**Title:** **Utilisation of Artificial Intelligence based Time-Series Prediction to validate Carbon Containment in Injection Well in Illinois Basin**

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**Abstract:**

This paper focuses on using time series injection data and monitoring information to predict changes in injection rates for the carbon sequestration well. The data we have used comes from the Illinois Basin - Decatur Project, a pilot CO2 project that demonstrated the practical feasibility of storing CO2 underground. The injection spanned three years, during which nearly 999,215 tonnes of CO2 was stored. Data was recorded across a pair of wells equipped with sensors to track pressure and temperature at various depths.

We perform the prediction using Long Short-Term Memory (LSTM) neural networks (NN). These changes, represented as deltas (Δ or inj\_diff) in injection rates between time t and time (t-1), are crucial indicators of carbon containment within the well. By correlating these rate changes with other well parameters, this approach serves as a checkpoint against unwanted and unexpected carbon containment breaches or downhole losses during the injection process.

Our work aims to show that machine learning methods can be useful to forecast these injection rate deltas based on monitoring data, thereby providing a way that is complimentary to traditional methods, to determine the effectiveness of carbon containment during injection.

**One-Sentence Summary:** Applying machine learning and predictive analytics via time series injection information and monitoring data on a carbon sequestration well to predict well injection rate deltas.

**Keywords (minimum 6):** low-carbon, time-series, neural network, LSTM, carbon capture, injection pressure, monitoring, migration

# Introduction

The burning of coal, oil, and natural gas has resulted in the generation of various greenhouse gases such as carbon dioxide (CO2), methane (CH4) and nitrous oxide (N2O) [1]. A report generated Liu et al revealed that global CO2 emissions for 2022 reached 36.1 GtCO2 [2]. Failure to effectively manage such substantial quantities will result in irreversible environmental consequences.

Carbon Capture Utilisation and Storage (CCUS) is one promising method to deal with the produced CO2 from anthropogenic sources. The idea is to capture CO2 from an emission point source and subsequent sequester it via injection into a suitable geological formation, with the explicit aim to store the CO2 safely, in a state of permanence. CCUS is now being viewed as a key technology that will assist us in reaching increasingly ambitious global anthropogenic climate change goals. Typically, CO2 geologic storage can be carried out in a number of different ways, including Enhanced Oil Recovery (EOR) processes, injection into virgin saline aquifers or into depleted oil and gas fields. These methods all have different project drivers, risks, and commercial implications. However, what these three methods have in common is the requirement that (a) there be a good understanding of the subsurface geological properties and (b) there be some ability to monitor and even predict CO2 containment behaviour at the well scale, be it during the injection phase or during the shut-in phase.

## The importance of real-time CO2 containment monitoring in the subsurface

Evaluating CO2 containment is a multiscale challenge, with measurement scales spanning orders of magnitude, from kilometres to nanometres. At the reservoir (kilometres to meters) scale, satellite-based remote sensing, 4D seismic monitoring, tiltmeters, downhole sensors and tracers deployed within injection wells can offer precise data on CO2 distribution. At the centimetre to nanometre scale, geochemical monitoring of produced fluids provides insights into CO2 interactions with subsurface formations. The intermediate scale (meters to centimetre) is where conventional “well-based” measurements are conducted. These include the monitoring of CO2 injection rates, well (annulus) pressures, casing pressure tests, and cased hole/production logging measurements. This enables a real-time assessment of CO2 injection efficiency and potential leakage.



There have been documented instances where the abovementioned techniques have worked well in CO2 containment monitoring. One example is the Equinor operated Sleipner Project in the North Sea where the operator utilised seismic surveys and downhole pressure measurements to demonstrate effective containment [4]. Yet, there are also documented instances where, despite extensive monitoring efforts, unexpected CO2 leakage behaviour does occur. The In Salah project in Algeria, led by BP, Statoil, and Sonatrach, is one such example [5]. The latter underscores the importance of continual vigilance and timely adaptive management in CO2 containment to mitigate risks effectively.

The above examples illustrate that it is sometimes not enough to rely solely on hardware based solutions like sensor measurements at the monitoring well. Rather, we postulate that subtle fluctuations in injection rates can act as a predicators for potential future containment breaches. By training a machine learning model to recognise these subtle fluctuations, potential containment breaches can be flagged prior to them occurring. If the model triggers in such events, the operator would simply need to shut the well in and investigate, for risk mitigation purposes.

## The Significance and Complexity of Optimising CO2 Injection Rates

Achieving optimised CO2 injection involves maximizing the rate and volume of CO2 while ensuring it remains in a supercritical state, thereby minimising phase transitions, vaporisation, and hydrate formation from the wellhead to the injection point. This necessitates meticulous consideration of three primary parameters: reservoir heterogeneity, pressure, and time.

Reservoir heterogeneity, encompassing permeability, porosity, and lithology, significantly influences injection rates. High-permeability formations facilitate rapid CO2 flow, while geological features such as layering, faults, and fractures can both enhance CO2 distribution and affect injection rates. Injecting CO2 too rapidly can induce skin effects, diminishing overall field injectivity. Moreover, reservoir pressure, inversely correlated with the volume of CO2 injected, must be carefully managed to prevent overfilling, which can lead to seismic activity and potential CO2 containment breach.



In essence, comprehending the intricate interplay between reservoir capacity and injection parameters is imperative for ensuring the efficiency and safety of CO2 sequestration endeavours. This understanding extends to recognising the temporal dynamics of CO2 injectivity and its relationship with various influencing factors over time. Through the analysis of historical CO2 injectivity data and its correlation with time-sensitive parameters, engineers can refine reservoir management strategies via modeling and scenario analysis. This approach allows for informed decision-making regarding CO2 storage and utilisation projects, ultimately advancing the efficacy and sustainability of carbon capture and storage initiatives.

