

International Journal of Greenhouse Gas Control
Utilisation of Artificial Intelligence based Time-Series Prediction to validate Carbon Containment in Injection Well in Illinois Basin
--Manuscript Draft--

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First Author:	Munish Kumar
Order of Authors:	Munish Kumar Kannappan Swaminathan
Abstract:	Carbon Capture Utilisation and Storage (CCUS) involves capturing CO ₂ emissions and securely storing them in geological formations. CCUS is gaining significance in global efforts to meet ambitious climate goals. The storage of CO ₂ typically occurs through injection into saline aquifers, depleted oil and gas fields, or for Enhanced Oil Recovery (EOR). However, all methods require a deep understanding of subsurface geology and the ability to monitor CO ₂ behaviour during injection and storage. Pilot projects like the Illinois Basin - Decatur Project demonstrated the practical feasibility of storing CO ₂ underground. The injection spanned three years, during which nearly 999,215 tonnes of CO ₂ was stored. Monitoring was carried out through a pair of wells equipped with sensors to track pressure and temperature at various depths. This paper focuses on using time series injection data and monitoring information to predict changes in injection rates for the carbon capture well. We perform the prediction using Long Short-Term Memory (LSTM) neural networks (NN). These changes, represented as deltas (Δ) in injection rates between time t and time (t-1), are crucial indicators of carbon containment and migration within the well. By correlating these rate changes with other well parameters, this approach serves as a checkpoint against unwanted carbon migration or losses during the injection process. Machine learning methods are applied to forecast these injection rate deltas based on monitoring data, thereby validating the effectiveness of carbon containment during injection.
Suggested Reviewers:	Alessandro Romagnoli A.Romagnoli@ntu.edu.sg PETER FANTKE PEFAN@DTU.DK Kamaljit Singh K.Singh@hw.ac.uk Praveen Linga chepl@nus.edu.sg Ning YAN ning.yan@nus.edu.sg Karen Lythgoe karen.lythgoe@ed.ac.uk
Response to Reviewers:	

Cover letter to the Editor

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

Name of the Corresponding Author: Munish Kumar

Name(s) of all other authors: Kannappan Swaminathan

Type of Manuscript: Research Article

This manuscript is appropriate for *the International Journal of Greenhouse Gas Control (IJGGC)* as to this authors knowledge, there is a limited pool of information combining engineering, data science and artificial intelligence for time series prediction and forecasting of fields undergoing carbon capture and storage. We primarily think this is due to the lack of publicly available data on how CO₂ wells behave once injection begins. We are both practicing energy professionals and hope that our work can be utilized by other like-minded scientists as they attempt to predict injection well behavior and better identify anomalies to ensure CO₂ containment in the long run.

We have realized, through this work, that having a holistic understanding of both practical petroleum engineering and data science within the carbon capture and storage realm can either help to derisk opportunities, or at the very minimum, explain why a project may perform in a sub-optimal manner. This makes our work important and the journal the appropriate avenue to publish it.

The manuscript has been checked by a native English speaker with expertise in the field of energy. In this authors opinion, this work would appeal to both a popular audience and scientific audience.

The manuscript, or its contents in some other form, has not been published previously by the author and is not under consideration for publication in another journal at the time of submission. The manuscript does not have any supporting information and/or Review-Only Material.

Yours sincerely,

Dr Munish Kumar

October 03, 2023

Response to Editor:

Thank you for arranging for the article review. We have made the revisions requested to the manuscript and addressed the comments from the reviewers individually within separate documents.

We would additionally like to share some feedback regarding the reviewers. Having incorporated the comments of the reviewers as best as we can, we would like to point out that:

- Reviewer #1 has accepted our paper with minor revisions. We note that he/she did not have major comments and was generally complementary. We have made the necessary changes requested.
- Reviewer #2 main point was for us to enhance the paper via deeper technical discussions and application, which we can appreciate. We (the authors) are both engineers by background and are fully supportive of “applied research” (which we hope this is) rather than more theoretical or abstract machine learning models. We have tried to incorporate this feedback through the inclusion of an additional paragraph where we discuss the business merits of this method.
- Reviewer #3 has asked for us to review the data from a more geological perspective. We appreciate this view, and have done our best to incorporate more of this in our paper. However, we want to point out that the reviewer must understand that our aim is machine learning and prediction, and not necessarily a detailed deep dive into the geology or reservoir properties of the data set. The reviewer has stated that there is no need for complicated methods to analyse CO₂ containment; the reviewer appears to be alone in this view as the other 3 reviewers have no such issue with the paper.
- Reviewer #4 appeared to be intrigued by our work and generally supportive, asking us to put in some arguments around the challenges of predicting CO₂ injection. We have incorporated this and think it will satisfy his/her requirements.

We hope this adequately addresses the concerns raised by the reviewers and look forward to hearing back from you.

Thank you

Dr Munish Kumar and Kannappan Swaminathan

Response to Reviewer #1:

Thank you for your feedback. We have made the revisions requested to the manuscript and addressed your comments in this document in blue. We hope this adequately addresses the concerns raised.

1. This work is a good demonstration of how machine learning and artificial intelligent can be used to effectively monitor carbon plume migration either from injection or monitoring wells by correlating change in injection rate to the behavior of other dynamic parameters. Although, the approach has been applied in many fields such reservoir parameters prediction, flow rate prediction, etc., the use of LSTM for data forecasting is adequately justified. It is the first application to injection rate monitoring in CCUS, although there is more room for model optimization and improvement. Overall, it is a well written manuscript and I recommend that it should be accepted with minor revision following some corrections.

Author Response: Thank you very much

2. Some of the information in the abstract can be moved to the introduction.

Line 12-18 should be moved to introduction.

Author Response: Noted; it is already mentioned in the introduction from lines 49-58 in the original manuscript. We have now removed it from the abstract entirely.

Line 60 – “Given the early stage of this technique, it is imperative to initiate pilot development and validate the technology” should be reworded.

CCUS technology is about 40-year-old not in pilot stage, there are many demonstrations of capabilities around the world especially in oil and gas industries.

Author Response: Noted, we have removed the statement.

Line 159-162-Please clarify or explain why 67% of data was used for training the model and 33% for validation. Why did use this percentage? Would 50:50 change the accuracy of the model?

Author Response: The 2/3: 1/3 training: validation ratio is a generalised “rule of thumb” and is just dependent on the programmers view at the time of code writing. In our experience, models can also be built with a 70:30 or 80:20 ratio.

We opted in this case to set aside more data as a validation set because we wanted to build a model that we hoped would be more insensitive to noise. In other words, the less data we use in our training set, the more generalised the model, but use too little and we ran the risk of underfitting, therefore limiting its usefulness as a predictor.

Similarly, if we used too much data for training, we would have created an overfitted model that would not be sufficiently generalised. This ratio was thus a good compromise in this author's opinion.

Line 328-32- Clarify the difference between figure 6a and 6b (Anomalies versus variation plot; notice that one is in months while the other appear to be in days in 2012)? In figure 6b, the injection difference does

not match the LSTM prediction very well. Can you explain why? Why are this data set chosen for the validation?

Author Response: The reviewer is correct in that 6(a) is in months and demonstrates that general variabilities can be captured by the model, as per design. 6(b), which is in days, then shows that as much as possible, small-scale perturbations are somewhat predicted, albeit not perfectly, because at such small scales, the data starts to behave like “noise”, with low amplitude, high frequency characteristics that any model would be hard pressed to predict 100%. At this scale it is most important to capture the statistical behaviour than point-for-point data.

To the editor, here are our responses/explanations based on the email:

International Journal of Greenhouse Gas Control

Reviewer's Responses to Questions

Note: In order to effectively convey your recommendations for improvement to the author(s), and help editors make well-informed and efficient decisions, we ask you to answer the following specific questions about the manuscript and provide additional suggestions where appropriate.

1. Are the objectives and the rationale of the study clearly stated?

Please provide suggestions to the author(s) on how to improve the clarity of the objectives and rationale of the study. Please number each suggestion so that author(s) can more easily respond.

Reviewer #1: This work is a good demonstration of how machine learning and artificial intelligent can be used to effectively monitor carbon plume migration either from injection or monitoring wells by

Author Response: Thank you

2. If applicable, is the application/theory/method/study reported in sufficient detail to allow for its replicability and/or reproducibility?

Please provide suggestions to the author(s) on how to improve the replicability/reproducibility of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #1: Mark as appropriate with an X:

Yes No N/A

Provide further comments here:

Author Response: Thank you

3. If applicable, are statistical analyses, controls, sampling mechanism, and statistical reporting (e.g., P-values, CIs, effect sizes) appropriate and well described?

Please clearly indicate if the manuscript requires additional peer review by a statistician. Kindly provide suggestions to the author(s) on how to improve the statistical analyses, controls, sampling mechanism, or statistical reporting. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #1: Mark as appropriate with an X:

Yes [x] No [] N/A []

Provide further comments here: The manuscript is in the domain of artificial intelligent. Perhap, mathematical modelling expert can provide more useful insight for the work. I recommend Prof. Hassan Hassanzadeh (University of Calgary), for further review of models.

[Author Response: Thank you](#)

4. Could the manuscript benefit from additional tables or figures, or from improving or removing (some of the) existing ones?

Please provide specific suggestions for improvements, removals, or additions of figures or tables. Please number each suggestion so that author(s) can more easily respond.

Reviewer #1: no

[Author Response: Thank you](#)

5. If applicable, are the interpretation of results and study conclusions supported by the data?

Please provide suggestions (if needed) to the author(s) on how to improve, tone down, or expand the study interpretations/conclusions. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #1: Mark as appropriate with an X:

Yes [x] No [] N/A []

Provide further comments here: The results from the models are well interpreted and are well supported in the conclusion.

[Author Response: Thank you](#)

6. Have the authors clearly emphasized the strengths of their study/theory/methods/argument?

Please provide suggestions to the author(s) on how to better emphasize the strengths of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #1: The study applies artificial intelligence to determine the effectiveness of CO₂ containment. It is a new application of method to CCS. The LSTM model can be expatiated more to help reader follow the application.

[Author Response: Thank you](#)

7. Have the authors clearly stated the limitations of their study/theory/methods/argument?

Please list the limitations that the author(s) need to add or emphasize. Please number each limitation so that author(s) can more easily respond.

Reviewer #1: Yes they did mentioned that the model can be improved by improving the feedback loop for better prediction accuracy.

[Author Response: Thank you](#)

8. Does the manuscript structure, flow or writing need improving (e.g., the addition of subheadings, shortening of text, reorganization of sections, or moving details from one section to another)?

Please provide suggestions to the author(s) on how to improve the manuscript structure and flow. Please number each suggestion so that author(s) can more easily respond.

Reviewer #1: It is easy to follow

[Author Response: Thank you](#)

9. Could the manuscript benefit from language editing?

Reviewer #1: No

[Author Response: Thank you](#)

Response to Reviewer #2:

Thank you for your feedback. We have made the revisions requested to the manuscript and addressed your comments in this document in blue. We hope this adequately addresses the concerns raised.

To the editor, here are our responses/explanations based on the email:

International Journal of Greenhouse Gas Control

Reviewer's Responses to Questions

Note: In order to effectively convey your recommendations for improvement to the author(s), and help editors make well-informed and efficient decisions, we ask you to answer the following specific questions about the manuscript and provide additional suggestions where appropriate.

1. Are the objectives and the rationale of the study clearly stated?

Please provide suggestions to the author(s) on how to improve the clarity of the objectives and rationale of the study. Please number each suggestion so that author(s) can more easily respond.

Reviewer #2: Although the authors have attempted to analyze some prediction methods, a deeper discussion would be expected. Otherwise, the motivation for this study may not be sufficiently strong.

Author Response: Thank you. We have included an additional section explaining the motivation in the introduction.

2. If applicable, is the application/theory/method/study reported in sufficient detail to allow for its replicability and/or reproducibility?

Please provide suggestions to the author(s) on how to improve the replicability/reproducibility of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #2: Mark as appropriate with an X:

Yes No N/A

Provide further comments here:

While basic metrics like mean square error and MAE are used to evaluate your regression model, such validation may not be strong enough. Therefore, it is suggested to design and incorporate other cross-validation techniques or specific metrics for a more robust evaluation.

Author Response: We thank the reviewer for this response, but the reviewer is mistaken. We did do a k-fold cross-validation methods for this work (line 255-256).

3. If applicable, are statistical analyses, controls, sampling mechanism, and statistical reporting (e.g., P-values, CIs, effect sizes) appropriate and well described?

Please clearly indicate if the manuscript requires additional peer review by a statistician. Kindly provide suggestions to the author(s) on how to improve the statistical analyses, controls, sampling mechanism, or statistical reporting. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #2: Mark as appropriate with an X:

Yes No N/A

Provide further comments here:

A more profound discussion should be provided to support the algorithm and its engineering applications.

[Author Response: Thank you. We have included a real-world case study in the introduction section.](#)

4. Could the manuscript benefit from additional tables or figures, or from improving or removing (some of the) existing ones?

Please provide specific suggestions for improvements, removals, or additions of figures or tables. Please number each suggestion so that author(s) can more easily respond.

Reviewer #2: The figure quality needs improvement; some numbers are unclear, such as in Figure 2. Please ensure consistency in formatting figures/tables within the context, such as the font in Figure 3.

Figure 4 requires correction; some information inside has overlapped, which does not meet publishing standards. Additionally, please check and rectify similar problems in all other figures.

[Author Response: Noted; we have edited where possible.](#)

5. If applicable, are the interpretation of results and study conclusions supported by the data?

Please provide suggestions (if needed) to the author(s) on how to improve, tone down, or expand the study interpretations/conclusions. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #2: Mark as appropriate with an X:

Yes No N/A

Provide further comments here:

A more profound discussion should be provided to support the algorithm.

[Author Response: Thank you. We have included this discussion in the introduction section.](#)

6. Have the authors clearly emphasized the strengths of their study/theory/methods/argument?

Please provide suggestions to the author(s) on how to better emphasize the strengths of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #2: No. The introduction part begins with human activities, which is too broad. It is suggested to concentrate on CCUS from the outset.

Author Response: Thank you. We have removed the first paragraph of the introduction.

7. Have the authors clearly stated the limitations of their study/theory/methods/argument?

Please list the limitations that the author(s) need to add or emphasize. Please number each limitation so that author(s) can more easily respond.

Reviewer #2: Deeper discussion is necessary rather than applying a machine learning method to CCUS.

Author Response: Thank you. We have highlighted its uses in the introduction.

8. Does the manuscript structure, flow or writing need improving (e.g., the addition of subheadings, shortening of text, reorganization of sections, or moving details from one section to another)?

Please provide suggestions to the author(s) on how to improve the manuscript structure and flow. Please number each suggestion so that author(s) can more easily respond.

Reviewer #2: The literature review has been separated from the introduction. However, these two parts lack correlation, and it is recommended to transition between them more smoothly.

Author Response: We thank the reviewer and have tried to synergize the section better.

9. Could the manuscript benefit from language editing?

Reviewer #2: Yes

Author Response: We thank the reviewer; however, we do not know what changes the reviewer is recommending. This reviewer is also alone in this recommendation, as the remaining 3 reviewers have not singled this out.

Response to Reviewer #3:

Thank you for your feedback. We have made the revisions requested to the manuscript and addressed your comments in this document in blue. We hope this adequately addresses the concerns raised.

To the editor, here are our responses/explanations based on the email:

International Journal of Greenhouse Gas Control

Reviewer's Responses to Questions

Note: In order to effectively convey your recommendations for improvement to the author(s), and help editors make well-informed and efficient decisions, we ask you to answer the following specific questions about the manuscript and provide additional suggestions where appropriate.

1. Are the objectives and the rationale of the study clearly stated?

Please provide suggestions to the author(s) on how to improve the clarity of the objectives and rationale of the study. Please number each suggestion so that author(s) can more easily respond.

Reviewer #3:

- a. main points in conclusion: As stated in line 412 & 413 of the Conclusion, the model was made to predict the injection rate changes of the CO₂ injection by using some of the 34 contemporaneously recorded other monitored parameters. And lines 418 & 419 state that the model's primary objective is to detect anomalies and alert operators to closely inspect the well for potential leaks.

Authors response: Thank you for the comment; there is nothing to action here.

- b. There is nothing in the report to show how just the single parameter of the injection rate changes are/can be linked to any anomalies to alert operators of any type of potential leak from the well. No cited publications for this specific linkage or theory. Shouldn't there be literature review of linkage and not just of modeling in the paper?

Authors response: We thank the reviewer for this response. It is observed from the data that a single delta injection parameter is intricately linked to the responses of multiple sensors deployed both laterally and vertically. Our methodology integrates data from these sensors to derive the single parameter, which serves as a key indicator of anomalous behavior in the system.

While our literature review has primarily focused on the modeling aspects of our research, we recognize the importance of providing context on the linkage between injection rate changes and leak detection. To address this, we have expanded our literature section to include relevant publications that discuss the theoretical underpinnings and empirical evidence supporting this linkage.

Furthermore, we would like to clarify that this area of research is novel, as stated in our literature review. Lastly, we would like to note that none of the other three reviewers raised this specific issue, which may suggest that the concern raised could stem from a misunderstanding or lack of familiarity with the intricacies of our research methodology.

- c. In highlights: Predicting this change can be used to provide a checkpoint against carbon plume migration and can determine if there are losses in the injection process. Not shown or explained in this paper on how knowing an injection rate can tell one about plume migration of CO₂ or injection well integrity.

Authors response: We thank the reviewer for this response. We think it will be hard to disagree with our view that changes in injection rate are an effective means to monitor the behavior of the injection process over time. But we are trying to extend this analysis further and determine whether we can find a way to link changes in injection rates to potential issues such as leaks or changes in reservoir behavior. By detecting deviations from expected injection patterns, operators can investigate further to determine the root cause of these anomalies, which may include integrity issues with the injection well or unwanted migration of CO₂.

