Numerical and Statistical Optimization of CO_2 Storage Performance for Emission Mitigation and Environmental Sustainability

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Abstract. Efficient CO_2 storage in permeable subsurface geologic reservoirs is crucial to the success of carbon capture and storage (CCS) for emission reduction. This study explores the operating conditions for CO_2 injection, such as the rate, pressure and temperature, using CFD-based simulation with ANSYS Fluent in conjunction with statistical optimization by RSM. Navier Stokes equations were used to formulate the model together with a porous media momentum sink and a transport equation for CO_2 saturation in a homogeneous porous-core. For the CCD experiments, values of parameter were varied from 5 to 15 mg/s (injection rate), from 250 to 350 bar (outlet pressure) and from 40 to 100°C (inlet temperature). The main response studied was CO_2 storage capacity (g of CO_2/m^3). RSM analysis revealed a quadratic relationship with R^2 = 0.8737, emphasizing that the interaction between injection rate and inlet temperature was the most influential factor affecting storage performance. The best operating parameters found were the feed flow rate of 7.89 mg/s, the inlet temperature equal to 93.61 °C and the outlet pressure 284.55 bar with an average CO_2/m^3 storage of about 214 g. These results indicate that a careful monitoring of the injection parameters can improve CO_2 storage efficiency and operational security.

1 Introduction

Current increases in atmospheric carbon dioxide (CO_2) concentrations present one of the largest contributors to global climate modifications; primarily as an outcome of the combustion of fossil fuels and industrial processes [1]. To mitigate these effects, a key option is the carbon capture and storage (CCS). CCS is the process of capturing CO_2 from industrial emissions and injecting it into deep geological reservoirs for long term storage [2], [3]. Porous geological formations, including deep saline aquifers and depleted hydrocarbon reservoirs, are considered among the most promising storage media due to their low cost per unit of stored CO_2 and their geologic stability [4].

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However, the performance of CO_2 injection and storage is significantly affected by the operational conditions such as the rate of injection, pressure and temperature. These determine the flow, storage (inside the sphere reserved for the CO_2) and viscosity of CO_2 injected [5]. Consequently, these parameters optimization are crucial to guarantee efficient storage and long term containment safety. Carbon Capture and Storage (CCS) has been one of the major technologies in Indonesia since it is very large CO_2 emitter with very vast geological storage. Indonesia's potential CO_2 storage capacity, based on the report by the Ministry of Energy and Mineral Resources (2024), stretches 577 gigatons in numerous basins. In particular, the Northeast Java Basin that includes the Tuban, Blora and Bojonegoro formations is an important potential site for CCS. New research has indicated that carbonate containing rocks, dolomite and calcite, are more reactive with injected CO_2 than silicate dominated reservoirs. This increased reactivity enhances mineral trapping capability but increases potential dissolution [6]. Previous studies, numerical and experimental, demonstrated the high sensitivity of storage capacity to geologic- and operational-related parameters. For example, Wang et al. [7] demonstrated by MATLAB simulation that permeability and pressure affect more CO_2 storage capacity than porosity does. Similarly, Liu [8] emphasized the importance of CO_2 solubility and mineral trapping in ultimate trapping efficiency. However, there has been little known of CO_2 on the behavior of Indonesian porous rock in a local scale, especially in the micro-scale injection condition such as its resemblance to underground media [9]. The present study attempts to fill this gap for numerical solutions with CFD results in the ANSYS Fluent and RSM to optimization of CO_2 flooding parameters in porous media. Flow simulation of the supercritical CO_2 is based on mass conservation and Darcy equation by employing RSM with central composite design (CCD). It's this perfect combination of injection rate, pressure and temperature that you're trying to achieve to maximise storage efficiency and secure geological stability. It is anticipated that such an integrated modelling and optimization framework can facilitate data-based decision-making for the design of a safe and efficient CCS programme in Indonesia's subsurface repositories.

2. Methods

2.1 Numerical Model

A two-phase flow model of the concurrent CO_2-brine as interpenetrating continuous phases was performed in this work with ANSYS Fluent using the Mixture Model. The Mixture Model was selected as it provides an accurate and computationally efficient approach to simulating systems in which one phase is present at low volume fractions, with continuous interaction between that phase and the predominant phase, without any physical discontinuities between them. This model reduces the difficulty of the problem to a solution of a single momentum equation for mass-averaged velocity of mixture and introduces a relative velocity in order to represent motion of dispersed phase with respect to continuous phase. This approach is suitable for simulating CO_2-brine flow system in which the interphase interactions and solubility effects occur over the entire computational domain. The continuity equation for the mixture model is given as [10]:

