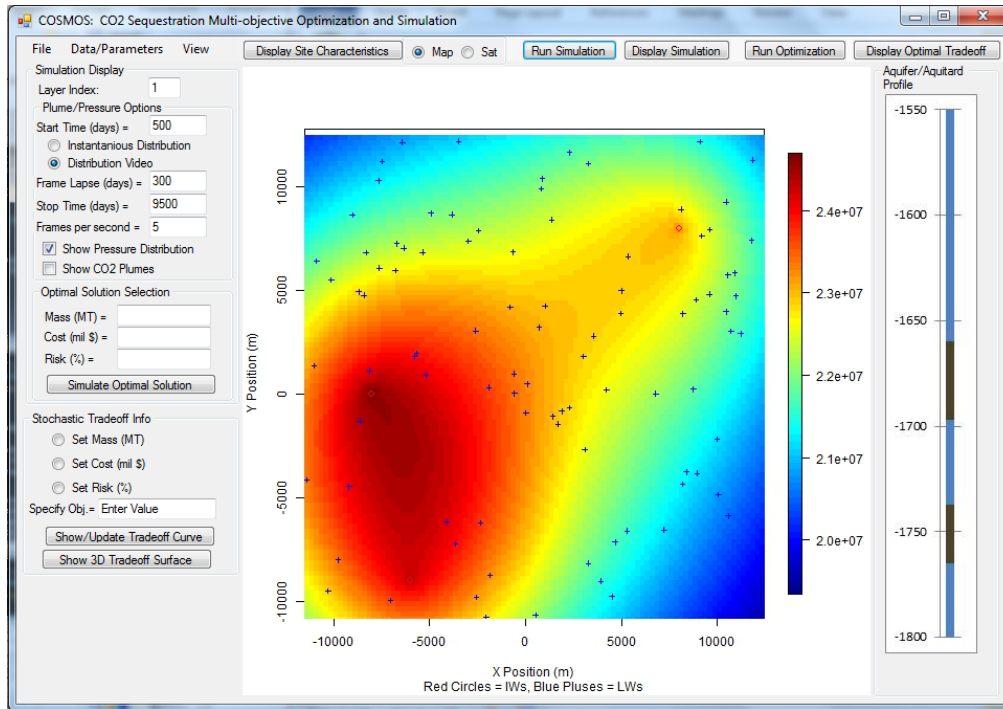
Figure 7. Plan view showing fluid pressure in the bottom aquifer after a period of injection