Secondly, while the paper primarily focuses on predicting injection rate deltas using machine learning techniques, it should be part of a larger framework for monitoring and managing CCUS operations. In practice, the predictive model would be integrated into a comprehensive monitoring and control system that includes real-time data from various sensors, geological monitoring, and reservoir simulations. By combining information from multiple sources, operators can gain a holistic understanding of the injection process and make informed decisions to ensure the safe and efficient operation of CCUS projects.

- d. Permit requires monitoring the injection well annulus pressures and periodic casing pressure tests and the use of reservoir saturation tool in the cased hole to try and detect CO₂ outside of the casing.

Authors response: We appreciate the reviewer's emphasis on the importance of existing monitoring methods such as annulus pressure monitoring, casing pressure tests, and the use of reservoir saturation tools. These approaches are indeed fundamental for ensuring the integrity and safety of injection wells in CCUS projects. In fact, the machine learning (ML) model uses some these parameters as inputs.

It's important to note that the ML method proposed in our study serves as an additional layer of monitoring and analysis, complementing these existing techniques. While traditional methods provide valuable real-time data and direct measurements, ML offers the potential to analyze large volumes of historical data, detect subtle patterns or anomalies, and predict future trends.

Moreover, we acknowledge the potential for ML to optimize operational expenses (OPEX) by reducing the frequency of certain tests or enabling more targeted monitoring strategies. By leveraging ML algorithms to identify trends and anomalies in the data, operators can make informed decisions about when and where to deploy traditional monitoring techniques, thereby maximizing their effectiveness and minimizing unnecessary costs.

We recognize the importance of integrating ML methods with established monitoring protocols and hardware-based tools to create a comprehensive and robust monitoring framework for CCUS projects. This synergy between empirical methods and data-driven analytics can enhance the overall safety, efficiency, and cost-effectiveness of carbon capture and storage operations.

2. If applicable, is the application/theory/method/study reported in sufficient detail to allow for its replicability and/or reproducibility?

Please provide suggestions to the author(s) on how to improve the replicability/reproducibility of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #3: Mark as appropriate with an X:

Yes No N/A

Provide further comments here:

- e. There is great detail of information on building the model, which in this case is built on training data that the authors' unsuccessfully attempted to "clean up" the not understood problems with the raw recorded parameter data. Part of the problem also centers around the understanding of basic hydrostatic formation pressures for the verification well data – there can't be zero formation pressures.

Authors response: We find this response a bit puzzling, because there are no zero values in the selected model as indicated in Table 4. We, in fact, describe how the zero values are handled. We utilize many different methods (forward or backward fill, dropping the rows with zero values), but for the sake of paper length, only document the final method we employ which is the forward fill method.

To the reviewers second point about values that are lower than formation pressure, we agree that the more correct method is ensure that there are no values below the formation pressure at the sensor depth. We have handled this via an additional step in the data cleaning stage (lines 213-214 in the revised manuscript).

3. If applicable, are statistical analyses, controls, sampling mechanism, and statistical reporting (e.g., P-values, CIs, effect sizes) appropriate and well described?

Please clearly indicate if the manuscript requires additional peer review by a statistician. Kindly provide suggestions to the author(s) on how to improve the statistical analyses, controls, sampling mechanism, or statistical reporting. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #3: Mark as appropriate with an X:

Yes No N/A

Provide further comments here:

- f. There are nearly no details on where the 11 pressure/temperature sensors are in the verification well and how the pressures were impacted by the baffles in the Mt. Simon in relation to the injection zone!

Authors response: Noted and this has now been addressed in the paper.

- g. No explanation on why the only Z05 (Zone 5) pressure/temperature sensor of the verification well was picked for the learning data. Zones 4-9 are above the baffles and are in a part of the aquifer that reacted very little to injection well pressures changes. For Zone 5, with a very, very slow buildup of the 25 psi pressures, took 3 years. It also took 100+ hours to see pressure changes at Z05 following

changes in injection while sensors at other elevations below the baffles had increases of 169 psi and 1 hour to see pressure changes.

Authors response: Our approach hinges on analyzing deltas, parameter changes, and trends rather than absolute values. As indicated in the correlation matrix presented in the paper, the time series trends from sensors in the verification well are highly collinear. This implies that including additional sensors from these zones would offer limited value in terms of enhancing the predictive capabilities of the model.

Moreover, sensitivity runs were conducted, as detailed in the "Sensitivity Runs" section, to explore various combinations of downhole sensors. These analyses further supported the decision to focus on the Z05 sensor. While we acknowledge that the different rates of pressure buildup across zones may reflect variations in reservoir properties that could impact storage volume, addressing such nuances falls outside the scope of our study. Our primary goal is to detect deviations from expected behavior and identify potential containment issues.

- h. Pressure readings through the 3 years of injection are shown in diagrams in several publications to give an overall bounds for some of the “clean up” parameters without directly going through the raw data in detail to find: pressure values below original formation pressures (which includes 0), injection well head pressure values above permitted and equipment capable highs, remove pressure changes after sensor re-installation that had jumps in pressure readings until sensors were re-installed again, pressure values stuck at one value for long periods, major time gaps (up to 3 months), and negative null values.

Authors response: We have now addressed this issue by incorporating these bounds as an additional layer of data cleaning process.

- i. Forward fill of pressure values in verification well data that are associated with very reactive sensors and high pressure changes for some times gaps which are as long as 3 month, would produce fairly fictitious values!

Authors response: There is no perfect method to deal with missing data; this is why experience matters. As authors, we have carefully monitored the data to make sure such a scenario does not occur; we exclude the data if it does.

- j. Text says 6 of the 33 parameter variables were used in the model and site Table 2 for the variable. Table 2 has 9 variables, and the two paired temperature/pressure were to only use one of the values – which ones were used and that makes 7 variables that were used?

Authors response: There were 33 parameters to begin with, after data-cleaning and checking collinearity, this was reduced to 8 excluding the target injection delta. This has been updated in the paper.

- k. Parameters such as in table 1 probably should be described what they represent. What is inj-diff and its units?

Authors response: This is now included in the nomenclature table in the appendix.

- l. Why isn’t the hold out data modeled injection rate changes shown? Figure 8 covers the time period when the injection rate was at its maximum of 42 to 44 tonnes/hr rate and there were two 0 injection time periods of 10 hours on the 20th and 3 hours on the 26th.

Authors response: We attempted to show the anomalies predicted by the injection pressure deltas and then based on that investigate the sensor parameters. We agree that showing the holding dataset is valuable and have now included it in the paper.

- m. Figure 5 for b Check file of small subset of data. The injection rates were at the typical 42-44 TPH rate which is a typical fluctuation range for that entire time period of b.

Authors response: Noted; thank you for the comment. It's important to clarify that our analysis primarily focuses on detecting anomalies and changes in data trends rather than absolute values. As such, the small fluctuations in injection rates, while within the expected range, still could contribute valuable information or rather this work is to determine if it does.

4. Could the manuscript benefit from additional tables or figures, or from improving or removing (some of the) existing ones?

Please provide specific suggestions for improvements, removals, or additions of figures or tables. Please number each suggestion so that author(s) can more easily respond.

Reviewer #3:

- n. Tables have data problems and no explanation of some of the data: . Table 4; What is the VW DH Sensor? Pressure or temperature? What is the Temp Sensor? VW Zero Value – there should be NO zero values for temperature or pressure.

Authors response: This has now been addressed in the paper as per the above.

- o. unless the authors converted the times to UTC, all the time data is local time.
Authors response: Noted and amended.

- p. Explain what is in the tables and figures. Explain what are the parameters in table 1 and 2 and the colored boxes in figure 8 – as examples.

Authors response: This has been edited and the figure changed in the paper.

- q. In table 8, do not know what is real input data and what is the predicted values. For Avg_CCS1_DH6325Ps_psi, the raw recorded data is all below 3300 psi with a short downward change of 230 psi on the 20th and 162 psi on the 26th. Doesn't match the data in table 8.

Author: Figure 8 has the incorrect dates; this has now been updated and it has been verified that there is no change in analysis. The raw recorded data for Avg_CCS1_DH6325PS_psi should correspond to the dates 20 Nov 2014 to 26 Nov 2014.

5. If applicable, are the interpretation of results and study conclusions supported by the data?

Please provide suggestions (if needed) to the author(s) on how to improve, tone down, or expand the study interpretations/conclusions. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #3: Mark as appropriate with an X:

Yes [] No [X] N/A []

Provide further comments here:

- r. Results for the success of the model was to run 67% of the data to teach the model and use the 33% held back data to run to predict injection rate changes. I believe this was supposed to be accomplished in Figure 8 which has no legend for viewer to figure out which data is which. Couldn't the predicted parameters be compared to the actual measured parameters of injection rate? Which is not in the graph! Visually it would be nice to see that data as a comparison and not a derivative of the data.
19. No results or explanation given for linking injection rate changes to containment issues.

Author: Noted and Ground Truth values have now been added to the paper.

6. Have the authors clearly emphasized the strengths of their study/theory/methods/argument?

Please provide suggestions to the author(s) on how to better emphasize the strengths of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #3:

- s. Hard to come up with a strength when study/theory cited in the title is so incomplete. Question the use a complicated Artificial Intelligence based Time-Series Prediction to predict injection rate changes using Well head injection pressure and temperature, annulus pressures, down hole pressures and temperatures, and two variables from the verification well 1007 feet away, when simple relationships can be examined and developed between just several of the injection well parameters without AI.

Authors response: While simple relationships between some injection well parameters can indeed be examined and developed without AI, our methodology offers distinct advantages in capturing nuanced patterns and interactions within the data that may not be readily apparent through traditional analyses. Furthermore, our aim is not solely to predict absolute values but rather to analyze deltas, changes, and trends in the data. For instance, consider the relationship between injection rate changes and pressure variations. This approach allows us to identify anomalies and trends that could indicate potential issues or opportunities for optimization.

While it's true that simpler analyses can be conducted for individual wells, the scalability of such methods becomes a significant challenge when dealing with a large number of wells. In contrast, Machine Learning and AI offer the capability to analyze vast quantities of data from numerous wells simultaneously, enabling operators to prioritize interventions based on predictive insights. For example, if there are thousands or even millions of wells in a field, AI-driven analytics can help identify the most critical areas requiring attention, thereby optimizing resource allocation and operational decision-making.

Lastly, this is a prototype, a start which is why we are using such a dataset that is simple, known and one can easily derive the expected result as pointed out by the reviewer to see what the model does and

see how well it does, what breaks the model, etc. The aim would be to scale this to more challenging situations and inputs.

7. Have the authors clearly stated the limitations of their study/theory/methods/argument?

Please list the limitations that the author(s) need to add or emphasize. Please number each limitation so that author(s) can more easily respond.

t. Reviewer #3: None stated.

Authors response: We acknowledge that while we may not have explicitly labeled them as 'limitations' in our paper, we have indeed addressed areas for improvement within our model. These include dealing with outliers/garbage values effectively, including a feedback loop and reduction of runtime optimization. These suggestions inherently represent limitations that need to be addressed in future iterations of this work.

8. Does the manuscript structure, flow or writing need improving (e.g., the addition of subheadings, shortening of text, reorganization of sections, or moving details from one section to another)?

Please provide suggestions to the author(s) on how to improve the manuscript structure and flow. Please number each suggestion so that author(s) can more easily respond.

Reviewer #3: Structure is not a problem

Authors response: Noted; thank you

9. Could the manuscript benefit from language editing?

Reviewer #3: No

Reviewer #3:

u. main points: As stated in line 412 & 413 of the Conclusion, the model was made to predict the injection rate changes of the CO₂ injection. And lines 418 & 419 state that the model's primary objective is to detect anomalies and alert operators to closely inspect the well for potential leaks. Using predicted parameters to validate CO₂ containment in the Well - title. In highlights: Predicting this change can be used to provide a checkpoint against carbon plume migration and can determine if there are losses in the injection process. Not shown or explained in this paper on how knowing an injection rate can tell one about migration of CO₂ or injection well integrity.

Authors response: Noted; we have edited where we can

v. Line 62 Mt. Simon Sandstone is the official name. Not Mount.

Authors response: Noted; edited

- w. Line 66 Injection started in Nov 2011 not 2009. Drilling was in 2009.

Authors response: Noted; edited

- x. Line 67 the distance between the Injection well and Verification well is 1007 ft as shown in Bauer et al. 2016.

Authors response: Noted; edited

- y. Line 79 What are the other losses?

Authors response: Noted; edited. We are referring to downhole losses, such as casing leaks, thief zones etc. Some of these changes are small, and conventional logging tools may not be able to detect them.

- z. Line 81 Do not understand how knowing injection rate changes, tells one the integrity of the well.

Permit requires monitoring the injection well annulus pressures and periodic pressure tests and the use of reservoir saturation tool in the cased hole to try and detect CO₂.

Authors response: Noted; periodic pressure tests, and use of logs implies an OPEX; a ML method is complimentary to these methods but can help lower costs for the operator by reducing the frequency such operations are conducted. We also want real-time monitoring; the methods recommended by the reviewer are not real-time.

Regarding the understanding of injection rate changes, they serve as indicators of potential anomalies in well behavior. For instance, a sudden change in injection rate, when all other parameters remain constant, could signal an issue that needs attention, such as a breach in containment. Therefore, our method aims to provide valuable insights into well integrity by analyzing these changes and identifying potential anomalies.

- aa. Line 94 hydrocarbon and water rates - RECOVERY? Rates

Authors response: Noted; edited.

- bb. Line 124 Data was - data is plural - Data were

Authors response: Noted; edited.

- cc. Line 133 Illinois Basin - Decatur Project hyphen missing

Authors response: Noted; edited.

- dd. Line 136 checkpoint against carbon migration. Authors are not working with any data showing where the CO₂ is or was located and how a single parameter of injection rate is a checkpoint for understanding CO₂ migration.

Author: the focus of our paper is on developing a machine learning model to serve as a tool for monitoring well integrity and CO₂ containment. While understanding the exact location of CO₂ migration is valuable, it falls outside the scope of our current study. The purpose of our model is to detect anomalies in parameters such as injection rate, which could indicate potential issues such as casing-tubing communication failure or reservoir saturation. These anomalies serve as checkpoints for operators to further investigate and take appropriate actions to ensure well integrity and CO₂ containment.

ee. Line 139 modelling variation in well and storage parameters to validate CO₂ containment. Of all the dynamic parameters, which are indicators or are associated with CO₂ containment and what is the definition for this? Or even where the CO₂ is located - CO₂ plume?

Authors response: Noted; edited.

ff. Line 142 No details on the annulus monitoring and nearly no details on where the sensors are located in the verification well and how the pressures were impacted by the baffles in the Mt. Simon in relation to the injection zone!

Authors response: Noted; but is this relevant to proving a ML model works? This paper is not meant to discuss the geologic metrics of the measured data. As explained earlier, we are accepting the data as is, and developing a method to help engineers detect anomalies. And even though there are baffles, pressure data indicates hydrostatic communication, and all sensor trends are highly co-linear.

gg. Line 145 TD of injection well is 7238 ft as shown in ref. 3.

Authors response: Noted; edited.

hh. Line 149 proper name is Precambrian

Authors response: Noted; edited.

ii. Line 153 Mt. St Simon delete St

Authors response: Noted; edited.

jj. Line 163 There are other problems in the data: Also pressure values stuck at one value for long periods, major time gaps (up to 3 months), in monitoring during removal of sensors, negative null values.

Authors response: Noted; All these values have been dealt with during the data cleaning process. There are no negative values, no null values. We use multiple inputs to the model in order to mitigate the frozen values. This will be treated as an improvement and has been indicated in the paper.

kk. Table 1 shows some of the data problems. Max value for WHCO2Inj of 39,032 psi - permit and the equipment limits are 2,380 psi.

Authors response: This is a comment and well noted. Table 1 is the raw value. Table 2 is the cleaned value which has now been incorporated to include the reviewer's comment.

ll. Line 171 (i) Would think that the first task for cleaning up the data would be to remove significant outliers, values below original formation pressures (which includes 0), injection well head pressure values above permitted and equipment capable highs, remove pressure changes after sensor re-installation that had jumps in pressure readings until sensors were re-installed again, then do forward fill for some times gaps which are as long as 3 month! This method has many pitfalls without going through the entire data set in detail and determining even small outliers, especially if you are working with only a 25 psi change in 3 years for Z05. Zone 5 was above a set of baffles in the Mt. Simon formation and the injection was below the baffles, resulting in a very slow 25 PSI increase over 3 years of injection with 100+ hours delay in pressure communication between the Injection well and the Z05 sensor. Data needs detailed visual screening.

Author: The data cleaning process now incorporates the reviewer's comment. As for the choice of sensor, the point here is there is pressure communication. Z05 sees the change albeit small. And the data shows that the Z05 and the other sensors are highly correlatable. That is, changes detected in the other sensors are also being detected in Z05. We ran sensitivities with other sensors, Z1, Z2 and Z3

and there is no major impact to the model's objective. As we are dealing with deltas, this is captured and Z5 was picked purely based on the lowest RMSE value.

mm. Table 2. Cleaned up data: VW1_Z05: minimum value of the measured formation pressure can not be lower than the original formation pressure. There is no withdrawal of formation waters to lower it! The original formation pressure for Zone 5 was 3051.8 psi. Going through the data in detail for Zone 5 data, one is looking for changes outside of this overall 25 psi change over 3 years. The median value in Table 2 is at the maximum pressure of about 3076 after 3 years. These values in this table for Z05 show the problems with this data to be easily cleaned up with the method used.

Author: This has now been addressed as per previous responses.

nn. Table 2. Cleaned up data: CCS1 well head injection pressures should be cleaned up so that permit required maximum levels of pressure (2,380 psi) and rate are the maximum values. These permitted maximum values are also near the equipment and pipeline maximum operating pressures.