# Literature Review

Various authors have tried numerous methods to forecast based on historical data. Work by De Gooijer and Hyndman [6], for instance, reviewed a series of time-series forecast models over a 25-year period, from 1985 to 2005. Their review highlighted various models being developed and applied in a myriad of scenarios related to finance, statistics and manufacturing, and included methods such as (a) exponential smoothing [7, 8], (b) Autoregressive Integrated Moving Average (ARIMA) [9], (c) seasonal models [10], (d) state space and structural models and the Kalman filter [11], (e) nonlinear models [12], (f) long-range dependence models, including the family of Autoregressive Fractionally Integrated Moving Average (ARFIMA) models [13], (g) Autoregressive Conditional Heteroskedasticity/Generalized Autoregressive Conditional Heteroskedasticity (ARCH/GARCH) models [14], and (h) count data forecasting [15].

Within reservoir engineering, the extrapolation of hydrocarbon and water recovery rates from geological formations into the future can be viewed as a type of time-series forecasting. Empirical solutions developed by Arps [16], referred to as decline curve analysis (DCA) technique is one of the earliest methods to address this problem. The method is based on a curve-fit principle, where one would attempt to fit either exponential, hyperbolic or harmonic curve to historical flow production rate as a function of time. Equation 1 shows the general form of the equation, while Equation 2 and Equation 3 are more specialised forms of the equation:

|  |  |  |
| --- | --- | --- |
| General Form (Hyperbolic Decline) |  | Equation 1 |
| Exponential Decline |  | Equation 2 |
| Harmonic Decline |  | Equation 3 |

where qt is the flow rate at time t (bbls/day), qi is the initial flow rate (bbls/day), t is time (day), Di is the initial decline rate (%), and b is the degree of curvature of the line (Arps’ decline-curve exponent). A hyperbolic curve would have 0 < b < 1 and a harmonic curve would have b = 1. The fitted curve is then used to predict future production rates and cumulative production [17]. This method was originally designed to work with high porosity-permeability reservoirs and tends to overestimate hydrocarbon recovery from unconventional (low permeability) reservoirs. Thus, various authors have tried to expand on this work [18, 19, 20, 21], and are mostly variations of the initial DCA method developed by Arps. For an effective DCA forecast, domain and field knowledge are key, but inherently the process is one of trial and error, and thus it is not uncommon for DCA results to have ‘low-best-high’ estimates.

With the advent of big data, fast computing and cheap memory, applying a machine learning (ML) and artificial intelligence (AI) solution for time-series forecasting seems a natural evolution. ML solutions were first introduced to the petroleum industry in the early 2000s. Applications of ML and AI include addressing prediction of reservoir parameters [22], history matching, of oil, gas and water production forecasting (flow rate prediction), pattern recognition in well logs and well tests analysis, production enhancement and prediction of failures, among others [23, 24, 25].

ML algorithms have been used to predict carbon emissions [23], leakage [24], CO2 absorption and adsorption [25], property prediction and process simulation [26], simulation of transportation, and geological behaviours as it relates to uncertainty analysis, sequestration, utilisation and EOR processes [26, 27, 28]. In the field of CCUS and well performance, work by Iskander et al [29] employs Long Short-Term Memory (LSTM) networks to forecast oil, water and CO2 production at future infill well locations, for both single phase and 3-phase fluid models. Data were in the form of a synthetic PUNQ-S3 reservoir model, combined with real-world observations from 8 production wells, which recorded daily production volumes over a decade from 2004-2014 [29]. Injection data from CO2 wells was not a direct input in the deep learning model, although it did play an indirect role in the oil and gas production data being recorded, as it swept the residual hydrocarbons and therefore resulted in an uplift in production rates.

We aim to develop on the work of Iskander and others by utilising ML and AI methods, and in particular LSTM, but focusing on the prediction of CCUS injection well performance, using the open-source information from the IBDP (Illinois Basin - Decatur Project) [3]. We will demonstrate how our developed LSTM model shows a correlation between the change in injection rate to the behaviour of other dynamic parameters [29].

One of the objectives of the model is to detect anomalies and alert operators to closely inspect the wells for potential leaks. While still adhering to local jurisdictional requirements of well annulus pressure monitoring, periodic pressure tests and cased hole logging, a ML model can be an additional method utilised to detect unexpected carbon leaks. We also view the model as another means for engineers to perform scenario based de-risking of exploration plays, via modelling variations in well and storage parameters to validate CO2 containment. The model will also aid in the understanding of the injection process and potentially can be used to “right size” injection rates, well operations and optimise costs.

# Scope and Methods

This paper aims to use time series injection information and monitoring data on a carbon sequestration well to predict carbon sequestration well injection rates deltas (D or inj\_diff) which is the difference in the injection rate (IR) at time t and time (t-1) i.e.

|  |  |  |
| --- | --- | --- |
|  |  | Equation 4 |

Our primary source of data is from the Illinois Basin - Decatur Project, a CO2 pilot project meant to demonstrate the capacity, injectivity, and containment of carbon storage in the Mount Simon Sandstone, the main carbon storage resource in the Illinois Basin and the Midwest Region (Figure 1(L)). The source of the injected CO2 is from ethanol production at the Archer Daniels Midland company’s plant. The CO2 is compressed, dehydrated and injected into the Mt. Simon Sandstone, which is primarily a saline aquifer approximately ~7,000 ft deep. Injection began in 2009 and continued for a 3-year period (Nov-2011 to Nov-2014). Cumulatively, ~999,215 tonnes of supercritical CO2 have been injected and geologically stored. A pair of injection and verification wells, ~1007ft apart, were drilled into the formation (Figure 1(R)). The wells were equipped with downhole sensors to monitor pressure and temperature at various depths of interest.