$$\frac{\partial}{\partial}(\rho_m) + \nabla . (\rho_m \vec{v}_m) = 0 \tag{1}$$

where $\rho_m = \sum_k \alpha_k \rho_k$ is the mixture density and $\vec{v}_m$ is the mass-average velocity of the mixture, defined as:

$$\vec{v}_m = \frac{\sum_k \alpha_k \rho_k \vec{v}_m}{\rho_m} \tag{2}$$

The momentum equation employs the altered Navier–Stokes equation with a momentum sink term derived as the viscous and inertial resistance of the porous media:

$$\rho\left(\frac{\partial v_i}{\partial t}+v_j\frac{\partial v_i}{\partial x_j}\right)=-\frac{\partial p}{\partial x_i}+\mu\nabla^2 v_i+F_i+S_i \quad (3)$$

$$S_i=-\left(\sum_{j=1}^{3}D_{ij}\mu v_j+\sum_{j=1}^{3}C_{ij}\rho|v|v_j\right) \quad (4)$$

where ρ is the mixture density, μ denotes the viscosity, represents gravitational body force, and is the porous resistance source term. The first term in describes viscous damping while the second is related to inertial resistance and where and can be obtained from permeability of medium under consideration and geometry. The Mixture model was used in the ANSYS Fluent multiphase framework for simulation. The simulation included two phases: carbon (CO_2) as the first phase and brine as second phase. The flow regime model method was turned on to properly predict drag and slip velocity across the domain. The formulation of the implicit body force solver was employed to improve the numerical stability in domains dominated by gravity and buoyancy, an important consideration for the accurate prediction of CO_2 migration and solubility in vertical or inclined geometries. The energy equation was enabled in order to describe thermal coupling between heat and mass transfer in the CO_2-brine system. The CO_2 thermophysical properties with respect to the real gas behavior as a function of temperature and pressure were calculated using Peng Robinson Equation of State (PR-EOS). The PR-EOS outputs CO_2 density, enthalpy and heat capacity as a function of pressure and temperature without the need for interpolations, ensuring that energy and momentum equations are thermodynamically consistent. [10].

$$p=\frac{RT}{v-b}-\frac{a\,\alpha(T)}{v(v+b)+b(v-b)} \quad (5)$$

$$\alpha(T)=[1+\kappa(1+\sqrt{T_r})]^2 \quad (6)$$

where a and b are substance-dependent constants, κ is the function of the acentric factor, and Tr is the reduced temperature. The use of this EOS enables accurate predicting of temperature-dependent CO_2 density, which is essential for simulating the dissolution and migration of CO_2 in brine[10].

migration of CO_2 in brine[10]. Interstitial reacting phase transfer between CO_2 and brine was characterized by Henry's law that relates concentration of dissolved CO_2 in the liquid with partial pressure of it in post injection gas. The Van't Hoff correlation was used to describe the temperature dependence of Henry's constant, according to [10]:

$$H(T)=H_0\exp\left[\frac{C}{R}\left(\frac{1}{T_0}-\frac{1}{T}\right)\right] \quad (7)$$

where $H_0 = 3.4 \times 10^{-4}$, C = 2400 K, and R is the universal gas constant.

This correlation was incorporated into the species mass transfer model dialog, with the reference Henry's constant and temperature dependence specified accordingly. The overall mass transfer coefficient between phases was set to 2×10^{-12} m/s, representing the diffusion- limited regime typical of CO_2 dissolution in brine [11].

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2.2 Boundary Conditions

The boundary conditions for CO_2 injection in porous media include inlet temperature and injection rate at the inlet face geometry. Porous media are designated as gas-phase or liquid- phase. Mass flow inlet is chosen as the boundary type at the CO_2 inlet surface. Transient simulation was conducted on the flow with a timestep size of 0.5 seconds and 20 iterations per timestep. Details of the parameters in both simulations are shown in Table 1.

Table 1. Parameter used in simulation

Parameters	Solution Method
Multiphase Model	Mixture
CO_2 Inlet Flowrate	5, 10, 15 mg/s
Inlet Temperature	40, 70, 100 ^{o}C
Outlet Pressure	250, 300, 350 bar
CO_2 Properties	Real gas-PengRobinson
Volume fraction and Body Force Formulation	Implicit
Energy	On
Turbulence Model	k-e (standard)
Pressure-Velocity Coupling	Coupled scheme
Gradient Discretization	Least squares cell based
Pressure	PRESTO!
Momentum	Second order upwind
Volume Fraction	Compressive
Turbulent Kinetic Energy	First order upwind
Turbulent Dissipation Rate	First order upwind

2.3 Statistical Analysis

Statistical analysis was performed using response surface methodology (RSM) with a central composite design (CCD). RSM was used to optimize process variables to enhance the operational conditions of CO_2 injection in porous media. This method is well-suited for fitting a quadratic surface model in sequential experiments. High sensitivity for suitability assessment [12]. Based on insights gained from CCD. A regression model was developed, and the experimental results were modeled using with trial version of Design Expert software. Three system parameters were selected in the CO_2 injection process: injection rate, inlet temperature and outlet pressure. The models were built based on the 16 CCD matrices that covered the entire factor design of the three factors in Table 2.