Author: This cleanup now been addressed as per previous responses. But we would like to point out that it does not necessarily mean all operators adhere to the permitted wellhead injection pressures.

oo. For all the diagrams with time. The original data is in local time not UTC - unless authors have converted it.

Author: Noted. Thank you.

pp. Line 342 Table 4 are the listings of input parameters in the model to test predicted output of the other parameters and as stated authors are predicting the changes in the injection rates by using other recorded contemporaneous data. Final model run has input of injection well head pressure, which can be related to volume from a project developed relationship and volume over time is injection rate. Why the complicated model then?

Author: Indeed, the final model includes input parameters such as injection well head pressure, which can theoretically be directly related to injection volume over time. However, the complexity of the model arises from its ability to capture nuanced relationships and detect anomalies that may not be apparent in straightforward correlations. For instance, while changes in injection well head pressure may directly influence injection rates in conventional scenarios, there could be instances where changes in other variables, not directly tied to well head pressure, impact injection rates.

Regarding the possibility of changes in injection rates without corresponding changes in well head pressure, while it may seem counterintuitive, it's conceivable in certain operational contexts. For instance, changes in downhole conditions, reservoir characteristics, or equipment performance could potentially influence injection rates independently of variations in well head pressure. Therefore, the model's complexity allows for the identification of such nuanced patterns and anomalies, providing a more comprehensive understanding of system behavior beyond simple correlations.

qq. Table 4; What is the VW DH Sensor? Pressure or temperature and which one? What is the Temp Sensor? VW Zero Value - there should be NO zero values for temperature or pressure.

Author: Thank you for pointing out the ambiguity. The VW WH DH Sensor refers to the pressure sensor. The table in the report has been amended. As for the zero values, this has now been addressed as per responses above.

rr. Figure 8. What are the different colored boxes? Don't understand the flat line data for Z05 from 20 Nov 2012 through about 24 Nov 2012. Pressures during this time period fluctuated from 3069.079 to 3069.65 psi and outside of it not being flat data, it doesn't even match the 3071.5+ values in this

graph, which are in 0.1 divisions and should show the raw data fluctuation range or that there are problems with the data clean up method.

Author: We have replaced Figure 8; we hope the results are clearer to the reviewer

- ss. References 3, Authors need corrections and Illinois Basin-Decatur Project - needs caps.

Authors response: Noted; edited.

- tt. References 10, 15, and 17 need authors fixed.

Authors response: Noted; edited.

- uu. If verification well data is used for predictions, one may want to use data from zones that were rapidly affected by pressure changes at the injection well. Zones 1 through 3 are below a baffle that affected injection transmitting changes in formation pressures in the Mt. Simon and are near the level of the CCS1 injection and reacted to CCS1 changes within about an hour and had maximum recorded pressure changes of 169 psi. Zones 4-9 are above the baffles and are in a part of the aquifer that reacted very little to pressure changes. For Zone 5, the very, very slow buildup of the 25 psi pressures took 3 years. Once when the sensor was pulled and reset, it took 5 months for it to restabilize to the original pressures.

Authors response : Our approach hinges on analyzing deltas, parameter changes, and trends rather than absolute values. As indicated in the correlation matrix presented in the paper, the time series trends from sensors in the verification well are highly collinear. This implies that including additional sensors from these zones would offer limited value in terms of enhancing the predictive capabilities of the model.

Moreover, sensitivity runs were conducted, as detailed in the "Sensitivity Runs" section, to explore various combinations of downhole sensor. Z05 is the best option in terms of RMSE which is how a LSTM ML model is evaluated on. While we acknowledge that the different rates of pressure buildup across zones may reflect variations in reservoir properties that could impact storage volume, addressing such nuances falls outside the scope of our study. Our primary goal is to detect deviations from expected behavior and identify potential containment issues.

Response to Reviewer #4:

Thank you for your feedback. We have made the revisions requested to the manuscript and addressed your comments in this document in blue. We hope this adequately addresses the concerns raised.

To the editor, here are our responses/explanations based on the email:

International Journal of Greenhouse Gas Control

Reviewer's Responses to Questions

Note: In order to effectively convey your recommendations for improvement to the author(s), and help editors make well-informed and efficient decisions, we ask you to answer the following specific questions about the manuscript and provide additional suggestions where appropriate.

1. Are the objectives and the rationale of the study clearly stated?

Please provide suggestions to the author(s) on how to improve the clarity of the objectives and rationale of the study. Please number each suggestion so that author(s) can more easily respond.

Reviewer #4: Yes. See detailed comments for additional input.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

2. If applicable, is the application/theory/method/study reported in sufficient detail to allow for its replicability and/or reproducibility?

Please provide suggestions to the author(s) on how to improve the replicability/reproducibility of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #4: Mark as appropriate with an X:

Yes [x] No [] N/A []

Provide further comments here: See detailed comments for additional input.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

3. If applicable, are statistical analyses, controls, sampling mechanism, and statistical reporting (e.g., P-values, CIs, effect sizes) appropriate and well described?

Please clearly indicate if the manuscript requires additional peer review by a statistician. Kindly provide

suggestions to the author(s) on how to improve the statistical analyses, controls, sampling mechanism, or statistical reporting. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #4: Mark as appropriate with an X:

Yes [x] No [] N/A []

Provide further comments here: See detailed comments for additional input.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

4. Could the manuscript benefit from additional tables or figures, or from improving or removing (some of the) existing ones?

Please provide specific suggestions for improvements, removals, or additions of figures or tables. Please number each suggestion so that author(s) can more easily respond.

Reviewer #4: No. Would only suggest clarifying the existing ones, as described in the detailed comments section.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

5. If applicable, are the interpretation of results and study conclusions supported by the data?

Please provide suggestions (if needed) to the author(s) on how to improve, tone down, or expand the study interpretations/conclusions. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #4: Mark as appropriate with an X:

Yes [] No [x] N/A []

Provide further comments here: As presented, the figures and text do not have enough stand-alone information to support the conclusions. See detailed comments for suggested improvements to improve clarity.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

6. Have the authors clearly emphasized the strengths of their study/theory/methods/argument?

Please provide suggestions to the author(s) on how to better emphasize the strengths of their study. Please number each suggestion so that the author(s) can more easily respond.

Reviewer #4: Yes. See detailed comments for additional input.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

7. Have the authors clearly stated the limitations of their study/theory/methods/argument?

Please list the limitations that the author(s) need to add or emphasize. Please number each limitation so that author(s) can more easily respond.

Reviewer #4: Somewhat. The authors clearly describe their methods, which is refreshing. They clearly describe what it can do, but a balanced approach may be in order to better describe some of the method's limitations.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

8. Does the manuscript structure, flow or writing need improving (e.g., the addition of subheadings, shortening of text, reorganization of sections, or moving details from one section to another)?

Please provide suggestions to the author(s) on how to improve the manuscript structure and flow. Please number each suggestion so that author(s) can more easily respond.

Reviewer #4: No.

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

9. Could the manuscript benefit from language editing?

Reviewer #4: No

Author Response: Noted, Thank you. We will address your comments in the “Detailed comments” section below

Reviewer #4:

1. Line 41. To improve clarity, remove the word "only".

Author Response: Edited; we have removed the line based on comments from reviewer #1

2. Reference 1. Although from a reputable source, this reference is only pointing to a news article. Especially for your first citation, I would encourage a more rigorously scrutinized source. Is there also a peer-reviewed source that contains the same information?

Author Response: Edited; we have added a new source.

3. Line 44. Coal, oil and natural gas are the largest used sources of fossil fuels, but not the only ones. Similarly CO₂, CH₄, and N₂O are the largest produced GHGs, but not the only ones. Clarify language by modifying text to read: "The burning of fossil fuels (such as coal, oil, and natural gas) has resulted in the generation of various GHGs, such as carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O).

Author Response: Edited; thank you

4. Reference 2. Please update reference, preferably to a report or peer-reviewed journal. Reference 2 is pointing to an online webpage from a reputable source that was last updated on 23 February 2024. The webpage does not indicate that the amount of CO₂ generated in 2020 to be ~3.11 million metric tons.

Author Response: Edited; we have added a new source.

5. Line 53. CO₂ storage can be carried out in a number of different ways, not just the 3 listed. Clarify language by modifying the text to read: "CO₂ geologic storage can be carried out in a number of different ways, including via injection into ..."

Author Response: Edited; thank you

6. Line 60. This paragraph requires the addition of peer-reviewed journal references.

Author Response: Edited; we have removed the line based on comments from reviewer #1

7. Reference 3. The reference author names and format need to be corrected for this and other references. For this particular reference, correct reference information: "Bauer RA, Will R, E. Greenberg S, Whittaker SG. Illinois Basin-Decatur Project. In: Davis TL, Landrø M, Wilson M, eds. Geophysics and Geosequestration. Cambridge University Press; 2019:339-370."

Author Response: Edited; thank you

8. Line 73. Here and elsewhere, clarify "carbon capture well" terminology. I believe you mean "capture sequestration well", as opposed to something to do with the carbon capturing process itself.

Author Response: Edited; thank you

9. Introduction section. A discussion should be added about CO₂ injection rates in general, what drives them, and why their calculation is a somewhat difficult problem for CO₂ sequestration. Of deep interest is the calculation of the maximum rate at which CO₂ can be injected into the subsurface by human operators. We are interested in the maximum rates of course because current climate models suggest that rather large amounts of CO₂ injected at high rates is needed to sequester CO₂ as fast as possible to mitigate climate change. Given that operators may want to have as high a rate as possible, what are the factors that actually determine the rate at which the operators are injecting CO₂ (e.g., the pressure rise in the aquifer, equipment malfunctions, etc)? This would be directly relatable to what you are predicting. Lastly, there should be a discussion about why AI can become a preferred method: among other things, some existing methods to estimate subsurface injection rates can become complex and/or costly when considering at a basin scale. I'm sure there are other reasons that can be stated as well. What are the other ways in which maximum injection rates are currently calculated? What are the tradeoffs in methods? There is often, no single right way of doing things.

Author Response: A paragraph with regards to optimum CO₂ injectivity has been added. In summary, achieving optimum CO₂ injectivity relies on various factors, including geological and reservoir properties such as permeability and heterogeneity, effective pressure management, maintenance of injection fluid properties, and appropriate pump and well design. The goal is to determine the injection rate that maximizes volume over time while ensuring the storage reservoir's capacity is not exceeded. This emphasis on optimum rather than maximum injection rate considers the need for sustainable CO₂ sequestration. Injecting too rapidly can lead to issues like premature reservoir filling or skin problems, reducing injectivity. Insights and methodologies from the oil and gas industry, such as nodal analysis, can inform our approach. However, further discussion on this topic falls outside the scope of this paper.

10. Line 94. Clarify text: "Within reservoir engineering, the prediction of hydrocarbon and water production rates from geological ..."
Author Response: Edited; thank you. This statement simply means that predicting flow rates are a time series problem where future rates are predicted based on historical rates.
11. Equation 2. The text in Lines 95-99 seems to indicate that Equation 2 is discussed in Reference 14. However, this equation is not included in Reference 14, Arps (1945). Additionally, there appears to be mathematical issue with this equation since one option has $b=0$, but then the exponent $1/b$ would be $1/0$, which is impossible to answer since division by zero is undefined. This equation should be corrected, correctly referenced, each variable should be defined and units stated (including t).
Author Response: Edited; thank you. The reviewer is incorrect; these equations are present in Pg 19, table 5. We express all 3 forms of the equation in the table and expand the explanation to include the range of values of b for each equation.
12. Line 118. This sentence is misleading. In the field of CCUS, there are currently well over 100+ fields with data collected. Additionally, "injector production" is confusing as well: An injection well adds fluid to the subsurface, but a production well removes fluid from the subsurface. Which is meant by this term? In general I would say that data has been collected (although data itself is sometimes difficult to share, which is a different issue.) Even in the ML realm, Reference 23 states "ML algorithms have been widely used in CCS research and achieved good effect...". The beginning of this paragraph should be re-written to be in line what the references show as well.
Author Response: Edited; thank you. We have replaced the word "injector production" with "well" performance. We have rewritten the paragraph slightly.
13. Line 123. The Iskander et al sentence is missing the reference number.
Author Response: Edited; thank you
14. Table 1. A description of what the 34 measurements are needed. For example, what is "Avg_PLT_CO2VentRate_TPH" actually measuring and what are the units? The short names are sometimes not very descriptive. Also, what does "Non-Zero Value" mean?
Author Response: We have edited the and address this in the nomenclature table.
15. Line 212. Another plus of LSTMs are that they are "effective at capturing long-term temporal dependencies without suffering from the optimization hurdles that plague recurrent networks", right? (Greff et al., 2015)
Author Response: Reference has been included; thank you

16. Figure 4. Y-axis appears to be truncated. Colorbar needs descriptor.

Author Response: Edited; thank you

17. Line 270. Why were these 6 variables in particular retained?

Author response: Many variables exhibit strong correlations, with coefficients exceeding 0.5 (See correlation matrix). To prevent multicollinearity issues, we retained only one variable from each group of highly correlated variables. Exceptions were made when variables originated from different sources, such as tubing and reservoir pressure at the observation well. Excluding the target injection delta variable, we selected eight variables for the machine learning application.

18. Figure 5. What is the y-axis with units on 5b?

Author response: tonnes per hour. Figure amended.

19. Figure 5 and 6. The 5b and 6b close up comparisons between the actual and LSTM predictions do not match up well. There should be some discussion about why this is okay (or not). Are the larger amplitude variations of greater interest in a real-world setting and is your model capturing those wiggle-for-wiggle? (Can't tell from the figure.) Are these smaller scale variations not of importance in a real-world setting? Is further decimation of the data necessary and/or useful?

Author Response: Fig 5 is just showing one example from a K-fold. It's a smaller data set, so the match will be poorer, but the model uses these numerous small data sets to ultimately tune the large scale macro model.

20. Line 318. How are you defining an anomaly? How is this useful in a real world example?

Author Response: In a CO₂ injection project, we anticipate maintaining a consistent optimum injection rate and injection pressure – therefore we define an anomaly as anything that disrupts the equilibrium seen in past measurements.

21. Table 4. A description of the Varied Parameters is needed. For example, what does "Z-Score Inj_Diff" actually mean? This actually appears to be two tables stitched together, they should be separated and separately described.

Author Response: Noted; we have split the table as requested although we think it makes for a less impactful presentation. We have explained what Z-score means in “Nomenclature”; its just a conventional statistical measurement, like mean or mode.

22. Table 5. Table 5 appears to be truncated. No column headers. Cannot evaluate.

Author Response: Noted; it is not truncated. We have added a new column header (there was a previous header there already) – we hope this is clearer

23. Figure 7. The comparisons do not appear to match up well even though the authors indicate that "all results show small perturbations around the unseeded value". There should be some discussion about why variations up to an order of magnitude difference is okay (or not).

Author Response: We remind the reviewer that the expectation that the results match perfectly when initial conditions change is an unreasonable one to make. Of course, the results will be different. What we want to demonstrate is that it is insensitive to initial seed values because results only change within +/- 10% of a base (unseeded value) case. We are measuring at fractions of a psi, after all.

24. Figure 8. Units needed on y-axis. X-axis units are unclear, is this days? What do the yellow and green boxes represent? Where are the four anomalies described in the text?

Author Response: This figure is replaced with something that we hope is clearer.

25. Line 418. Your motivation is important and should also be stated in the introduction to better emphasize the strength of your technique.

Author Response: Noted; we have emphasized this again in the introduction and conclusion.

26. Conclusions. How would a significant equipment failure (or similar event) in the training dataset be represented? Would the data need to be cleaned, or would it be able to cope? What if there was such a failure in the testing dataset? In an operational example? What would happen?

Author Response: Equipment failure can indeed lead to anomalous readings in the sensor data. For instance, if the pump malfunctions, it would likely affect the injection well's wellhead pressure, which in turn would be detected by the downhole sensors. The model would recognize this deviation from the normal operating pattern as an anomaly, prompting operators to investigate and address the issue promptly. Moreover, such anomalies serve as indicators that the containment of CO₂ is intact, providing assurance of safety and operational integrity. On the other hand, if there is a failure in the wellbore, the anomaly would likely manifest in the nearest sensor of the injection well. However, there may not be corresponding changes in the injection pressure or other sensors in the well.

Nonetheless, this anomaly would still trigger an alert regarding the injection delta, signaling operations to investigate further. Once confirmed, actions such as shutting in the well and initiating wellbore repair procedures would be taken promptly to maintain operational efficiency and prevent any potential environmental or safety concerns.

Highlights

- CCUS is one method to deal with produced CO₂.
- Prediction how the CO₂ behaves in the subsurface once injected is difficult.
- We aim to use LSTM neural networks to predict injection deltas, which are changes that occur during the injection process.
- The input data source comprises measurements taken from sensors located a distance away in a monitoring well.
- Predicting this change can be used to provide a checkpoint against carbon plume migration and can determine if there are losses in the injection process.

1 **Title: Utilisation of Artificial Intelligence based Time-Series Prediction to validate**

2 **Carbon Containment in Injection Well in Illinois Basin**

3

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5

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8

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10

11 **Abstract:**

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

17

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

23

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

27

28 **One-Sentence Summary:** Applying machine learning and predictive analytics via time series injection
29 information and monitoring data on a carbon sequestration well to predict well injection rate deltas.
30
31 **Keywords (minimum 6):** low-carbon, time-series, neural network, LSTM, carbon capture, injection pressure,
32 monitoring, migration
33

34 **Introduction**

35 The burning of coal, oil, and natural gas has resulted in the generation of various greenhouse gases such as
36 carbon dioxide (CO_2), methane (CH_4) and nitrous oxide (N_2O) [1]. A report generated Liu et al revealed that
37 global CO_2 emissions for 2022 reached 36.1 Gt CO_2 [2]. Failure to effectively manage such substantial
38 quantities will result in irreversible environmental consequences.