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Figure 1: (L) Location map of the Illinois Basin – Decatur Project (IBDP). (R) Schematic illustration of the formation layers, location of perforation intervals in the CCS1 injector well (green cylinders) and the location of the verification well (VW1). Image taken from [3]

## Datasets

During this three-year period, a substantial amount of data was collected from both an injection and monitoring well, 1007 ft apart. The injection well was drilled to a total depth (TD) of ~7238 ft, and was drilled with a 26” bit to 355 ft, and cased with a 20” casing to surface. A 17 ½” hole size then followed to a TD of 5339 ft, and an intermediate casing string 13 3/8” in diameter was set. The reservoir section was drilled in a 12 ½” hole size to ~ 7056 ft and completed with a 9 5/8” production casing and 4 ½” tubing. The perforations were made at the base (i.e. above the Precambrian) Mt. Simon Sandstone, which was a relatively thick reservoir of ~1620 ft. A total of 3 geophones were set at 4925 ft, 5743 ft and 6137 ft along with a pressure / temperature gauge mandrel at 6325 ft. The monitor well was drilled to a total TD of 7272 ft; it had a surface casing (13 3/8” to 377 ft, followed by intermediate casing of 9 5/8” to 5322 ft and 5 ½” casing across the Mt. St Simon Sandstone, which contained a 3 component geophone array) [3].

1. *Data Collection and Preparation*

A total of 34 parameters were measured from the injection and verification well. The parameters measured comprised of both surface and downhole measurements which were acquired at five second intervals over three full years. The sheer volume of data required that the time scale be downscaled to hourly intervals, taking the parameter average over the hour. 27,665 hours of data (training data) was used to build a suitable model. 67% of the “training” data set was used to train the model. The remaining 33% was used as a “validation” dataset. The model built off this data was finally used to predict 201 hours of D into the future (“hold out” data). Given in Table 1 is the descriptive statistics of the provided data; we refer readers to the nomenclature table for the definition of the variables. We note that there are a series of “null values” (including negative null values) and non-numeric numbers, missing rows, time gaps and note that for some of the input data measurements, there are significant outliers.

**Table 1:** Data Statistics

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Measurement | Non-Zero  Value | Mean Value | Standard Deviation | Minimum Value | 25th  Percentile | Median Value | 75th  Percentile | Maximum Value |
| Avg\_PLT\_CO2VentRate\_TPH | 27398.0 | 2.1 | 133.2 | 0.0 | 0.0 | 0.1 | 0.2 | 18333.2 |
| Avg\_CCS1\_WHCO2InjPs\_psi | 27270.0 | 1239.9 | 817.7 | 0.0 | 1235.5 | 1338.9 | 1361.0 | 39032.4 |
| Avg\_CCS1\_WHCO2InjTp\_F | 27398.0 | 89.8 | 48.3 | 0.0 | 93.0 | 96.3 | 96.9 | 2879.4 |
| Avg\_CCS1\_ANPs\_psi | 27304.0 | 560.9 | 445.9 | 0.0 | 523.5 | 564.9 | 604.8 | 24105.6 |
| Avg\_CCS1\_DH6325Ps\_psi | 27398.0 | 3244.2 | 173.5 | 0.0 | 3233.0 | 3286.1 | 3324.7 | 3515.9 |
| Avg\_CCS1\_DH6325Tp\_F | 27398.0 | 127.7 | 7.2 | 0.0 | 127.2 | 130.1 | 131.1 | 135.7 |
| Avg\_VW1\_WBTbgPs\_psi | 26127.0 | 1801.8 | 999.4 | 0.0 | 2173.5 | 2322.4 | 2379.8 | 4954.7 |
| Avg\_VW1\_WBTbgTp\_F | 26061.0 | 80.8 | 44.3 | 0.0 | 103.4 | 104.2 | 105.0 | 120.1 |
| Avg\_VW1\_ANPs\_psi | 23487.0 | 525.0 | 3988.7 | 0.0 | 0.5 | 4.7 | 16.9 | 31993.5 |
| Avg\_VW1\_Z11D4917Ps\_psi | 26688.0 | 1597.5 | 873.3 | 0.0 | 2070.3 | 2073.4 | 2074.1 | 2378.0 |
| Avg\_VW1\_Z11D4917Tp\_F | 26709.0 | 81.7 | 44.2 | 0.0 | 103.7 | 105.2 | 106.5 | 108.6 |
| Avg\_VW1\_Z10D5001Ps\_psi | 26688.0 | 1627.9 | 889.9 | 0.0 | 2106.9 | 2112.4 | 2116.6 | 2420.6 |
| Avg\_VW1\_Z10D5001Tp\_F | 26709.0 | 81.2 | 44.0 | 0.0 | 101.8 | 104.7 | 105.0 | 110.9 |
| Avg\_VW1\_Z09D5653Ps\_psi | 26688.0 | 1961.1 | 1071.9 | 0.0 | 2534.0 | 2547.5 | 2551.1 | 2785.4 |
| Avg\_VW1\_Z09D5653Tp\_F | 26709.0 | 87.4 | 47.3 | 0.0 | 111.5 | 112.8 | 113.5 | 114.9 |
| Avg\_VW1\_Z08D5840Ps\_psi | 26189.0 | 1604.8 | 1289.3 | 0.0 | 0.0 | 2627.3 | 2637.4 | 4446.2 |
| Avg\_VW1\_Z08D5840Tp\_F | 25878.0 | 69.0 | 56.4 | 0.0 | 0.0 | 114.0 | 115.0 | 353.2 |
| Avg\_VW1\_Z07D6416Ps\_psi | 25985.0 | 2199.2 | 1273.0 | 0.0 | 0.0 | 2911.6 | 2925.3 | 3195.0 |
| Avg\_VW1\_Z07D6416Tp\_F | 25985.0 | 88.8 | 50.8 | 0.0 | 116.5 | 116.9 | 118.6 | 145.1 |
| Avg\_VW1\_Z06D6632Ps\_psi | 25500.0 | 2315.6 | 1308.6 | 0.0 | 3012.2 | 3026.1 | 3031.3 | 3380.4 |
| Avg\_VW1\_Z06D6632Tp\_F | 25500.0 | 90.9 | 50.8 | 0.0 | 116.6 | 118.6 | 119.4 | 124.3 |
| Avg\_VW1\_Z05D6720Ps\_psi | 23955.0 | 2106.0 | 1447.2 | 0.0 | 0.0 | 3069.6 | 3073.6 | 3365.9 |
| Avg\_VW1\_Z05D6720Tp\_F | 23955.0 | 82.3 | 55.0 | 0.0 | 0.0 | 118.5 | 119.4 | 122.1 |
| Avg\_VW1\_Z04D6837Ps\_psi | 26600.0 | 2347.5 | 1369.0 | 0.0 | 0.0 | 3148.0 | 3153.5 | 3331.9 |
| Avg\_VW1\_Z04D6837Tp\_F | 26600.0 | 91.0 | 51.6 | 0.0 | 118.8 | 119.5 | 119.9 | 125.8 |
| Avg\_VW1\_Z03D6945Ps\_psi | 24361.0 | 2350.9 | 1495.7 | 0.0 | 0.0 | 3299.9 | 3320.6 | 3457.9 |
| Avg\_VW1\_Z03D6945Tp\_F | 25932.0 | 182.3 | 368.5 | 0.0 | 0.0 | 121.3 | 122.8 | 1602.9 |
| Avg\_VW1\_Z02D6982Ps\_psi | 26423.0 | 2456.6 | 1459.1 | 0.0 | 0.0 | 3316.2 | 3332.0 | 3499.6 |
| Avg\_VW1\_Z02D6982Tp\_F | 26423.0 | 91.3 | 52.7 | 0.0 | 32.0 | 121.3 | 122.0 | 124.3 |
| Avg\_VW1\_Z01D7061Ps\_psi | 25307.0 | 2300.2 | 1521.4 | 0.0 | 0.0 | 3318.2 | 3327.3 | 3445.1 |
| Avg\_VW1\_Z01D7061Tp\_F | 25108.0 | 85.9 | 55.4 | 0.0 | 0.0 | 121.4 | 122.6 | 133.9 |
| Avg\_VW1\_Z0910D5482Ps\_psi | 26709.0 | 1855.6 | 1017.6 | 0.0 | 2353.3 | 2374.9 | 2416.1 | 2758.3 |
| Avg\_VW1\_Z0910D5482Tp\_F | 26709.0 | 86.3 | 46.7 | 0.0 | 110.5 | 111.5 | 112.0 | 113.7 |
| inj\_diff | 27397.0 | 0.0 | 82.7 | -11021.1 | -0.1 | 0.0 | 0.1 | 7033.5 |