COSMOS also returns the optimal trade-off surface (Figure 8) between three competing objectives; maximize mass of CO_2 sequestered, minimize risk, and minimize project cost. Two dimensional tradeoff curves (Figure 9) may be displayed for specific objective values.
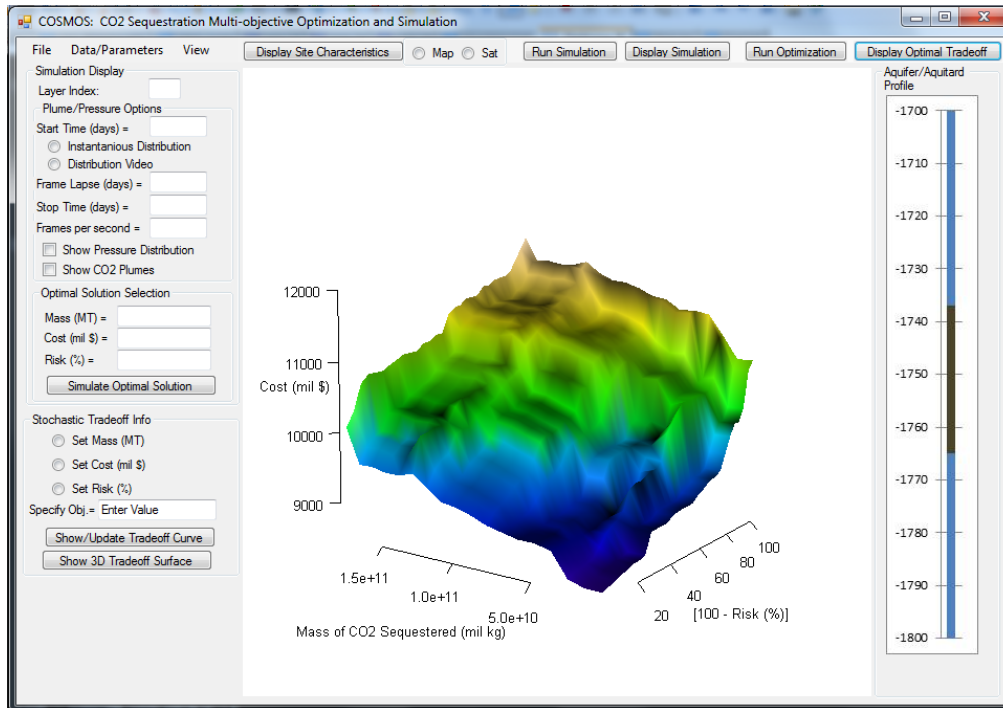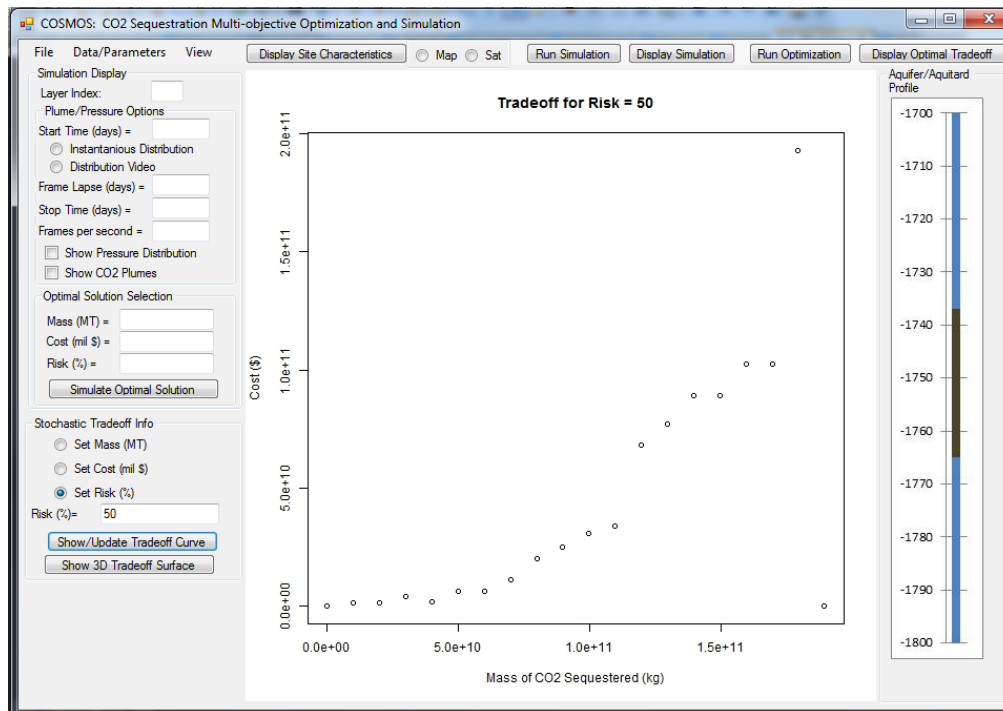

Figure 8. Example of an optimal tradeoff surface between three competing objects for a potential injection site

Figure 9. Example of an optimal tradeoff curve between Project Cost ($) and Mass Sequestered when setting Risk to 50%

5. Computational Efficiency

Due to the iterative nature of genetic search and Monte Carlo processes, large numbers of simulations are needed for stochastic optimization. This framework utilizes *parallel computing* and *simulation archiving* to improve computational efficiency.

Parallel Computing

As described above, CO_2 leakage must be estimated for multiple injection scenarios for each generation. Leakage estimation calculations for a given generation are independent and therefore may be processed in parallel (i.e. simultaneously) rather than sequentially. Users of this framework are able to specify the maximum number of parallel leakage estimations occurring at one time.

Simulation Archiving

Simulation archiving prevents the GA from recalculating objective values for identical scenarios. A record is kept of GA input data and objective values for each simulation processed.

6. Conclusions and Future Application

The methodology of a general stochastic optimization framework has been presented. A semi-analytical algorithm is used to estimate quantities of CO_2 leakage.

The next phase of this research involves testing and improvement of the framework. First, stochastic optimization will be performed for a hypothetical project at the Michigan Technological University (MTU) test site near Thompsonville, MI. This site is a nearly depleted oil reservoir with a great wealth of data, making it attractive for computational

testing. In addition, an option to use a gravitational search algorithm (GSA) rather than a GA will be created. Performance measures such as convergence rate, computational efficiency, and final objective values of the GSA will be compared to those of the GA.

Due to the large set of assumptions made by the semi-analytical CO_2 leakage algorithm, this framework may only be used for initial site planning and characterization. However, once full developed, this tool has potential for initial carbon sequestration project planning and performing initial screening and ranking of large sets of potential carbon sequestration sites.

Acknowledgements

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