39

40 Carbon Capture Utilisation and Storage (CCUS) is one promising method to deal with the produced CO_2
41 from anthropogenic sources. The idea is to capture CO_2 from an emission point source and subsequent
42 sequester it via injection into a suitable geological formation, with the explicit aim to store the CO_2 safely, in
43 a state of permanence. CCUS is now being viewed as a key technology that will assist us in reaching
44 increasingly ambitious global anthropogenic climate change goals. Typically, CO_2 geologic storage can be
45 carried out in a number of different ways, including Enhanced Oil Recovery (EOR) processes, injection into
46 virgin saline aquifers or into depleted oil and gas fields. These methods all have different project drivers, risks,
47 and commercial implications. However, what these three methods have in common is the requirement that (a)
48 there be a good understanding of the subsurface geological properties and (b) there be some ability to monitor
49 and even predict CO_2 containment behaviour at the well scale, be it during the injection phase or during the
50 shut-in phase.

51

52 **The importance of real-time CO_2 containment monitoring in the subsurface**

53 Evaluating CO_2 containment is a multiscale challenge, with measurement scales spanning orders of
54 magnitude, from kilometres to nanometres. At the reservoir (kilometres to meters) scale, satellite-based remote
55 sensing, 4D seismic monitoring, tiltmeters, downhole sensors and tracers deployed within injection wells can
56 offer precise data on CO_2 distribution. At the centimetre to nanometre scale, geochemical monitoring of
57 produced fluids provides insights into CO_2 interactions with subsurface formations. The intermediate scale
58 (meters to centimetre) is where conventional “well-based” measurements are conducted. These include the

59 monitoring of CO₂ injection rates, well (annulus) pressures, casing pressure tests, and cased hole/production
60 logging measurements. This enables a real-time assessment of CO₂ injection efficiency and potential leakage.

61
62 There have been documented instances where the abovementioned techniques have worked well in CO₂
63 containment monitoring. One example is the Equinor operated Sleipner Project in the North Sea where the
64 operator utilised seismic surveys and downhole pressure measurements to demonstrate effective containment
65 [4]. Yet, there are also documented instances where, despite extensive monitoring efforts, unexpected CO₂
66 leakage behaviour does occur. The In Salah project in Algeria, led by BP, Statoil, and Sonatrach, is one such
67 example [5]. The latter underscores the importance of continual vigilance and timely adaptive management in
68 CO₂ containment to mitigate risks effectively.

69
70 The above examples illustrate that it is sometimes not enough to rely solely on hardware based solutions
71 like sensor measurements at the monitoring well. Rather, we postulate that subtle fluctuations in injection
72 rates can act as predictors for potential future containment breaches. By training a machine learning model
73 to recognise these subtle fluctuations, potential containment breaches can be flagged prior to them occurring.
74 If the model triggers in such events, the operator would simply need to shut the well in and investigate, for
75 risk mitigation purposes.

76
77 **The Significance and Complexity of Optimising CO₂ Injection Rates**

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

82
83 Reservoir heterogeneity, encompassing permeability, porosity, and lithology, significantly influences
84 injection rates. High-permeability formations facilitate rapid CO₂ flow, while geological features such as
85 layering, faults, and fractures can both enhance CO₂ distribution and affect injection rates. Injecting CO₂ too

86 rapidly can induce skin effects, diminishing overall field injectivity. Moreover, reservoir pressure, inversely
87 correlated with the volume of CO₂ injected, must be carefully managed to prevent overfilling, which can lead
88 to seismic activity and potential CO₂ containment breach.

89
90 In essence, comprehending the intricate interplay between reservoir capacity and injection parameters is
91 imperative for ensuring the efficiency and safety of CO₂ sequestration endeavours. This understanding extends
92 to recognising the temporal dynamics of CO₂ injectivity and its relationship with various influencing factors
93 over time. Through the analysis of historical CO₂ injectivity data and its correlation with time-sensitive
94 parameters, engineers can refine reservoir management strategies via modeling and scenario analysis. This
95 approach allows for informed decision-making regarding CO₂ storage and utilisation projects, ultimately
96 advancing the efficacy and sustainability of carbon capture and storage initiatives.

97 **Literature Review**

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

107
108 Within reservoir engineering, the extrapolation of hydrocarbon and water recovery rates from geological
109 formations into the future can be viewed as a type of time-series forecasting. Empirical solutions developed
110 by Arps [16], referred to as decline curve analysis (DCA) technique is one of the earliest methods to address
111 this problem. The method is based on a curve-fit principle, where one would attempt to fit either exponential,

112 hyperbolic or harmonic curve to historical flow production rate as a function of time. Equation 1 shows the
113 general form of the equation, while Equation 2 and Equation 3 are more specialised forms of the equation:

114

General Form

(Hyperbolic Decline)

$$q(t) = \frac{q_i}{(1 + bD_i t)^{1/b}} \quad \text{Equation 1}$$

Exponential Decline

$$q(t) = q_i e^{-dt} \quad \text{Equation 2}$$

Harmonic Decline

$$q(t) = \frac{q_i}{(1 + bD_i t)} \quad \text{Equation 3}$$

115
116 where q_t is the flow rate at time t (bbls/day), q_i is the initial flow rate (bbls/day), t is time (day), D_i is the initial
117 decline rate (%), and b is the degree of curvature of the line (Arps' decline-curve exponent). A hyperbolic
118 curve would have $0 < b < 1$ and a harmonic curve would have $b = 1$. The fitted curve is then used to predict
119 future production rates and cumulative production [17]. This method was originally designed to work with
120 high porosity-permeability reservoirs and tends to overestimate hydrocarbon recovery from unconventional
121 (low permeability) reservoirs. Thus, various authors have tried to expand on this work [18, 19, 20, 21], and
122 are mostly variations of the initial DCA method developed by Arps. For an effective DCA forecast, domain
123 and field knowledge are key, but inherently the process is one of trial and error, and thus it is not uncommon
124 for DCA results to have 'low-best-high' estimates.

125
126 With the advent of big data, fast computing and cheap memory, applying a machine learning (ML) and
127 artificial intelligence (AI) solution for time-series forecasting seems a natural evolution. ML solutions were
128 first introduced to the petroleum industry in the early 2000s. Applications of ML and AI include addressing
129 prediction of reservoir parameters [22], history matching, of oil, gas and water production forecasting (flow
130 rate prediction), pattern recognition in well logs and well tests analysis, production enhancement and
131 prediction of failures, among others [23, 24, 25].

132

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

143

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

148

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

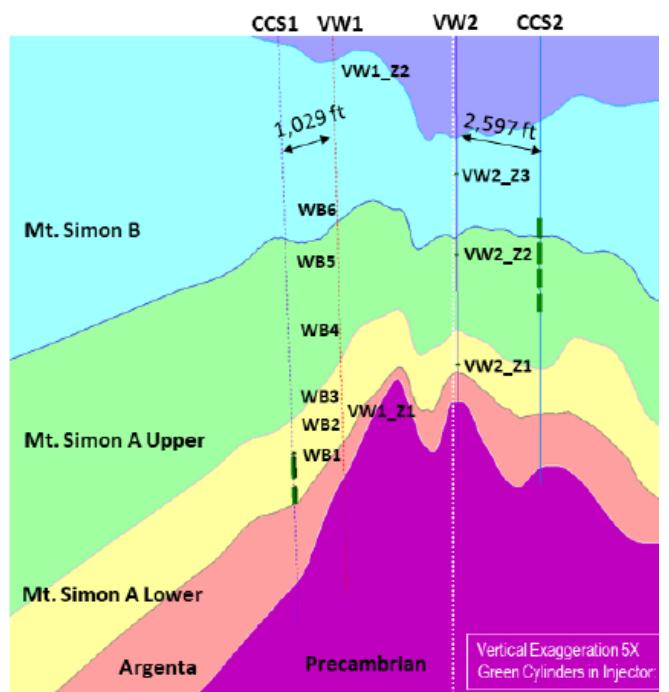
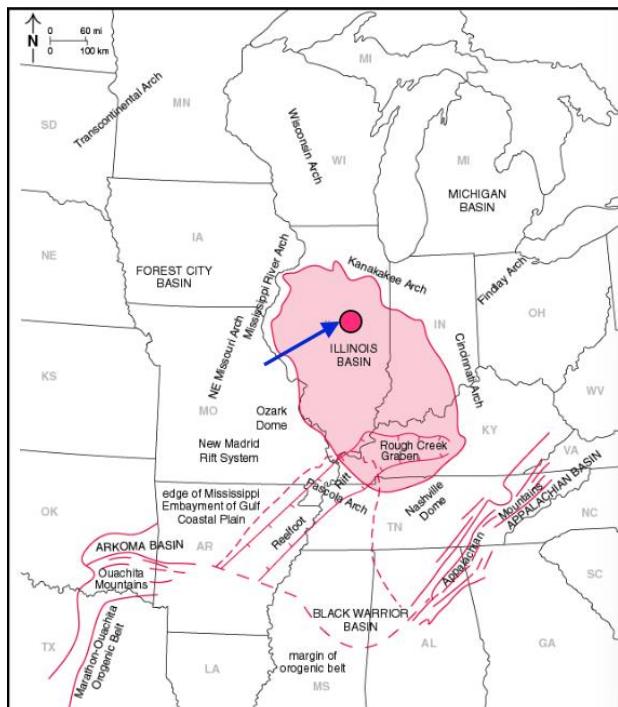
156

157 **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 (Δ or inj_diff) which is the difference in the injection rate (IR) at time t and time (t-1) i.e.

$$\Delta = IR_t - IR_{t-1} \quad \text{Equation 4}$$

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.



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

176

177 **Datasets**

178 During this three-year period, a substantial amount of data was collected from both an injection and
179 monitoring well, 1007 ft apart. The injection well was drilled to a total depth (TD) of ~7238 ft, and was drilled
180 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
181 5339 ft, and an intermediate casing string 13 3/8" in diameter was set. The reservoir section was drilled in a
182 12 ½" hole size to ~ 7056 ft and completed with a 9 5/8" production casing and 4 ½" tubing. The perforations
183 were made at the base (i.e. above the Precambrian) Mt. Simon Sandstone, which was a relatively thick
184 reservoir of ~1620 ft. A total of 3 geophones were set at 4925 ft, 5743 ft and 6137 ft along with a pressure /
185 temperature gauge mandrel at 6325 ft. The monitor well was drilled to a total TD of 7272 ft; it had a surface
186 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.
187 St Simon Sandstone, which contained a 3 component geophone array) [3].

188

189 A. Data Collection and Preparation

190 A total of 34 parameters were measured from the injection and verification well. The parameters measured
191 comprised of both surface and downhole measurements which were acquired at five second intervals over
192 three full years. The sheer volume of data required that the time scale be downscaled to hourly intervals, taking
193 the parameter average over the hour. 27,665 hours of data (training data) was used to build a suitable model.
194 67% of the “training” data set was used to train the model. The remaining 33% was used as a “validation”
195 dataset. The model built off this data was finally used to predict 201 hours of Δ into the future (“hold out”
196 data). Given in Table 1 is the descriptive statistics of the provided data; we refer readers to the nomenclature
197 table for the definition of the variables. We note that there are a series of “null values” (including negative
198 null values) and non-numeric numbers, missing rows, time gaps and note that for some of the input data
199 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

202

203

B. Cleaning Data

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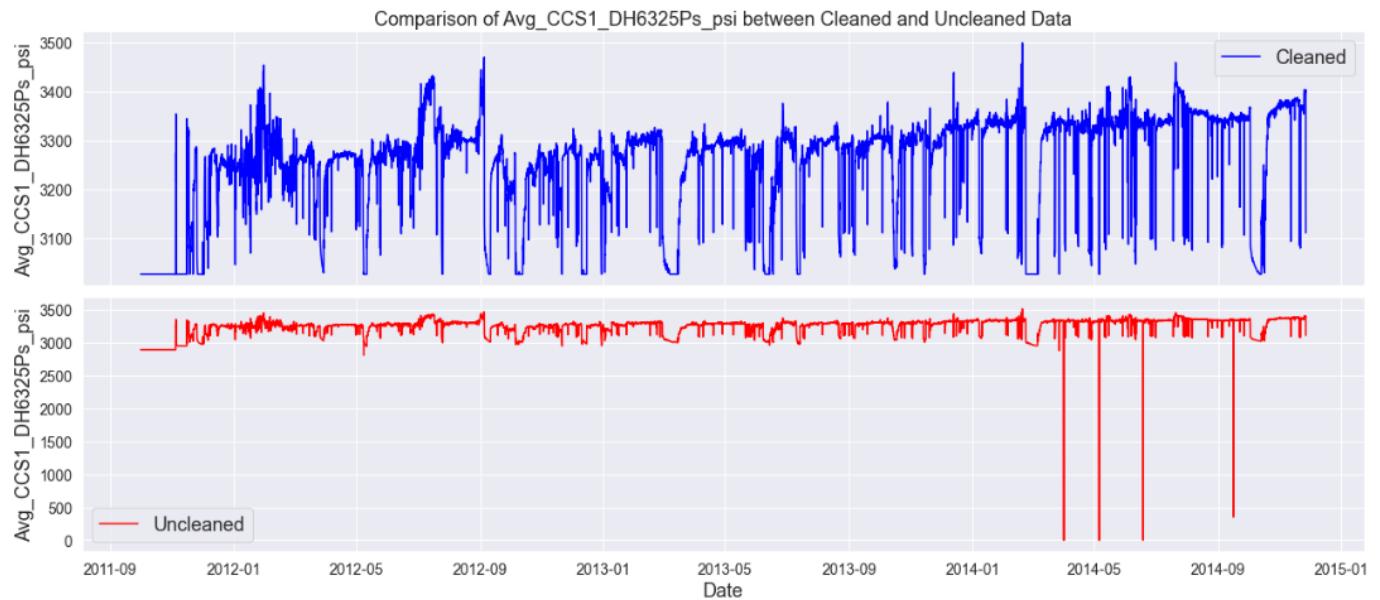
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218

219

$$Z = \frac{x_i - \tilde{x}}{MAD} \quad \text{Equation 5}$$

x_i is a single data value, \tilde{x} 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.



220
221 Figure 2: An example of the measurement before (lower image) and after (upper image) data cleaning.
222
223

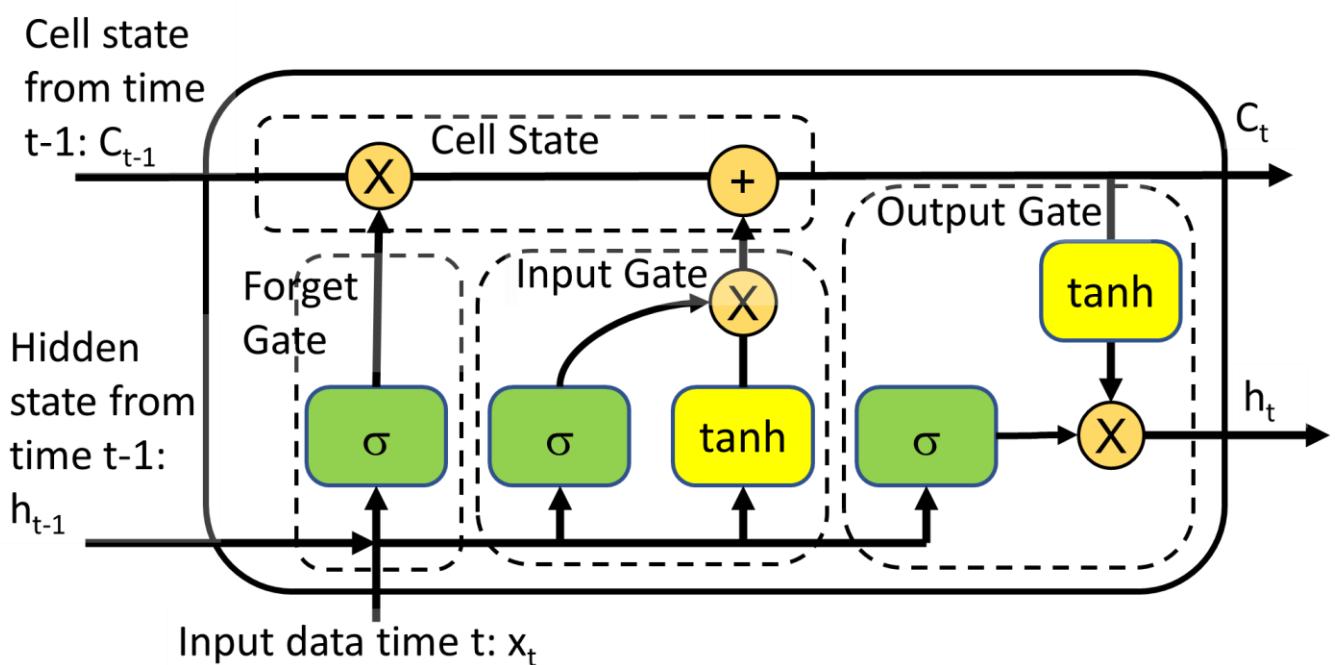
224
225 *C. Machine Learning Model Selection - Long Short-Term Memory (LSTM) vs. Autoregressive Integrated
226 Moving Average (ARIMA)*

227 In the choice of ML model to apply, we had to decide between a statistical approach based on ARIMA, or
228 alternatively, the use of a non-linear algorithm such as neural networks (NN). Many authors have investigated
229 comparing such methods and in various fields. What we noted from our review of the work was there was a
230 general agreement that approaches like ARIMA would not only require less inputs, but would be less of a
231 “black-box”, which NNs are known to be [30, 31, 32].
232

233 ARIMA has been applied by previous authors to forecast oil production data [33]. The “autoregressive”
234 piece of ARIMA deals with finding a correlation between a specific value and a prior/lagged value, essentially
235 seeing if a variable has any correlation to its past values. The “integrated” piece deals with making data
236 stationary, essentially ensuring that properties of the data (such as mean and variance), are constant over time.
237 The “moving average” piece of the model finds the dependency between a specific value, and the error from
238 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

239 models being produced with high frequency data, where accuracy on an hourly basis was important, found
240 that the error rate compounds significantly when the forecasting horizon is extended beyond a day [34].