1. *Cleaning Data*

We reviewed the attributes for the data, and were especially concerned about discontinues, non-numerical data or data that were clearly outliers (e.g. ~25,000 psi WHP at injection well or 0 psi downhole gauge pressure). We utilised 4 methods to clean the data, in order of operation (i) we firstly performed a computational fill of all the missing and null values with a “forward fill’ operation, with the last valid observation being propagated forward. We do this on the assumption that missing values retain the properties of the previous cell i.e. there has been no change in the data between time *t* and time (*t-1*), (ii) a Z-score method where

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| --- | --- | --- |
|  |  | Equation 5 |

xi is a single data value, is the median of the data set and MAD is the median absolute deviation of the dataset, (iii) removing values of formation pressure that we know to be technically invalid and (iv) a final visual check of the data, removing outliers that we view as being deleterious to the interpretation. Shown in Figure 2 is an example of the impact that data cleaning has on the data quality. We see that our process has removed spikiness in the data and smoothed out some of the small-scale perturbations, resulting in a more manageable dynamic range.

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Figure 2: An example of the measurement before (lower image) and after (upper image) data cleaning.

1. *Machine Leaning Model Selection - Long Short-Term Memory (LSTM) vs. Autoregressive Integrated Moving Average (ARIMA)*

In the choice of ML model to apply, we had to decide between a statistical approach based on ARIMA, or alternatively, the use of a non-linear algorithm such as neural networks (NN). Many authors have investigated comparing such methods and in various fields. What we noted from our review of the work was there was a general agreement that approaches like ARIMA would not only require less inputs, but would be less of a “black-box”, which NNs are known to be [30, 31, 32].

ARIMA has been applied by previous authors to forecast oil production data [33]. The “autoregressive” piece of ARIMA deals with finding a correlation between a specific value and a prior/lagged value, essentially seeing if a variable has any correlation to its past values. The “integrated” piece deals with making data stationary, essentially ensuring that properties of the data (such as mean and variance), are constant over time. The “moving average” piece of the model finds the dependency between a specific value, and the error from a moving average model applied to previous values. ARIMA models are therefore useful in forecasting time series data and are especially useful when trying to predict time series data that is non-stationary. While Ning et al observed that ARIMA was robust in predicting rates of oil production across wells, our review of ARIMA models being produced with high frequency data, where accuracy on an hourly basis was important, found that the error rate compounds significantly when the forecasting horizon is extended beyond a day [34].

LSTM is a type of recurrent NN which uses useful patterns from sequential data to provide accurate forecasts [23]. It learns from previous outputs to provide better results the following time. A typical LSTM has 3 layers (i) an input gate which assigns weights based on the significance of different variables, (ii) a forget gate to retain only useful information, and (iii) an output gate which manages the information flow. LSTM holds a memory cell (known as a cell state) which retains captured information over longer time periods and preserves useful constituents using its input and forget gates, hence avoiding the vanishing gradient issue associated with traditional NNs. LSTMs are particularly useful for non-linear problems where there does not appear to be strict mathematical relationships between variables. Unlike recurrent NNs, LSTMs can account for long-term temporal effects without encountering optimisation hurdles like vanishing gradients [35]. In our review of LSTM vs ARIMA models, we have found a common consensus in various fields that LSTM performed better, with reduced error rates but with significantly increased processing time [32, 31].