3 Results and Discussion

3.1 CO_2 Storage Capacity

The simulated CO_2 storage capacities with the different combinations of injection rate (A), outlet pressure (B) and inlet temperature (C) are presented in Table 2 by using the numerical simulation with ANSYS Fluent, as well as the prediction based on statistics calculation via RSM. The CCD experimental matrix is used to systematically investigate the main and interaction effects of three factors.

Table 2. Central composite matrix design with a response to experimental results and predictions on the CO2 injection process

Run	Injection Rate (A) in mg/s	Pressure (B) in Bar	Temperature (C) in ^oC	Storage Capacity (Respon) g CO_2/m^3	
				Ansys Simulation (Actual)	RSM Model (Predicted)
1	5 (-1)	250 (-1)	40 (-1)	67,7	83,9
2	5 (-1)	250 (-1)	100 (1)	107,7	84,0
3	5 (-1)	350 (1)	40 (-1)	135,2	111,5
4	5 (-1)	350 (1)	100 (1)	132,3	117,3
5	15 (1)	250 (-1)	40 (-1)	211,5	211,5
6	15 (1)	250 (-1)	100 (1)	54,1	81,4
7	15 (1)	350 (1)	40 (-1)	211,1	238,5
8	15 (1)	350 (1)	100 (1)	108,1	95,5
9	18,4 (1,68)	300 (0)	70 (0)	211,5	190,2
10	1,6 (-1,68)	300 (0)	70 (0)	53,9	69,9
11	10 (0)	384,1 (1,68)	70 (0)	153,8	132,6
12	10 (0)	215,2 (-1,68)	70 (0)	151,5	167,6
13	10 (0)	300 (0)	120,4 (1,68)	38,3	67,2
14	10 (0)	300 (0)	19,5(-1,68)	206,5	172,1
15	10 (0)	300 (0)	70 (0)	182,6	183,0
16	10 (0)	300 (0)	70 (0)	182,6	183,0

The regression model derived from RSM is expressed as:

$$\begin{aligned} Storage\ Capacity = {} & 183 - 35.7A + 10.4B + 31.1C + 1.4\,AB - 37.2\,AC \\ & - 4.8BC - 18.7A^2 - 11.6\,B^2 - 22.3C^2 \end{aligned} \tag{8}$$

This quadratic equation meaningfully represents the nonlinear effects of injection parameters and storage capacity. The negative coefficients of the quadratic terms (A2, B2, C2) imply a decreasing efficiency at rates higher than optimum when injection rate or temperatures are too high and gas mobility will be increased resulting in less retention due to low solubility. The AB term is positive, suggested a synergistic effect on CO_2 storage when both injection rate and pressure are increased in the same range.

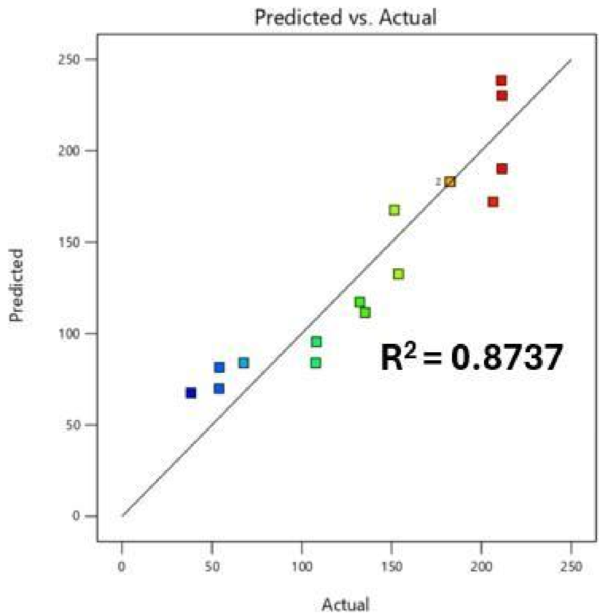

Fig. 1. Normal probability plot on CO_2 storage capacity based on the RSM.

Figure 1 shows the comparison between storage capacity actual and predicted storage capacities of the model with a good performance (R^2 = 0.8737). This value verified statistical analysis results, nearly twenty-eight seven percent of the variance in CO_2 retention capacity was explained by the regression model which was good correlation between numerical simulations and response surface prediction values. The points are tightly clustered along the diagonal line, implying very little discrepancy between predicted and observed values.