241
242 LSTM is a type of recurrent NN which uses useful patterns from sequential data to provide accurate
243 forecasts [23]. It learns from previous outputs to provide better results the following time. A typical LSTM
244 has 3 layers (i) an input gate which assigns weights based on the significance of different variables, (ii) a
245 forget gate to retain only useful information, and (iii) an output gate which manages the information flow.
246 LSTM holds a memory cell (known as a cell state) which retains captured information over longer time periods
247 and preserves useful constituents using its input and forget gates, hence avoiding the vanishing gradient issue
248 associated with traditional NNs. LSTMs are particularly useful for non-linear problems where there does not
249 appear to be strict mathematical relationships between variables. Unlike recurrent NNs, LSTMs can account
250 for long-term temporal effects without encountering optimisation hurdles like vanishing gradients [35]. In our
251 review of LSTM vs ARIMA models, we have found a common consensus in various fields that LSTM
252 performed better, with reduced error rates but with significantly increased processing time [32, 31].
253



254 Figure 3: Schematic of LSTM network
255

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

260

261 *D. Model Performance and Hyperparameter Optimization*

262 We access the model performance using a host of measures, from training and validation loss to mean
263 absolute error (MAE - Equation 6), mean squared error (MSE - Equation 7), root mean squared error (RMSE
264 - Equation 8) and the coefficient of determination (R^2 - Equation 9). The training and validation loss functions
265 serve to determine how well the model is performing and to prevent overfitting. During training, the model
266 learns by iteratively adjusting its parameters to minimize a defined loss function. The training loss measures
267 the discrepancy between the model's predictions and the actual target values on the training data. The goal is
268 the minimization of this loss, as it indicates how well the model is fitting the training data. The validation loss
269 is the other component of this and is computed by evaluating the model's performance on a separate validation
270 dataset, not used for training. It serves as an estimate of how well the model generalizes to unseen data.

271

MAE:
$$\frac{1}{n} \sum_{i=1}^n |y_i - x_i| \quad \text{Equation 6}$$

MSE:
$$\frac{1}{n} \sum_{i=1}^n (y_i - x_i)^2 \quad \text{Equation 7}$$

RMSE:
$$\sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - x_i)^2} \quad \text{Equation 8}$$

R^2 :
$$1 - \frac{\sum (y_i - x_i)^2}{\sum (x_i - \bar{x})^2} \quad \text{Equation 9}$$

272

273 Equation 6 to Equation 9 show the other measurement metrics, with y_i as the predicted value, x_i as the true
274 value, \bar{x} as the mean of x_i and n as the total number of data points. MAE measures the average absolute
275 difference between the predicted and actual values and provides an absolute measure of the model's

276 performance. MSE measures the average squared difference between the predicted and actual values and
277 amplifies larger errors due to the squaring operation. RMSE is the square root of MSE and provides a measure
278 of the average magnitude of errors. It is useful for interpreting errors in the same units as the target variable.
279 R² measures the proportion of the variance in the target variable that is explained by the model. It ranges from
280 0 to 1, where 1 indicates a perfect fit and 0 indicates a poor fit.

281
282 While MAE, MSE, RMSE, and R² are evaluation metrics used to assess the model's performance after
283 training, the (training and validation) loss functions are specific to the training process. These loss functions
284 guide the model's learning by providing gradients for updating the model's parameters. However, the
285 suitability of the model is ultimately guided by scores where the MAE, MSE and RMSE are low, while the
286 R² is high.

287
288 The NN model is tuned by varying a series of “hyperparameters”. A hyperparameter is a characteristic of
289 a model that is external to the model and whose value cannot be estimated from data. The hyperparameters
290 that were optimized included the (i) learning rate, (ii) the epochs, (iii) the number of neurons, (iv) the
291 magnitude of dropout, (v) batch size, (vi) the choice of optimiser and finally (vii) the choice of activation
292 function. To account for idiosyncrasies in the data (noise, patterns, outliers, etc.), k-fold cross-validation was
293 run to validate the stability of the model.

294
295 **Results and Discussion**

296 **Data Preparation**

297 We observed significant collinearity of > 0.8 across most of the data set. Most were paired couplet
298 measurements of “Temperature” and “Pressure” at various gauge depths. Keeping both parameters adds no
299 additional information to the predictive model and in fact may be detrimental, with potential overfitting.
300 Therefore, a single element from each of the variable pairs is eliminated to allow for a more stable model.
301 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.

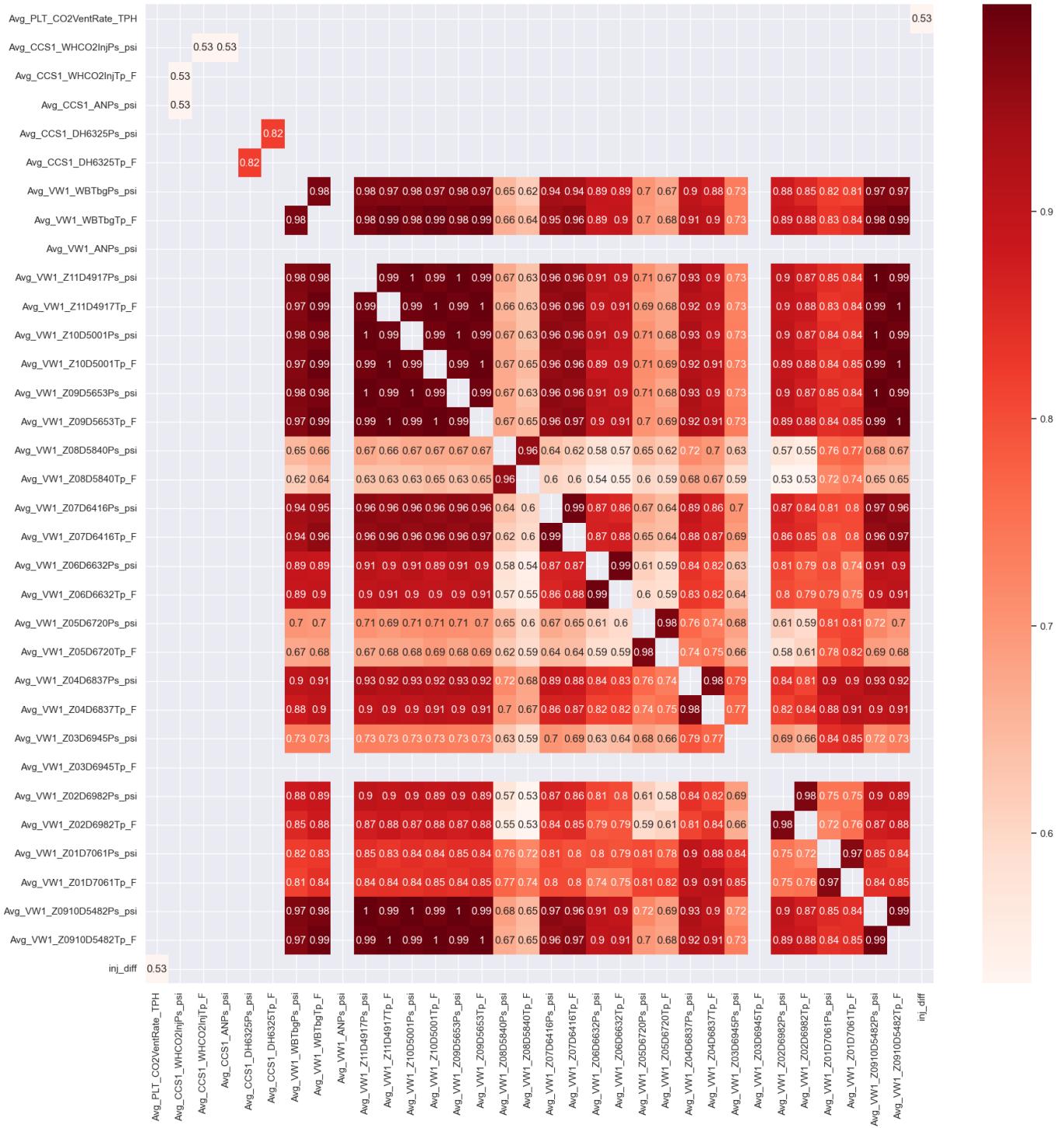


Figure 4: Correlation Matrix – Pairwise Correlation. It ranges from -1 to 1, -1 being a perfect negative correlation and +1 being a perfect positive correlation. The color scale visually depicts this: dark/warm show strong correlations

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

313

314 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

315

316 LSTM Model Architecture

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

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

330

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

334

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

342

343

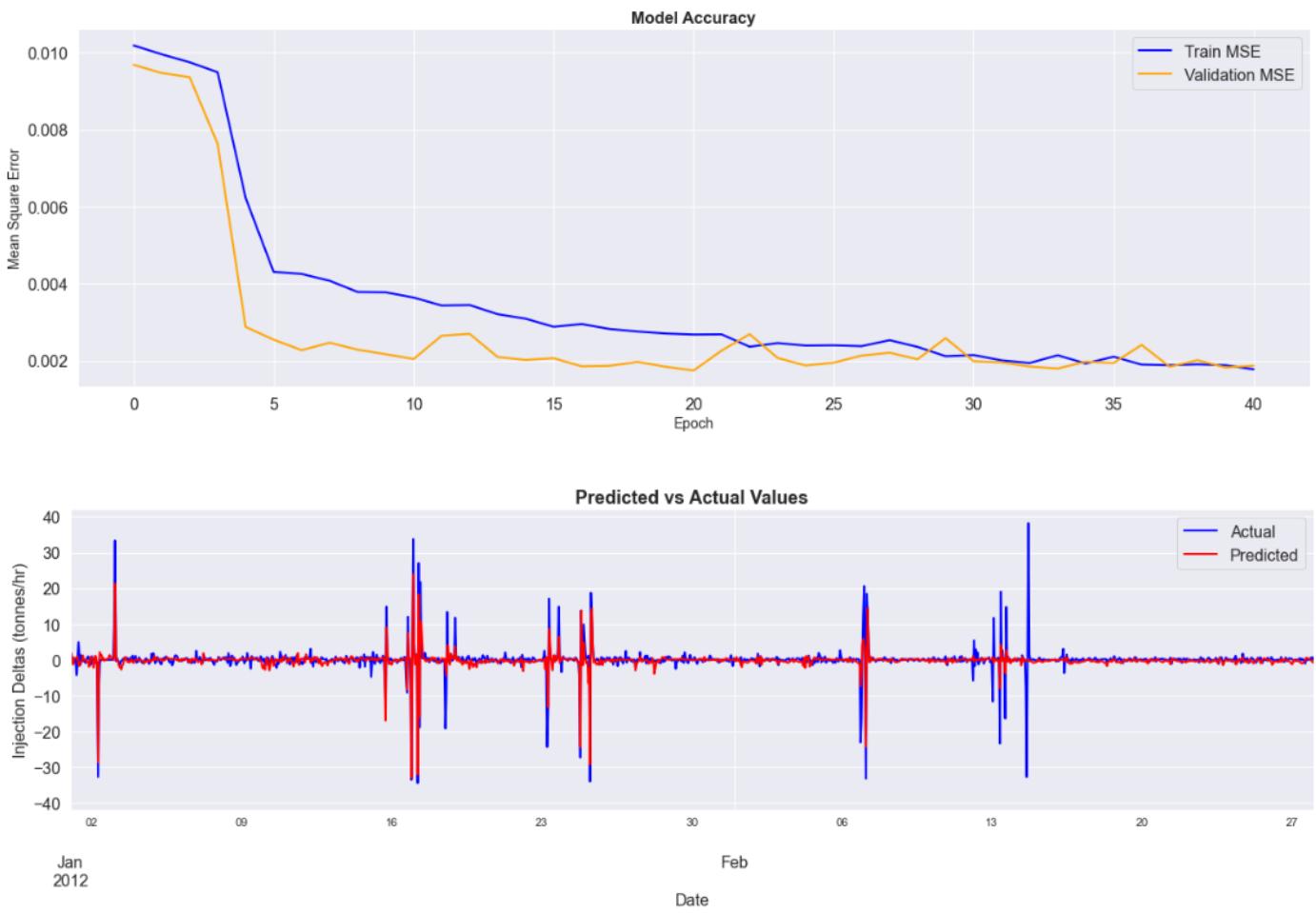
Table 3: Variation in Hyperparameter Values, Final Selected Values and Parameter descriptor

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: $f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

344

345 Figure 5 shows the MSE output of the training (train) and validation (val) sets for one of our K-folds. MSE
 346 is on the y-axis and epoch is on the x-axis. We observe the convergence between train and val, telling us that
 347 the model accuracy is improving per epoch. The point of convergence is arrived at by gradient descent and
 348 tells us the point of minimum information loss. In this example, we achieved convergence at around epoch =
 349 30, with losses increasing beyond that.



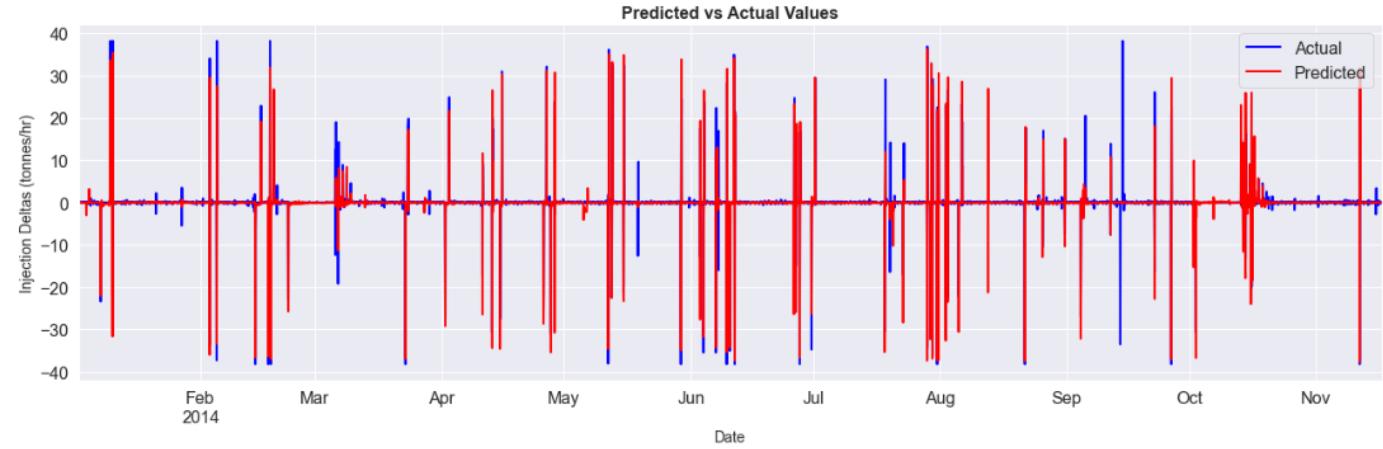
350
351 Figure 5: (Upper) MSE output of the training and validation set (Lower) Check file of a small subset of
352 data; output from the K-fold set.
353

354 355 Prediction on Validation Data

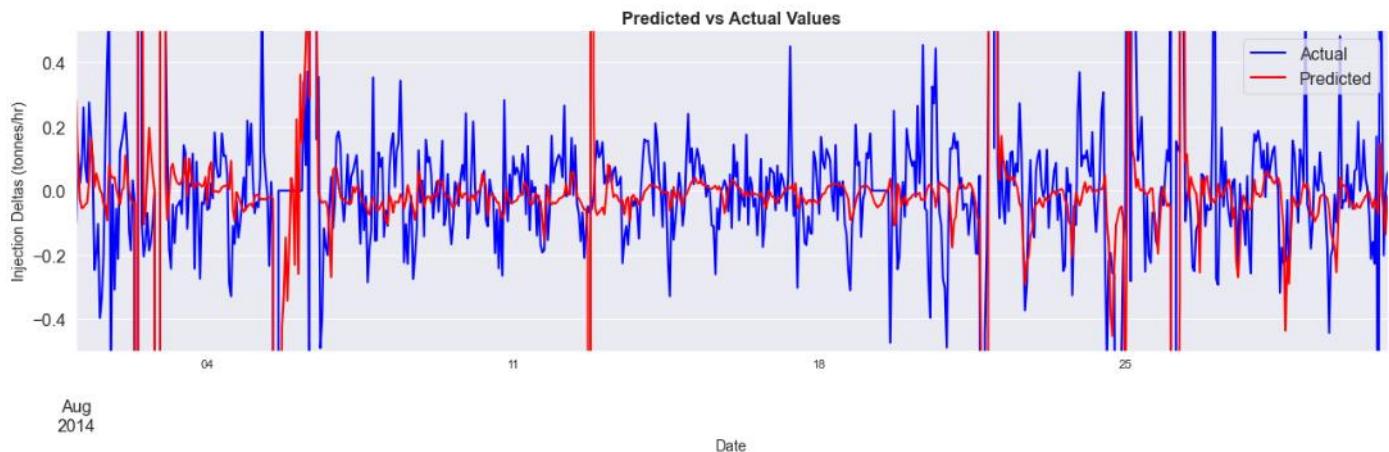
356 We deployed our developed model on our validation data. Given in Figure 6 is the comparison between
357 the predicted injection rate deltas versus the actual injection rate deltas in our validation set. The results
358 demonstrate the model's capability to successfully identify and replicate actual anomalies, which provides
359 evidence that the model is predictive in nature. Moreover, Figure 6 illustrates that the model can accurately
360 capture both large scale high frequency signal, as well as smaller scale fluctuations in the injection deltas
361 (admittedly, the subtle variations are harder to capture as these change at ranges of $\pm 1\text{psi}$ and can be described
362 to be in the domain of "noise"), indicating the robustness of the LSTM model.
363

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

369



370



371

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

374

375 Generalising the model

376 This LSTM model was built from (what is fundamentally) a single data set i.e. from a specific geological
377 rock type, whose CO₂ flow behaviour is constrained by its own petrophysical and reservoir engineering
378 properties. We think further generalisation of the model is necessary to truly confirm these findings. As we

379 do not have data from other geological settings, we attempted generalisation through a series of sensitivity
380 runs. We did this in 2 ways (a) selecting a single seed value but varying the input parameters fed into the
381 model and (b) by randomising the seed value itself but keeping the input parameters constant.