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Figure 3: Schematic of LSTM network

We settled on the choice of LSTM because we realised that the data we were analysing was likely to contain non-seasonal, high frequency information, where accuracy was going to be important [36]. Additionally, the were numerous variables provided which we did not know the relative importance of in prediction without a working model.

1. *Model Performance and Hyperparameter Optimization*

We access the model performance using a host of measures, from training and validation loss to mean absolute error (MAE - Equation 6), mean squared error (MSE - Equation 7), root mean squared error (RMSE - Equation 8) and the coefficient of determination (R2 - Equation 9). The training and validation loss functions serve to determine how well the model is performing and to prevent overfitting. During training, the model learns by iteratively adjusting its parameters to minimize a defined loss function. The training loss measures the discrepancy between the model's predictions and the actual target values on the training data. The goal is the minimization of this loss, as it indicates how well the model is fitting the training data. The validation loss is the other component of this and is computed by evaluating the model's performance on a separate validation dataset, not used for training. It serves as an estimate of how well the model generalizes to unseen data.

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| --- | --- | --- |
| MAE: |  | Equation 6 |
| MSE: |  | Equation 7 |
| RMSE: |  | Equation 8 |
| R2: |  | Equation 9 |

Equation 6 to Equation 9 show the other measurement metrics, with yi as the predicted value, xi as the true value, as the mean of xi and n as the total number of data points. MAE measures the average absolute difference between the predicted and actual values and provides an absolute measure of the model's performance. MSE measures the average squared difference between the predicted and actual values and amplifies larger errors due to the squaring operation. RMSE is the square root of MSE and provides a measure of the average magnitude of errors. It is useful for interpreting errors in the same units as the target variable. R2 measures the proportion of the variance in the target variable that is explained by the model. It ranges from 0 to 1, where 1 indicates a perfect fit and 0 indicates a poor fit.

While MAE, MSE, RMSE, and R2 are evaluation metrics used to assess the model's performance after training, the (training and validation) loss functions are specific to the training process. These loss functions guide the model's learning by providing gradients for updating the model's parameters. However, the suitability of the model is ultimately guided by scores where the MAE, MSE and RMSE and low, while the R2 is high.

The NN model is tuned by varying a series of “hyperparameters”. A hyperparameter is a characteristic of a model that is external to the model and whose value cannot be estimated from data. The hyperparameters that were optimized included the (i) learning rate, (ii) the epochs, (iii) the number of neurons, (iv) the magnitude of dropout, (v) batch size, (vi) the choice of optimiser and finally (vii) the choice of activation function. To account for idiosyncrasies in the data (noise, patterns, outliers, etc.), k-fold cross-validation was run to validate the stability of the model.

# Results and Discussion

## Data Preparation

We observed significant collinearity of > 0.8 across most of the data set. Most were paired couplet measurements of “Temperature” and “Pressure” at various gauge depths. Keeping both parameters adds no additional information to the predictive model and in fact may be detrimental, with potential overfitting. Therefore, a single element from each of the variable pairs is eliminated to allow for a more stable model. Exceptions were made if variables were found to be from different sources e.g. tubing and reservoir pressure at the observation well for instance. This is also in line with conventional reservoir engineering concepts where temperature and pressure are correlated.

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Figure 4: Correlation Matrix – Pairwise Correlation. It ranges from -1 to 1, -1 being a perfect negative correlation and +1 being a perfect positive correlation. The color scale visually depicts this: dark/warm show strong correlations

Excluding the target injection delta variable, eight variables were retained for the machine learning application and are summarised in Table 2 for the entire dataset. All data is numerical data types. The total data size is 27,665 values per column, for a total of 248,784 data points which was approximately ~26% of the original data base.

Table 2: Statistics of the cleaned dataset

|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| Measurement | Non-Zero  Value | Mean Value | Standard Deviation | Minimum Value | 25th  Percentile | Median Value | | 75th  Percentile | Maximum Value |
| Avg\_PLT\_CO2VentRate\_TPH | 27,665 | 1.015 | 3.94 | 0 | 0 | 0.06 | | 0.15 | 60 |
| Avg\_CCS1\_WHCO2InjPs\_psi | 27,665 | 1253 | 191 | 701 | 1233 | 1339 | | 1361 | 1882 |
| Avg\_CCS1\_WHCO2InjTp\_F | 27,665 | 91 | 12 | 59 | 93 | 96 | 97 | | 120 |
| Avg\_CCS1\_ANPs\_psi | 27,665 | 554 | 102 | 149 | 523 | 565 | | 605 | 977 |
| Avg\_CCS1\_DH6325Ps\_psi | 27,665 | 3254 | 106 | 3006 | 3234 | 3286 | | 3326 | 3516 |
| Avg\_CCS1\_DH6325Tp\_F | 27,665 | 128 | 4.58 | 117 | 127 | 130 | 131 | | 136 |
| Avg\_VW1\_WBTbgPs\_psi | 27,665 | 2248 | 452 | 60 | 2233 | 2343 | | 2421 | 4817 |
| Avg\_VW1\_Z05D6720Ps\_psi | 27,665 | 3043 | 233 | 282 | 3061 | 3072 | | 3075 | 3366 |
| inj\_diff | 27,665 | 0.03 | 3.74 | -38 | -0.08 | 0 | | 0.07 | 38 |

## LSTM Model Architecture

We have employed a stacked LSTM architecture, with 2 layers, for this evaluation. In a stacked LSTM model, the output sequence of one LSTM layer serves as the input sequence for the next LSTM layer in the stack. This allows for a hierarchical representation of the input data, with each LSTM layer capturing different levels of abstraction or temporal dependencies. The second layer of the stacked model feeds the results to the output layer. We also use dropout to reduce the risk associated with overfitting. Finally, there is a dense layer which predicts the output, a single timestep at a time.