3.2 Respond surface methodology (RSM)

The response surface methodology (RSM) was utilized to find the best process conditions of CO_2 injection by correlating the main process factors: inlet temperature (C), outlet pressure (B) and injection rate (A) with the capture amount. This interaction among these three parameters is shown in Fig.2. The relationship between injection rate and inlet temperature is a lower injection rate enhances storage ability better for intermediate to low temperatures. This observation is consistent with thermodynamic expectations, as the higher temperature puts CO_2 into a more supercritical like state with greater density and thus favoring dissolution in brine.

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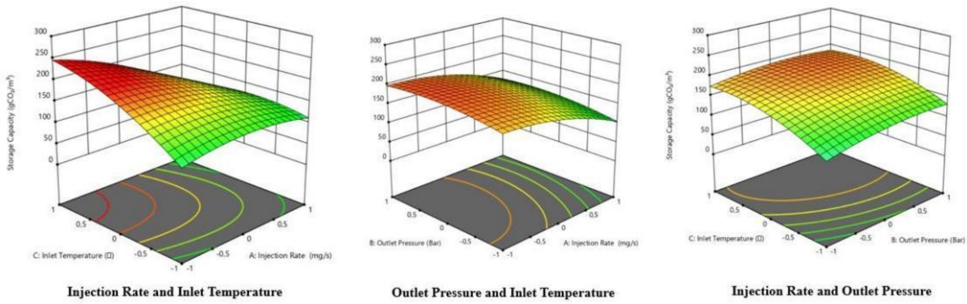

Fig. 2. Contour plot on CO_2-storage capacity based on the RSM.

3.3 Optimal CO_2 injection operational condition

The optimal operational conditions of CO_2 injection were obtained by the Design Expert, as presented in Fig. 3. The optimization aimed at maximizing CO_2 storage capacity with respect to injection rate, inlet temperature and outlet pressure. The ideal operating conditions corresponded to a feed rate of 7.89 mg/s, an inlet temperature of 93.61 °C and an outlet pressure of 284.55 bar at which the maximum modelled storage capacity reached up to 214.73 g CO_2/m^3. These results demonstrate that the optimized parameters from RSM offer an effective combination for enhancing CO_2 storage performance, consistent with the numerical simulation trends where temperature, pressure, and flow rate interactively impact the overall storage capacity.

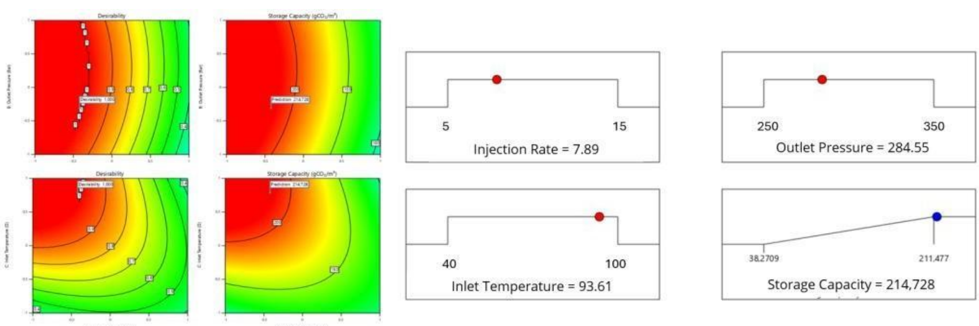

Fig. 3. Optimize condition plot on CO_2-storage capacity based on the RSM.

4 Conclusion

The results show that CO_2 storage performance in porous media is greatly affected by the interaction between injection rate, inlet temperature, and outlet pressure. The quadratic regression model created using response surface methodology (RSM) accurately captures these relationships, as demonstrated by an R^2 value of 0.8737, confirming good agreement between simulated and predicted data. Optimal injection parameters were found at 7.89 mg/s, 93.61 °C, and 284.55 bar, resulting in a maximum predicted storage capacity of 214.7 g CO_2/m^3. This indicates that a balanced combination of moderate-to-high temperature and injection rate under high pressure enhances CO_2 solubility and storage efficiency. Overall, combining CFD-based simulation with RSM offers a dependable framework for optimizing CO_2 injection conditions to maximize storage capacity while ensuring operational safety and system stability.

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A.J.A.N – CFD simulation, RSM modeling, result interpretation, writing, and editing.
A.I.A.W. – data curation, simulation insights, critical review of the manuscript.
R.P.A. – experimental design support, supervision & verification, methodological guidance.
G.W. – conceptualization, supervision, project administration

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