382

383 *(a) Single Seed, Variable Inputs*

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

387

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

394

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

401
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

402
403 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

404
405 Randomness406 NN themselves are not inherently stochastic, as they follow deterministic mathematical operations, and the
407 inputs, weights, and biases are all fixed values during inference. However, the stochastic nature of the NN
408 model becomes apparent when seed values are varied; different seed values result in different results.409
410 Our next test for the generality of the model involved running various seed values (we utilised 10 different
411 values) and determining if both high and low amplitude delta values could be predicted. Seven selected results
412 are displayed in Table 6 while Figure 7 to show the range of comparison with respect to the first unseeded
413 run.414
415 We observe that while all runs can predict the anomalies, the signature of the minor differences varies
416 between seed values (Table 6). We also observe that the RMSE and R2 values on the validation set all lie

417 within a small range ($\pm 10\%$ or up to 0.2 psi absolute) of the unseeded value (Figure 7). Thus, to account for
418 randomness and to retain the unbiased nature of the model, an unseeded model is selected for deployment.

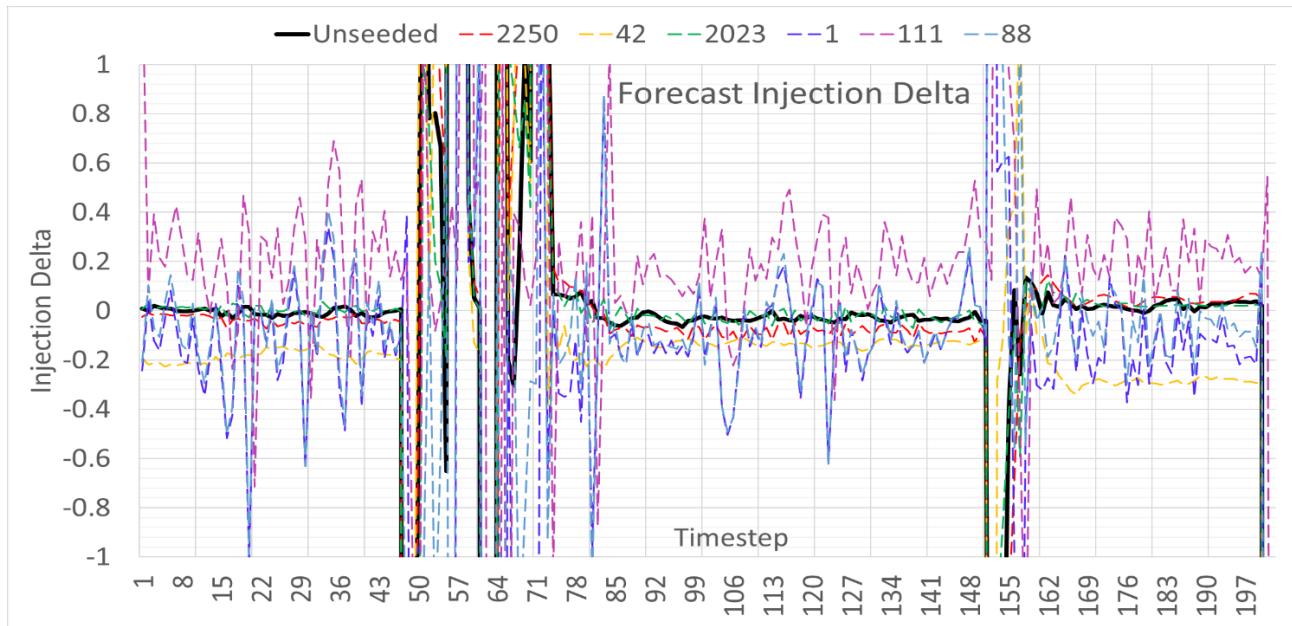
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420

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

421



422

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

424

Evaluation against the “Hold-out” Data

425

We test the predictive capability of the model by passing downhole sensor measurements never seen by
426 the model (our “hold out” data set), to determine if the model can detect injection rate anomalies.
427

428

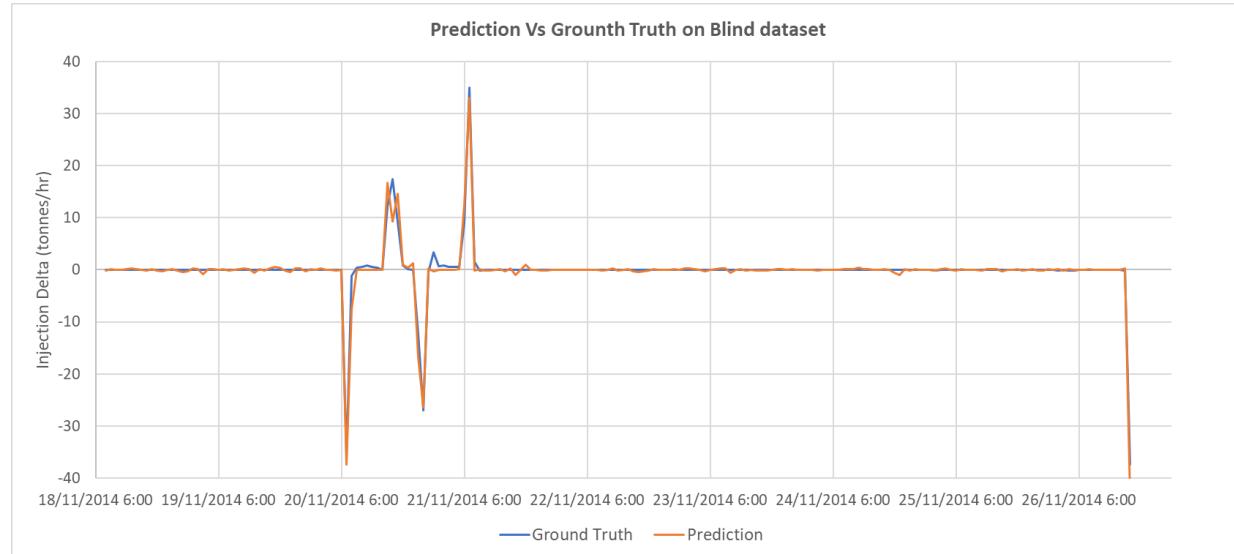
429 Figure 8 shows the results of this test, where our model has successfully predicated the presence of four
430 anomalies in the injection rates. When we plot this prediction against what the actual injection rates were (our
431 “ground truth” data), we observe a near perfect overlap in results.

432 **Error! Reference source not found.**

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

437

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



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

444

445 **Discussion & Recommendations**

446 We think there are several ways to further enhance the model's performance. First, incorporating the
447 response of the operator when an anomaly is marked as safe reduces the likelihood of flagging similar

448 anomalies in the future. This feedback loop mechanism can help refine the model's predictive accuracy and
449 ensure more reliable results over time.

450

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

454

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

459

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

463

464 **Conclusion**

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

469

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

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

484
485 We also recommended a series of improvements and model enhancements in this paper which would
486 increase the machine learning model's predictive ability, potentially providing operators with timely alerts for
487 potential leaks while optimizing operational efficiency and cost-effectiveness.

488
489 **Nomenclature**

GHG	greenhouse gas
CO ₂	carbon dioxide
CH ₄	methane
N ₂ O	nitrous oxide
EPA	Environmental Protection Agency
CCUS	Carbon Capture Utilisation and Storage
EOR	Enhanced Oil Recovery
Δ	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
q_i	initial rate (bbls/day)
D_i	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
R^2	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

490

491 **Acknowledgements**

492

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494

495 **Reference**

496

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499

1 Title: Utilisation of Artificial Intelligence based Time-Series Prediction to validate

2 Carbon Containment in Injection Well in Illinois Basin

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11 Abstract:

Carbon Capture Utilisation and Storage (CCUS) involves capturing CO₂ emissions and securely storing them in geological formations. CCUS is gaining significance in global efforts to meet ambitious climate goals. The storage of CO₂ typically occurs through injection into saline aquifers, depleted oil and gas fields, or for Enhanced Oil Recovery (EOR). However, all methods require a deep understanding of subsurface geology and the ability to monitor CO₂ behaviour during injection and storage.

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Pilot projects like the Illinois Basin-Decatur Project demonstrated the practical feasibility of storing CO₂ underground. The injection spanned three years, during which nearly 999,215 tonnes of CO₂ was stored. Monitoring was carried out through a pair of wells equipped with sensors to track pressure and temperature at various depths.

This paper focuses on using time series injection data and monitoring information to predict changes in injection rates for the carbon capture 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.

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

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34
35 Our work aims to show that Machine learning methods are applied to can be useful to forecast these injection
36 rate deltas based on monitoring data, thereby validating providing a way that is complimentary to traditional
37 methods, to determine the effectiveness of carbon containment during injection.

38
39 **One-Sentence Summary:** Applying machine learning and predictive analytics via time series injection
40 information and monitoring data on a carbon capture-sequestration well to predict well injection rate deltas.
41

42 **Keywords (minimum 6):** low-carbon, time-series, neural network, LSTM, carbon capture, injection pressure,
43 monitoring, plume-migration
44

45 **Introduction**

46 ~~Undoubtedly, human activities stand as a prominent cause behind the surge in greenhouse gas (GHG)~~
47 ~~emissions and the subsequent global warming. The escalation of carbon dioxide (CO₂) levels can primarily be~~
48 ~~attributed to swift industrialization and population expansion, which have only accelerated since the 1960s~~

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49 The burning of fossil fuels (such as coal, oil, and natural gas) has resulted in the generation of various
50 greenhouse gases such as carbon dioxide (CO₂), methane (CH₄) and nitrous oxide (N₂O) generation.^{[1][4]} A
51 report generated by the United States Environmental Protection Agency (EPA) evaluated the amount of CO₂
52 generated in 2020 to be 3.11 million metric tons.^{Liu et al revealed that global CO₂ emissions for 2022 reached}
53 36.1 GtCO₂.^{[2][2]} Failure to effectively manage such substantial quantities will result in irreversible
54 environmental consequences.

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56 Carbon Capture Utilisation and Storage (CCUS) is one promising method to deal with the produced CO₂
57 from anthropogenic sources. The idea is to capture CO₂ from an emission point source and subsequent
58 sequester it via injection into a suitable geological formation, with the explicit aim to store the CO₂ safely, in
59 a state of permanence. CCUS is now being viewed as a key technology that will assist us in reaching
60 increasingly ambitious global anthropogenic climate change goals. Typically, CO₂ geologic storage can be
61 carried out in a number of different ways, including Enhanced Oil Recovery (EOR) processes. CO₂-storage is
62 carried out in one of three ways – via injection into virgin saline aquifers or into depleted oil and gas fields;
63 or if used for Enhanced Oil Recovery (EOR) processes. These methods all have different project drivers, risks,
64 and commercial implications. However, what these 3three methods have in common is the requirement that
65 (a) there be a good understanding of the subsurface geological properties and (b) there be some ability to
66 monitor and even predict CO₂ migrationcontainment behaviour at the well scale, be it during the injection
67 phase or during the shut-in phase.

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68
69 The importance of real-time CO₂ migrationcontainment monitoring in the subsurface

Evaluating CO₂ migration containment is hard to predict, given its dynamic nature and its interaction with geological formations. CO₂ behaviour in the subsurface 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 and migration paths. At the centimetre to nanometre scale, geochemical monitoring of produced fluids provides insights into CO₂ interactions with subsurface formations.

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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.

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Given the early stage of this technique, it is imperative to initiate pilot development and validate the technology. The Illinois Basin Decatur Project is one such study which aimed 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. 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, ~700ft apart, were drilled into the formation. The wells were equipped with downhole sensors to monitor pressure and temperature at various depths of interest.

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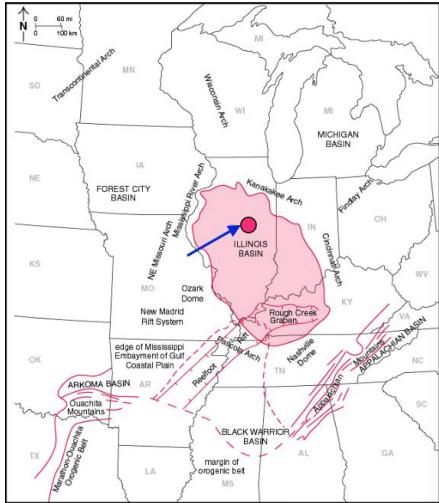


Figure 1: Location map of the Illinois Basin—Decatur Project (IBDP). Image taken from [3]

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In general, such there have been documented instances where the abovementioned techniques have worked well in CO₂ migration 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 of the CO₂ plume [4]–[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]–[5]. The latter underscores the importance of continual vigilance and timely adaptive management in CO₂ E&CUS containment projects to mitigate risks effectively.

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The above examples illustrate that it is sometimes not enough to rely solely on hardware based solutions like sensor measurements at the monitoring well are a much needed first line of defence but is not foolproof. Rather, we postulate that subtle fluctuations in injection rates can act as predictors 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, if such sensor

11 measurements are coupled with machine learning algorithms, such that subtle patterns and anomalies can be
12 detected, this may potentially act to mitigate risk further.

13

14 **The Significance and Complexity of Optimising CO₂ Injection Rates**

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

19

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

26

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

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135 Operators are interested in the maximum rate at which CO₂ should be injected into the subsurface, as
136 current climate models suggest large volumes of CO₂ need to be sequestered quickly to mitigate climate
137 change effects. However, the determination of optimal rates of CO₂ injection is a challenge
138
139 Given that operators may want to have as high a rate as possible, what are the factors that actually determine
140 the rate at which the operators are injecting CO₂ (e.g., the pressure rise in the aquifer, equipment malfunctions,
141 etc.)? This would be directly relatable to what you are predicting. Lastly, there should be a discussion about
142 why AI can become a preferred method: among other things, some existing methods to estimate subsurface
143 injection rates can become complex and/or costly when considering at a basin scale. I'm sure there are other
144 reasons that can be stated as well. What are the other ways in which maximum injection rates are currently
145 calculated? What are the tradeoffs in methods? There is often no single right way of doing things.

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147 This paper aims to use time series injection information and monitoring data on a carbon capture well to
148 predict carbon capture well injection rates deltas (Δ) which is the difference in the injection rate (IR) at time t
149 and time (t-1) i.e.

$$\Delta = IR_t - IR_{t-1}$$

Equation 1

150
151 CO₂ injectivity, or the rate at which CO₂ can be effectively injected into subsurface reservoirs, depends on
152 a multitude of factors. Geological and reservoir parameters such as permeability, porosity, and lithology
153 significantly influence injection rates. High permeability formations facilitate faster CO₂ flow, while
154 variations in reservoir characteristics, including layering, faults, and fractures, can impact CO₂ distribution
155 and flow patterns. Reservoir heterogeneity must be carefully understood to accurately predict injection rates.
156 Pressure management is crucial to prevent reservoir overpressurization, induced seismicity, or CO₂ leakage.
157 Injecting too rapidly may fill the reservoir prematurely or cause skin issues, reducing injectivity. Additionally,
158 maintaining CO₂ in a supercritical state from the wellhead to the injection point minimizes phase transitions,
159 vaporization, and hydrate formation, ensuring efficient injection. Injection pump and well design must also
160 be optimized to handle the desired rate at pressure and temperature. Achieving optimum injectivity requires

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161 balancing these factors to maximize both rate and volume. Injecting too rapidly may fill the reservoir
162 prematurely or cause skin issues, reducing injectivity. Therefore, a comprehensive understanding of reservoir
163 capacity and injection parameters is essential to ensure efficient and sustainable CO₂ sequestration.

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164 Correlating the change in injection rate to the behaviour of other parameters in the well can be used to
165 provide a checkpoint against carbon migration from the well or other losses during the process. Utilisation of
166 a machine learning (ML) method to predict injection rate deltas based on monitoring well data can be used to
167 validate carbon containment throughout the injection of the well as well.

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169 Literature Review

170 Various authors have tried numerous methods to forecast future trends based on past data/historical data.
171 Work by De Gooijer and Hyndman [6][6], for instance, reviewed a series of time-series forecast models over
172 a 25-year period, from 1985 to 2005. Their review highlighted various models being developed and applied
173 in a myriad of scenarios related to finance, statistics and manufacturing, and included methods such as (a)
174 exponential smoothing [7, 8][7, 8], (b) Autoregressive Integrated Moving Average (ARIMA) [9][9], (c)
175 seasonal models [10][10], (d) state space and structural models and the Kalman filter [11][11], (e) nonlinear
176 models [12][12][12], (f) long-range dependence models, including the family of Autoregressive Fractionally
177 Integrated Moving Average (ARFIMA) models [13][13], (g) Autoregressive Conditional
178 Heteroskedasticity/Generalized Autoregressive Conditional Heteroskedasticity (ARCH/GARCH) models
179 [14][14], and (h) count data forecasting [15][15].