We tested the performance of the model by varying the hyperparameters given in Table 3. We utilised K-fold cross validation for hyper parameter tuning, ensuring that we kept the time series harmony. By this, what we mean is we split the time series sequence into samples but retained the sequence of information. With each split, a model is trained using (k-1) folds of the training data. The model is then validated against the remaining fold. A final model is scored on the held-out fold, with scores averaged across the splits. We used this to refine our hyperparameters, and finally took an average of values you see in Table 3.

Each hyperparameter serves a specific purpose and it is fundamentally an iterative process to tune these parameters such that the model outputs are optimised. We broadly define each hyperparameter here, sharing more details in Table 3. The same table also shows our final selected values based on an optimised MSE value.

The learning rate refers to the model’s degree of responsiveness to errors. Epochs refer to the number of iterations across the entire dataset, while neurons are the fundamental nodes/building blocks used to process inputs. Dropout refers to the proportion of randomly selected neurons which get deactivated (to prevent overfitting) and batch size addresses the quantity of inputs processed before updating the model. An optimiser algorithm is needed to minimize the loss function, by finding the optimal set of parameter values that lead to improved network performance. Finally, the activation function is a mathematical function which introduces non-linearity to the layer of neurons.

Table 3: Variation in Hyperparameter Values, Final Selected Values and Parameter descriptor

|  |  |  |  |  |
| --- | --- | --- | --- | --- |
| Measure | Minimum | Maximum | Final | Parameter Descriptor |
| Learning Rate (lr) | 0.001 | 0.1 | 0.01 | The rate at which the parameters (weights and biases) of the network are updated during the training process. It essentially controls how quickly or slowly the network learns from the gradients of the loss function. |
| Epochs | 10 | 100 | 50 | This parameter determines how many times the learning algorithm will iterate over the entire training dataset. Each iteration has the following steps (a) forward propagation, (b) loss computation, (c) backpropagation, and (d) update. These steps are repeated in the training dataset until all samples have been processed. This completes one epoch. |
| Neurons | 10 | 50 | 20 | Each neuron takes multiple inputs, performs a computation on those inputs, and produces an output. The computation typically involves applying a weighted sum of the inputs, followed by the application of an activation function. |
| Dropout | 0.1 | 0.25 | 0.25 | This parameter introduces noise or randomness into the network by temporarily removing a portion of the neurons from the calculation in each training iteration. By doing so, dropout prevents complex co-adaptations between neurons, reducing the reliance of the network on specific neurons and promoting the learning of more robust and generalized representations. |
| Batch Size | 30 | 100 | 50 | This parameter refers to the number of training examples that are processed together in a single forward and backward pass during training. |
| Optimiser | - | - | Adam | ADAM (Adaptive Moment Estimation) is an optimization algorithm used to update the weights of neural networks during the training process. It automatically adjusts the learning rate for each parameter based on the history of gradients. This was chosen as the default optimizer as it has the ability to converge quickly as well |
| Activation | - | - | tanh | The hyperbolic tangent function maps the input to a value between -1 and 1. It has an S-shaped curve like the sigmoid function but is symmetric around the origin. The formula for tanh is: |

Figure 5 shows the MSE output of the training (train) and validation (val) sets for one of our K-folds. MSE is on the y-axis and epoch is on the x-axis. We observe the convergence between train and val, telling us that the model accuracy is improving per epoch. The point of convergence is arrived at by gradient descent and tells us the point of minimum information loss. In this example, we achieved convergence at around epoch = 30, with losses increasing beyond that.

A graph showing the number of the same model

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Description automatically generated with medium confidence



Figure 5: (Upper) MSE output of the training and validation set (Lower) Check file of a small subset of data; output from the K-fold set.

## Prediction on Validation Data

We deployed our developed model on our validation data. Given in Figure 6 is the comparison between the predicted injection rate deltas versus the actual injection rate deltas in our validation set. The results demonstrate the model's capability to successfully identify and replicate actual anomalies, which provides evidence that the model is predictive in nature. Moreover, Figure 6 illustrates that the model can accurately capture both large scale high frequency signal, as well as smaller scale fluctuations in the injection deltas (admittedly, the subtle variations are harder to capture as these change at ranges of ± 1psi and can be described to be in the domain of “noise”), indicating the robustness of the LSTM model.

The fact that the model can capture both large and small-scale measures strengthen our view that the model is indeed reliable in handling the variety of conditions experienced in the field during CO2 injection, and hints at its ability to effectively mimic the intricate patterns found within field injection rate data. The successful reproduction of significant anomalies as well as subtle variations highlights the model's potential to provide valuable insights and reliable predictions in this domain.

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Figure 6: (Upper) Able to match anomalies in injection delta (Lower) Able to mimic the small variations in the injection delta.

## Generalising the model

This LSTM model was built from (what is fundamentally) a single data set i.e. from a specific geological rock type, whose CO2 flow behaviour is constrained by its own petrophysical and reservoir engineering properties. We think further generalisation of the model is necessary to truly confirm these findings. As we do not have data from other geological settings, we attempted generalisation through a series of sensitivity runs. We did this in 2 ways (a) selecting a single seed value but varying the input parameters fed into the model and (b) by randomising the seed value itself but keeping the input parameters constant.

### Single Seed, Variable Inputs

We used a single seed value (2250) but varied six of the selected as a test for model generalisation. Our first iteration (Run 1 in Table 4) is with a default hyperparameter setting, where the predicted injection delta is zero for all test timesteps; this yielded an RMSE value of 5.54 (Run 1 in Table 5).

Several adjustments were made to the inputs from that base case defined in run 1. These modifications included (a) scaling all columns within a range of -1 to 1 (runs 2 to 6), (b) replacing, as one of the input variables, the VW DH Z09 sensor with the VW DH Z05 sensor (runs 4 to 6), (c) incorporating well head pressure (WHP) sensor data (runs 2 to 4, run 6), (d) using temperature sensor data (runs 5 and 6), (e) increasing the Z-score band for the target column from 20 to 25 (runs 3 to 6), and (f) utilizing corrected values of zero for the VW DH sensor (runs 3 to 6).

By analysing the results of these runs and comparing them to the base and default settings, it is possible to determine the most optimal configuration that yields improved accuracy and reliability in predicting injection deltas. This series of sensitivity runs showed us that the model performs most optimally based on the configuration in run 6. It additionally tells us that the model is sensitive to scaling, and our Z-score tolerance bands.

Table 4: Inputs to test for the effect of randomness in the model

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Varied  Parameter | Run 1  (Base Case) | Run 2 | Run 3 | Run 4 | Run 5 | Run 6  (Final Model) |
| Scaling | N | Y (0,1) | Y (-1,1) | Y (-1,1) | Y (-1,1) | Y (-1,1) |
| VW DH Sensor | NA | Z01 | Z05 | Z05 | Z01 | Z05 |
| Injection WHP Sensor | NA | Y | Y | N | Y | Y |
| Temp Sensor | NA | N | N | Y | Y | Y |
| Z-Score Tolerance | NA | 25 | 25 | 25 | 25 | 25 |

Table 5: RMSE and R2 output values to determine if the model is accurately able to account for randomness

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| Parameter | Run 1  (Base Case) | Run 2 | Run 3 | Run 4 | Run 5 | Run 6  (Final Model) |
| Test RMSE | 5.54 | 1.82 | 1.98 | 1.50 | 1.48 | 1.49 |
| Val RMSE | NA | 2.20 | 1.90 | 2.01 | 1.71 | 1.49 |
| Val R2 | NA | 0.63 | 0.72 | 0.69 | 0.78 | 0.83 |

*Randomness*

NN themselves are not inherently stochastic, as they follow deterministic mathematical operations, and the inputs, weights, and biases are all fixed values during inference. However, the stochastic nature of the NN model becomes apparent when seed values are varied; different seed values result in different results.

Our next test for the generality of the model involved running various seed values (we utilised 10 different values) and determining if both high and low amplitude delta values could be predicted. Seven selected results are displayed in Table 6 while Figure 7 to show the range of comparison with respect to the first unseeded run.

We observe that while all runs can predict the anomalies, the signature of the minor differences varies between seed values (Table 6). We also observe that the RMSE and R2 values on the validation set all lie within a small range (±10% or up to 0.2 psi absolute) of the unseeded value (Figure 7). Thus, to account for randomness and to retain the unbiased nature of the model, an unseeded model is selected for deployment.

Table 6: RMSE and R2 value of sensitivity runs to test randomness of model

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Variables | Run 1  (Base Case) | Run 2 | Run 3 | Run 4 | Run 5 | Run 6 | Run 7 |
| Seed Value (SV) | Unseeded | 2250 | 42 | 2023 | 1 | 111 | 88 |
| Val RMSE | 1.79 | 1.55 | 1.69 | 1.69 | 1.64 | 1.87 | 1.70 |
| Val R2 | 0.83 | 0.82 | 0.78 | 0.78 | 0.79 | 0.73 | 0.78 |

|  |
| --- |
|  |

Figure 7: Injection Delta forecasts of sensitivity run to test randomness of model – all results show small perturbations around the unseeded value

*Evaluation against the “Hold-out” Data*

We test the predictive capability of the model by passing downhole sensor measurements never seen by the model (our “hold out” data set), to determine if the model can detect injection rate anomalies.

Figure 8 shows the results of this test, where our model has successfully predicated the presence of four anomalies in the injection rates. When we plot this prediction against what the actual injection rates were (our “ground truth” data), we observe a near perfect overlap in results.

We observe that for the negative injection deltas, there are corresponding decreases in injection pressure implying a decreased CO2 injection rate. The prediction data also shows corresponding increase in injection pressure during positive injection deltas, implying an increased injection rate. Corresponding changes can also be seen on the other inputs such as temperature and CO2 vent rate.

The fact that our model can predict these anomalies using measured sensor data is encouraging; as an operator who is interpreting this result, it would be prudent to firstly ask if these injection deltas are expected. If they are not, then it behoves the operator to investigate/ monitor the well to determine what sort of remedial action should be taken.

|  |
| --- |
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Figure 8: Input (blue line) and prediction (red line) on blind “hold out” dataset

# Discussion & Recommendations

We think there are several ways to further enhance the model's performance. First, incorporating the response of the operator when an anomaly is marked as safe reduces the likelihood of flagging similar anomalies in the future. This feedback loop mechanism can help refine the model's predictive accuracy and ensure more reliable results over time.

Secondly, exploring alternative methods for outlier removal, and implementing advanced techniques to identify and handle outliers effectively will improve the model's ability to identify genuine anomalies, while minimizing false positives.

Thirdly, the workflow of the model can be improved to reduce runtime. This optimization involves running multiple sets of model ensembles, and aggregating their outputs to obtain a more “generalised” model. Generalising the model can further enhance performance and provide more reliability when it comes to anomaly detection.

Lastly, we also think the results of the model need integration with other monitoring technology; 4D seismic monitoring, tiltmeters, downhole sensors, tracers deployed and geochemical monitoring are just some examples of other data sets that should be incorporated.

# Conclusion

The IBDP project involved injection of ~1000 tonnes/day of CO2 into a single well, for a three year, resulting in ~995, 215 cumulative tonnes of CO2 being injected. In view of the growing importance of CCUS in achieving climate targets, we believe the wealth of open-source time-series data from this project can be applied to derisk CCUS monitoring.

In this work, we demonstrated how an LSTM based machine learning model has been developed and implemented to predict injection deltas of active CO2 injection. We demonstrate that our predicted models do well based on RMSE and R2 scores against both the training and validation data sets. Our model was able to predict both large and small anomalies, and we demonstrated that the model is sufficiently generalised for this single input data source.