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180 Within reservoir engineering, the prediction of the extrapolation of hydrocarbon and water recovery rates
181 from geological formations into the future can be attributed viewed as a type of time-series forecasting
182 problem. Empirical solutions developed by Arps [16][16], referred to as decline curve analysis (DCA)
183 technique is one of the earliest methods to address this problem. The method is based on a curve-fit principle,
184 where one would attempt to fit either exponential, hyperbolic or harmonic curve to historical flow production
185 rate as a function of time. Equation 1 shows the general form of the equation, while Equation 2 and Equation
186 3 are more specialised forms of the equation:

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General Form(Hyperbolic Decline)

$$q(t) = \frac{q_i}{(1 + bD_i t)^{1/b}}$$

Equation 1

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Exponential Decline

$$q(t) = q_i e^{-dt}$$

Equation 2

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Harmonic Decline

$$q(t) = \frac{q_i}{(1 + bD_i t)}$$

Equation 3

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where q_i is the flow rate at time t (bbls/day), q_i is the initial flow rate (bbls/day), t is time (day), D_i is the initial decline rate (%/units), and b is the degree of curvature of the line (Arps' decline-curve exponent). An exponential curve fit would have $b = 0$, 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][17-18, 19, 20][17, 18, 19, 20], and are mostly variations of the initial DCA method developed by Arps. For an effective DCA forecast, domain and field knowledge is 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.

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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][24], 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][22, 23, 24].

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In the field of CCUS and injector production performance, there is little to no available data related to time series and forecasting. This can be attributed to the early stages of development of both domains. Literature

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

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222 We aim to develop on the work of Iskander and others by utilising ML and AI methods, and in particular
223 LSTM, but focusing on the prediction of CCUS injection well performance, using the open-source information
224 from the IBDP (Illinois Basin—Decatur Project) [3][34]. We will demonstrate how our developed LSTM
225 model shows a correlation between the change in injection rate to the behaviour of other dynamic parameters
226 [29][28].

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227
228 One of the objectives of the model is to detect anomalies and alert operators to closely inspect the wells for
229 potential leaks. While still adhering to local jurisdictional requirements of well annulus pressure monitoring,
230 periodic pressure tests and cased hole logging. While the primary purpose of the ML model is as an
231 additional method utilised to checkpoint against detect unexpected carbon migration leaks, either at the well
232 location or from other losses during the injection process, we We also view the model as another means for
233 engineers to perform scenario based de-risking of exploration plays, via modelling variations in well and
234 storage parameters to validate CO₂ containment. The model will also aid in the understanding of the injection
235 process and potentially can be used to “right size” injection rates, well operations and optimise costs.

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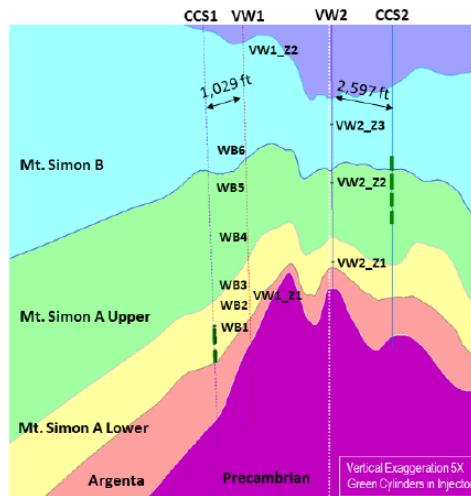
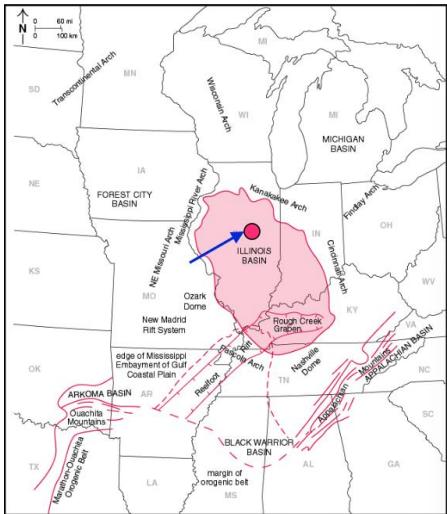
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237 **Scope and Methods**

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

241
$$\Delta = IR_t - IR_{t-1} \quad \text{Equation 4}$$

242
243 Our primary source of data is from the Illinois Basin - Decatur Project, a CO₂ pilot project meant to
244 demonstrate the capacity, injectivity, and containment of carbon storage in the Mount Simon Sandstone, the
245 main carbon storage resource in the Illinois Basin and the Midwest Region (Figure 1(L)). The source of the
246 injected CO₂ is from ethanol production at the Archer Daniels Midland company's plant. The CO₂ is
247 compressed, dehydrated and injected into the Mt. Simon Sandstone, which is primarily a saline aquifer
248 approximately ~7,000 ft deep. Injection began in 2009 and continued for a 3-year period (Nov-2011 to Nov-
249 2014). Cumulatively, ~999,215 tonnes of supercritical CO₂ have been injected and geologically stored. A pair
250 of injection and verification wells, ~1007ft apart, were drilled into the formation (Figure 1(R)). The wells
251 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). Image taken from [3](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]

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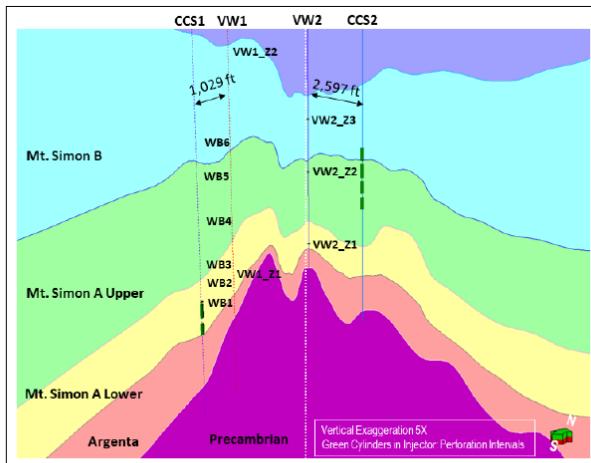


Figure 69. Location of perforation intervals in injectors (green cylinders) and pressure gauges in monitoring wells along the cross-sections I-I' (left) and II-II' (right).

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260 [Figure 2 depicts the formation layers, CC1—Injection well and the VW1, which is the verification well. It](#)
261 [also shows the perforations in the injection well in relation to the sensors at the VW1.](#)

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262 Datasets

263 During this three-year period, a substantial amount of data was collected from both an injection and
264 monitoring well, [1007700](#) ft apart. The injection well was drilled to a total depth (TD) of [~7051-7238](#) ft, and
265 was drilled with a 26" bit to 355 ft, and cased with a 20" casing to surface. A 17 1/2" hole size then followed
266 to a TD of 5339 ft, and an intermediate casing string 13 3/8" in diameter was set. The reservoir section was
267 drilled in a 12 1/2" hole size to ~ 7056 [ft, and ft and](#) completed with a 9 5/8" production casing and 4 1/2" tubing.
268 The perforations were made at the base (i.e. above the pPre-Ecambrian) Mt. St-Simon Sandstone, which was
269 a relatively thick reservoir of ~1620 ft. A total of 3 geophones were set at 4925 ft, 5743 ft and 6137 ft along
270 with a pressure / temperature gauge mandrel at 6325 ft. The monitor well was drilled to a total TD of 7272 ft;
271 it had a surface casing (13 3/8" to 377 ft, followed by intermediate casing of 9 5/8" to 5322 ft and 5 1/2" casing
272 across the Mt. St Simon Sandstone, which contained a 3 component geophone array) [\[3\]\[3\]](#).

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274 A. *Data Collection and Preparation*

275 A total of 34 parameters were measured from the injection and verification well. The parameters measured
276 comprised of both surface and downhole measurements which were acquired at five second intervals over
277 three full years. The sheer volume of data required that the time scale be downscaled to hourly intervals, taking
278 the parameter average over the hour. 27,665 hours of data (training data) was used to build a suitable model.
279 67% of the “training” data set was used to train the model. The remaining 33% was used as a “validation”
280 dataset. The model built off this data was finally used to predict 201 hours of Δ into the future (“hold out”
281 data). Given in Table 1 is the descriptive statistics of the provided data; [we refer readers to the nomenclature](#)
282 [table for the definition of the variables](#). We note that there are a series of “null values” [\(including negative](#)
283 [null values\)](#) and non-numeric numbers, missing rows, [time gaps](#) and note that for some of the input data
284 measurements, there are significant outliers.

285

286

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

287

288 **B. Cleaning Data**

289 We reviewed the attributes for the data, and were especially concerned about discontinues, non-numerical
 290 data or data that were clearly outliers (e.g. ~25,000 psi WHP at injection well or 0 psi downhole gauge
 291 pressure). We utilised 3–4 methods to clean the data, in order of operation (i) we firstly performed a
 292 computational fill of all the missing and null values with a “forward fill” operation, with the last valid
 293 observation being propagated forward. We do this on the assumption that missing values retain the properties
 294 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
 295 method where

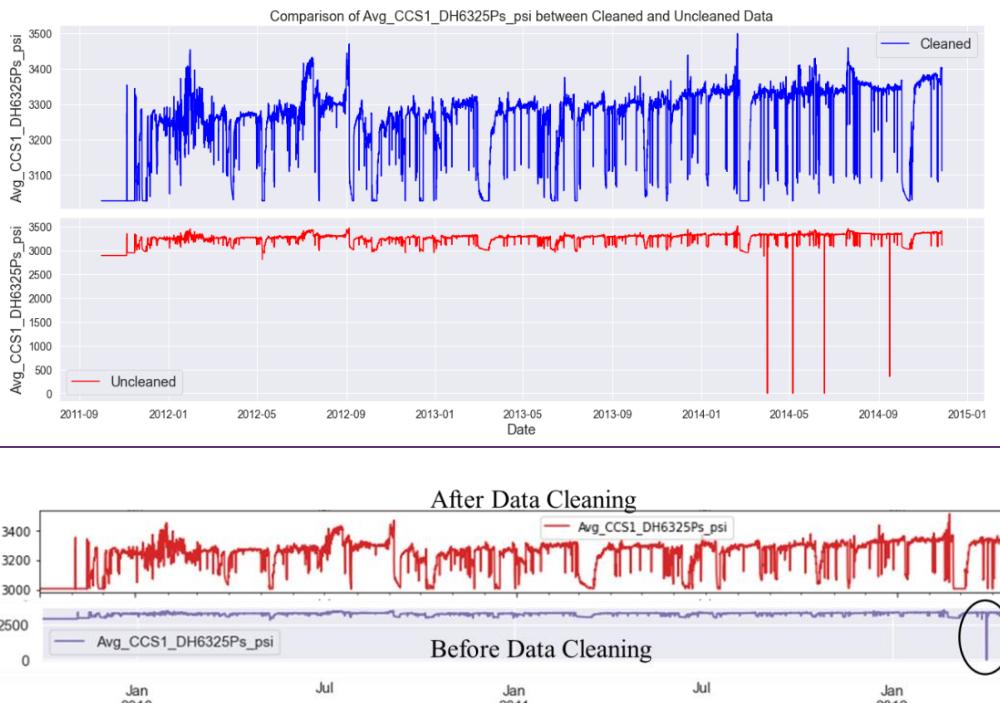
296

$$Z = \frac{x_i - \tilde{x}}{MAD} \quad \text{Equation 5}$$

297

298 x_i is a single data value, \tilde{x} is the median of the data set and MAD is the median absolute deviation of the
 299 dataset. [\(iii\) removing values of formation pressure and that we know to be technically invalid and](#) [\(iiiiv\)](#) a
 300 [final](#) visual check of the data, removing outliers that we view as being deleterious to the interpretation. Shown
 301 in Figure 2 is an example of the impact that data cleaning has on the data quality. We see that our process has
 302 removed spikiness in the data and smoothed out some of the small-scale perturbations, resulting in a more
 303 manageable dynamic range.

304



305
306
307 Figure 2: An example of the measurement before (lower image) and after (upper image) data
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319

[cleaning](#)[cleaning.](#)

C. Machine Learning 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][29, 30, 31].

ARIMA has been applied by previous authors to forecast oil production data [33][32]. The “autoregressive” piece of ARIMA deals with finding a correlation between a specific value and a prior/lagged value, essentially

320 seeing if a variable has any correlation to its past values. The “integrated” piece deals with making data
321 stationary, essentially ensuring that properties of the data (such as mean and variance), are constant over time.
322 The “moving average” piece of the model finds the dependency between a specific value, and the error from
323 a moving average model applied to previous values. ARIMA models are therefore useful in forecasting time
324 series data and are especially useful when trying to predict time series data that is non-stationary. While Ning
325 et al observed that ARIMA was robust in predicting rates of oil production across wells, our review of ARIMA
326 models being produced with high frequency data, where accuracy on an hourly basis was important, found
327 that the error rate compounds significantly when the forecasting horizon is extended beyond a day [34][33].
328

329 LSTM is a type of recurrent NN which uses useful patterns from sequential data to provide accurate
330 forecasts [23][22]. It learns from previous outputs to provide better results the following time. A typical LSTM
331 has 3 layers (i) an input gate which assigns weights based on the significance of different variables, (ii) a
332 forget gate to retain only useful information, and (iii) an output gate which manages the information flow.
333 LSTM holds a memory cell (known as a cell state) which retains captured information over longer time periods
334 and preserves useful constituents using its input and forget gates, hence avoiding the vanishing gradient issue
335 associated with traditional NNs. LSTMs are particularly useful for non-linear problems where there does not
336 appear to be strict mathematical relationships between variables. Unlike recurrent NNs, LSTMs are able to can
337 account for long-term temporal effects without encountering optimisation hurdles like vanishing gradients
338 [35][34]. In our review of LSTM vs ARIMA models, we have found a common consensus in various fields
339 that LSTM performed better, with reduced error rates but with significantly increased processing time [32,
340 31][31, 30].
341

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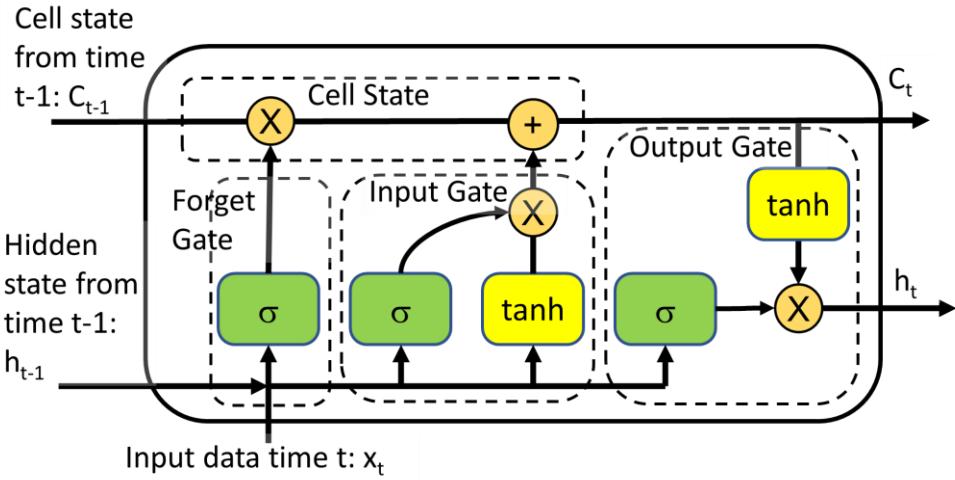


Figure 3: Schematic of LSTM network

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][35]. Additionally, there were numerous variables provided which we did not know the relative importance of in prediction without a working model.

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349 D. Model Performance and Hyperparameter Optimization

We assess 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 (R^2 - 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.

359

MAE:	$\frac{1}{n} \sum_{i=1}^n y_i - x_i $	Equation 6	Formatted Table
MSE:	$\frac{1}{n} \sum_{i=1}^n (y_i - x_i)^2$	Equation 7	
RMSE:	$\sqrt{\frac{1}{n} \sum_{i=1}^n (y_i - x_i)^2}$	Equation 8	
R ² :	$1 - \frac{\sum (y_i - x_i)^2}{\sum (x_i - \bar{x})^2}$	Equation 9	

360

361 Equation 6 to Equation 9 show the other measurement metrics, with y_i as the predicted value, x_i as the true
 362 value, \bar{x} as the mean of x_i and n as the total number of data points. MAE measures the average absolute
 363 difference between the predicted and actual values and provides an absolute measure of the model's
 364 performance. MSE measures the average squared difference between the predicted and actual values and
 365 amplifies larger errors due to the squaring operation. RMSE is the square root of MSE and provides a measure
 366 of the average magnitude of errors. It is useful for interpreting errors in the same units as the target variable.
 367 R² measures the proportion of the variance in the target variable that is explained by the model. It ranges from
 368 0 to 1, where 1 indicates a perfect fit and 0 indicates a poor fit.

369

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

375

376 The NN model is tuned by varying a series of "hyperparameters". A hyperparameter is a characteristic of
 377 a model that is external to the model and whose value cannot be estimated from data. The hyperparameters
 378 that were optimized included the (i) learning rate, (ii) the epochs, (iii) the number of neurons, (iv) the

379 magnitude of dropout, (v) batch size, (vi) the choice of optimiser and finally (vii) the choice of activation
380 function. To account for idiosyncrasies in the data (noise, patterns, outliers, etc.), k-fold cross-validation was
381 run to validate the stability of the model.