The model can detect anomalies which operators can use when determining which wells to inspect for potential leaks, especially in scenarios where multiple wells are used for injection. By passing the measured data through the model, one can determine at which well location downhole losses were observed during the injection process. The model can also help engineers to perform computational based de-risking of geological formations, by understanding how changing certain storage parameters impacts CO2 containment. The model will also aid in the understanding of the injection process and optimising well operations and costs, reducing the reliance on periodic (or ad-hoc depending on operator budget) tests like well annulus pressures, casing tests, and use of cased hole reservoir saturation tools.

We also recommended a series of improvements and model enhancements in this paper which would increase the machine learning model’s predictive ability, potentially providing operators with timely alerts for potential leaks while optimizing operational efficiency and cost-effectiveness.



# Nomenclature

|  |  |
| --- | --- |
| GHG | greenhouse gas |
| CO2 | carbon dioxide |
| CH4 | methane |
| N2O | nitrous oxide |
| EPA | Environmental Protection Agency |
| CCUS | Carbon Capture Utilisation and Storage |
| EOR | Enhanced Oil Recovery |
| D | injection rates deltas |
| IR | injection rate |
| ML | machine learning |
| ARIMA | Autoregressive Integrated Moving Average |
| ARFIMA | Autoregressive Fractionally Integrated Moving Average |
| ARCH/GARCH | Autoregressive Conditional Heteroskedasticity/ Generalized Autoregressive Conditional Heteroskedasticity |
| DCA | decline curve analysis |
| qi | initial rate (bbls/day) |
| Di | initial decline rate (units) |
| b | degree of curvature of the line |
| AI | artificial intelligence |
| LSTM | Long Short-Term Memory |
| IBDP | Illinois Basin - Decatur Project |
| TD | total depth |
| MAD | median absolute deviation |
| NN | neural networks |
| MAE | mean absolute error |
| MSE | mean squared error |
| RMSE | root mean squared error |
| R2 | coefficient of determination |
| lr | Learning Rate |
| ADAM | Adaptive Moment Estimation |
| Z score | a statistical measurement describing a value to the mean of a group of values |
| CCS1\_ANPs\_psig | CCS1 annulus pressure in psi |
| CCS1\_DHPs\_psig | CCS1 downhole pressure in psi |
| CCS1\_DHTp\_F | CCS1 downhole temperature in Deg F |
| CCS1\_WHCO2InjPs\_psi | CCS1 wellhead pressure in psi |
| CCS1\_WHCO2InjTp\_F | CCS1 wellhead temperature in Deg F |
| PLT\_CO2InjRate\_TPH | CO2 injection rate in tonnes per hour |
| PLT\_CO2VentRate\_TPH | CO2 vent rate in tonnes per hour |
| VW1\_ANPs\_psig | Validation well (VW1) annulus pressure in psi |
| VW1\_PTbgPs\_psig | VW1 tubing pressure in psi |
| VW1\_PTbgTp\_F | VW1 tubing temperature in Deg F |
| VW1\_Z01D7061Ps\_psi | VW1 Zone01 pressure (7061 ft) in psi |
| VW1\_Z01D7061Tp\_F | VW1 Zone01 temperature (7061 ft) in Deg F |
| VW1\_Z02D6982Ps\_psi | VW1 Zone02 pressure (6982 ft) in psi |
| VW1\_Z02D6982Tp\_F | VW1 Zone02 temperature (6982 ft) in Deg F |
| VW1\_Z03D6945Ps\_psi | VW1 Zone03 pressure (6945 ft) in psi |
| VW1\_Z03D6945Tp\_F | VW1 Zone03 temperature (6945 ft) in Deg F |
| VW1\_Z04D6837Ps\_psi | VW1 Zone04 pressure (6837 ft) in psi |
| VW1\_Z04D6837Tp\_F | VW1 Zone04 temperature (6837 ft) in Deg F |
| VW1\_Z05D6720Ps\_psi | VW1 Zone05 pressure (6720 ft) in psi |
| VW1\_Z05D6720Tp\_F | VW1 Zone05 temperature (6720 ft) in Deg F |
| VW1\_Z06D6632Ps\_psi | VW1 Zone06 pressure (6632 ft) in psi |
| VW1\_Z06D6632Tp\_F | VW1 Zone06 temperature (6632 ft) in Deg F |
| VW1\_Z07D6416Ps\_psi | VW1 Zone07 pressure (6416 ft) in psi |
| VW1\_Z07D6416Tp\_F | VW1 Zone07 temperature (6416 ft) in Deg F |
| VW1\_Z08D5840Ps\_psi | VW1 Zone08 pressure (5840 ft) in psi |
| VW1\_Z08D5840Tp\_F | VW1 Zone08 temperature (5840 ft) in Deg F |
| VW1\_Z0910D5482Ps\_psi | VW1 Zone0910 pressure (5482 ft) in psi |
| VW1\_Z0910D5482Tp\_F | VW1 Zone0910 temperature (5482 ft) in Deg F |
| VW1\_Z09D5653Ps\_psi | VW1 Zone09 pressure (5653 ft) in psi |
| VW1\_Z09D5653Tp\_F | VW1 Zone09 temperature (5653 ft) in Deg F |
| VW1\_Z10D5001Ps\_psi | VW1 Zone10 pressure (5001 ft) in psi |
| VW1\_Z10D5001Tp\_F | VW1 Zone10 temperature (5001 ft) in Deg F |
| VW1\_Z11D4917Ps\_psi | VW1 Zone11 pressure (4917 ft) in psi |
| VW1\_Z11D4917Tp\_F | VW1 Zone11 temperature (4917 ft) in Deg F |
| inj\_diff | difference in the injection rate (IR) at time t and time (t-1) in psi |

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