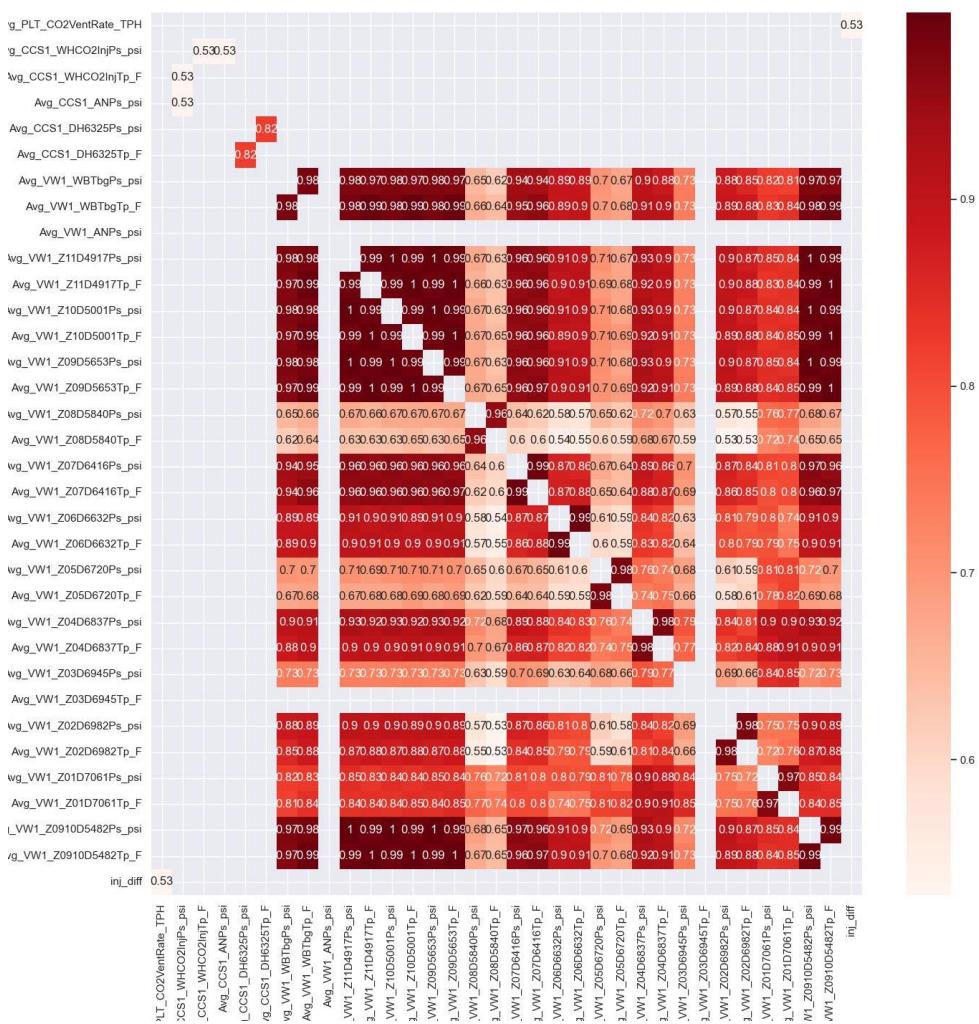
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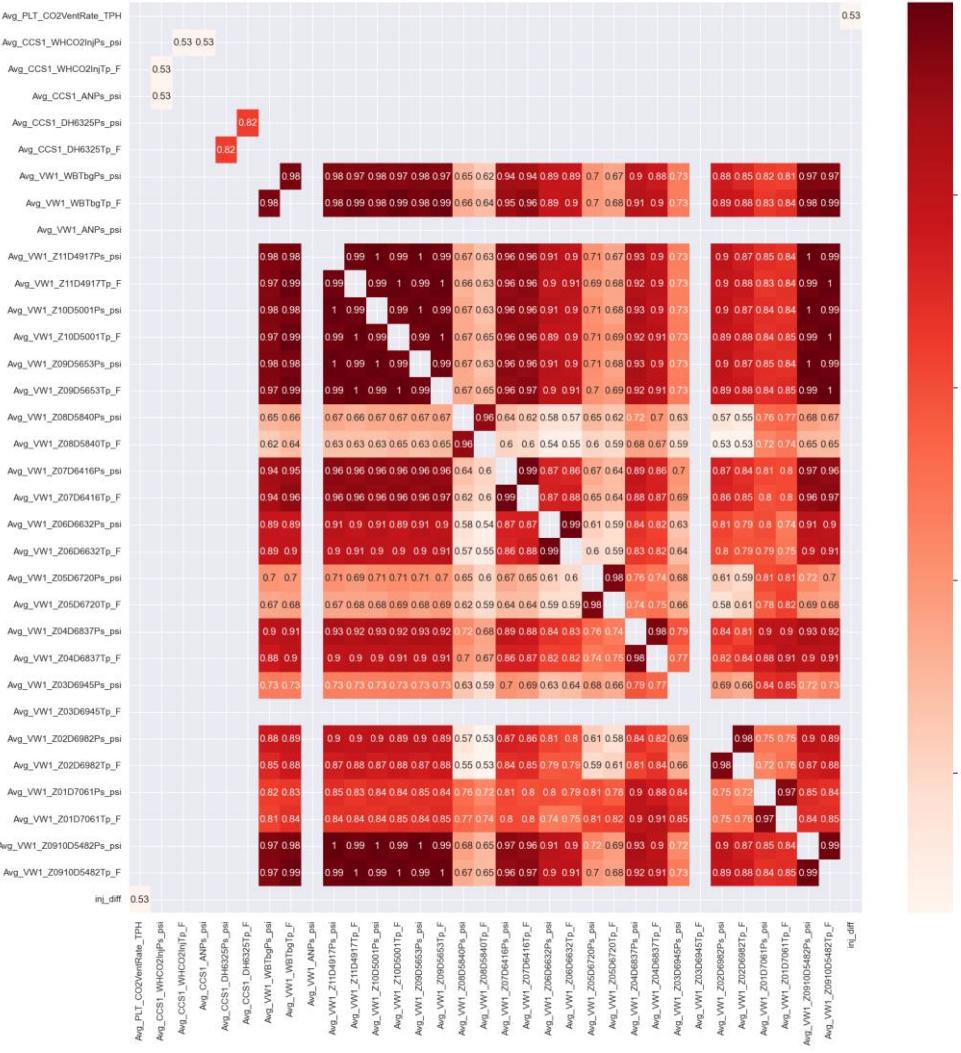
383 **Results and Discussion**

384 **Data Preparation**

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

392





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

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398 Excluding the target injection delta variable, ~~six~~^{eight} variables were retained for the machine learning
 399 application and are summarised in Table 2 for the entire dataset. All data is numerical data types. The total
 400 data size is 27,665 values per column, for a total of 248,784 data points which was approximately ~26% of
 401 the original data base.
 402

403 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	<u>27.665</u>	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

404
 405 **LSTM Model Architecture**

406 We have employed a stacked LSTM architecture, with 2 layers, for this evaluation. In a stacked LSTM
 407 model, the output sequence of one LSTM layer serves as the input sequence for the next LSTM layer in the
 408 stack. This allows for a hierarchical representation of the input data, with each LSTM layer capturing different
 409 levels of abstraction or temporal dependencies. The second layer of the stacked model feeds the results to the
 410 output layer. We also use dropout to reduce the risk associated with overfitting. Finally, there is a dense layer
 411 which predicts the output, a single timestep at a time.
 412

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

419

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

423

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

431

432 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: $f(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$

433

434 Figure 5 shows the MSE output of the training (train) and validation (val) sets for one of our K-folds. MSE
 435 is on the y-axis and epoch is on the x-axis. We observe the convergence between train and val, telling us that
 436 the model accuracy is improving per epoch. The point of convergence is arrived at by gradient descent and
 437 tells us the point of minimum information loss. In this example, we achieved convergence at around epoch =
 438 30, with losses increasing beyond that.

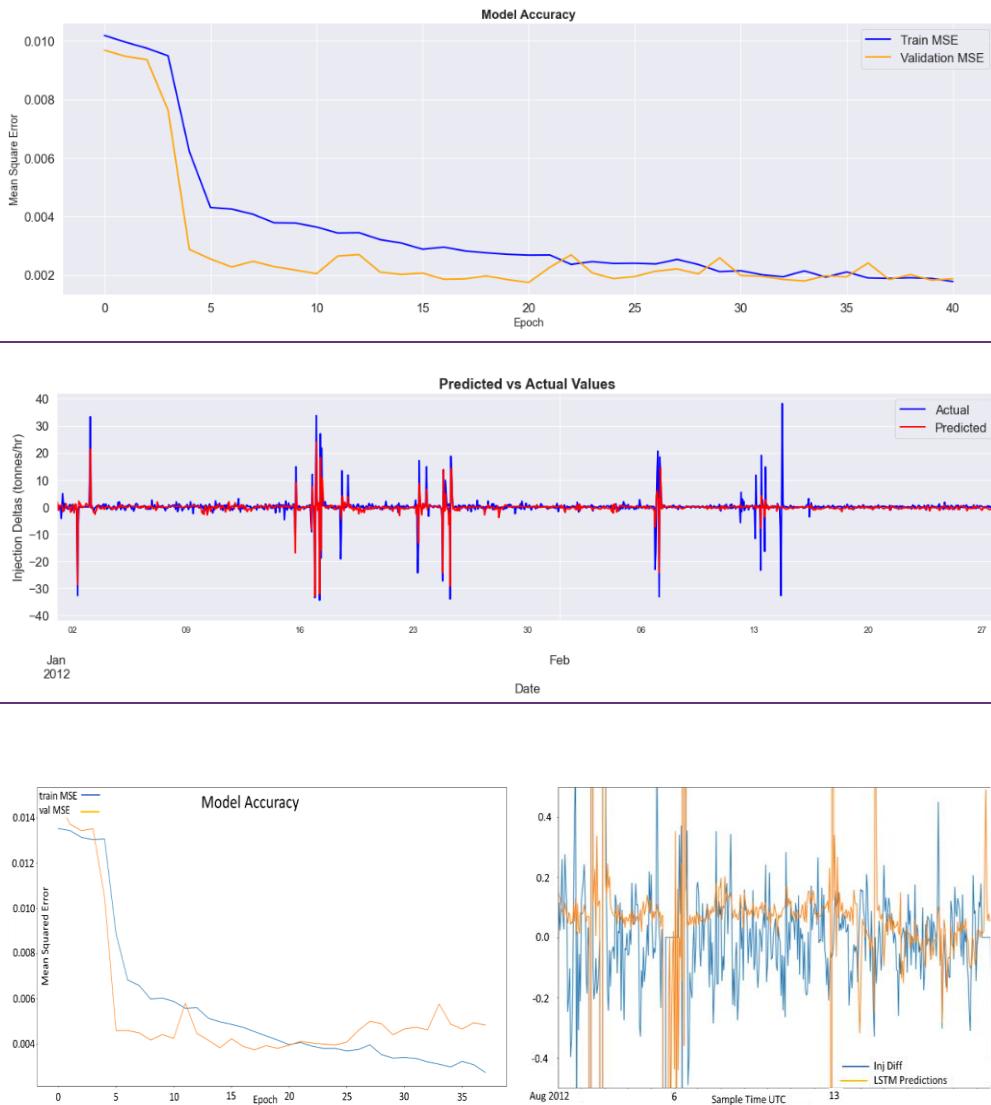
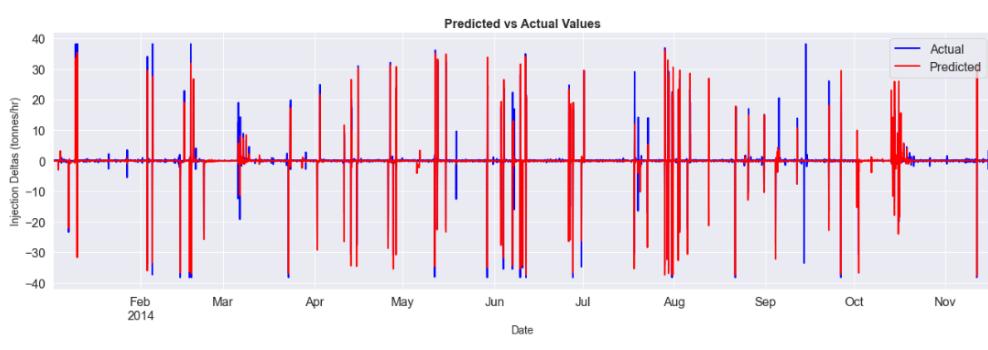
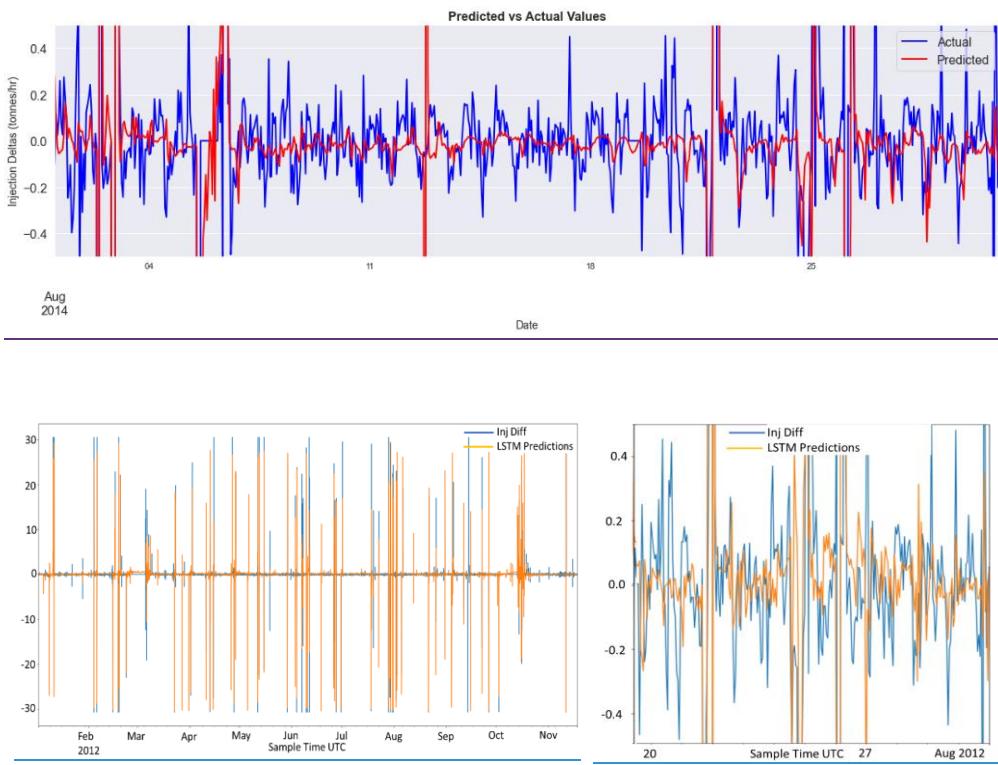


Figure 5: (a) Upper) MSE output of the training and validation set (b) Lower) Check file of a small subset of data; output from the K-fold set.

446 We deployed our developed model on our ~~hold-out~~^{validation} data. Given in Figure 6 is the comparison
447 between the predicted injection rate deltas versus the actual injection rate deltas in our validation set. The
448 results demonstrate the model's capability to successfully identify and replicate actual anomalies, which
449 provides evidence that the model is predictive in nature. Moreover, Figure 6 illustrates that the model ~~is able~~
450 ~~to can~~ accurately capture both large scale high frequency signal, as well as smaller scale fluctuations in the
451 injection deltas ([admittedly, the subtle variations are harder to capture as these change at ranges of \$\pm 1\text{psi}\$ and](#)
452 [can be described to be in the domain of “noise”](#)), indicating the robustness of the LSTM model.

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





461
462
463 Figure 6: (a) Able to match anomalies in injection delta (b) Able to mimic the small
464 variations in the injection delta.
465

466 Generalising the model

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

473
474 (a) Single Seed, Variable Inputs

475 We used a single seed value (2250) but varied six of the selected as a test for model generalisation. Our
476 first iteration (Run 1 in Table 4) is with a default hyperparameter setting, where the predicted injection delta
477 is zero for all test timesteps; this yielded an RMSE value of 5.54.[\(Run 1 in Table 5\)](#).
478

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

485
486 By analysing the results of these runs and comparing them to the base and default settings, it is possible to
487 determine the most optimal configuration that yields improved accuracy and reliability in predicting injection
488 deltas. This series of sensitivity runs showed us that the model performs most optimally based on the
489 configuration in run 6. It additionally tells us that the model is sensitive to scaling, and our Z-score tolerance
490 bands.

492 Table 4: RMSE and R2 value of sensitivity runs Inputs to test for the effect of randomness of 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(0,1)	Y (-1,1)Y(0,1)	Y (-1,1)Y(-1,1)	Y (-1,1)Y(-1,1)	Y (-1,1)
VW DH Sensor	NA	Z01Z09	Z05Z01	Z05Z05	Z01Z05	Z05
Injection WHP Sensor	NA	YY	YY	NY	YN	Y
Temp Sensor	NA	NN	NN	YN	YY	Y
Z-Score Inj_DiffTolerance	NA	2520	2525	2525	2525	25
VW Zero Values	NA	Yes	No	No	No	No
Test-RMSE	5.54	2.65	4.82	4.98	4.50	4.34
Val-RMSE	NA	4.75	2.20	4.90	2.04	4.73
Val-R2	NA	0.73	0.63	0.72	0.69	0.77

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494 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	1.822.65	1.981.82	1.501.98	1.501.48	1.491.31
Val RMSE	NA	2.204.75	1.902.20	2.044.90	2.041.71	4.731.49
Val R2	NA	0.630.73	0.720.63	0.690.72	0.690.78	0.8377

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496 Randomness

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

500
501 Our next test for the generality of the model involved running various seed values (we utilised 10 different
502 values) and determining if both high and low amplitude delta values could be predicted. Six-Seven selected

503 results are displayed in Table 6 while Figure 7 to show the range of comparison with respect to the first
 504 unseeded run.

505

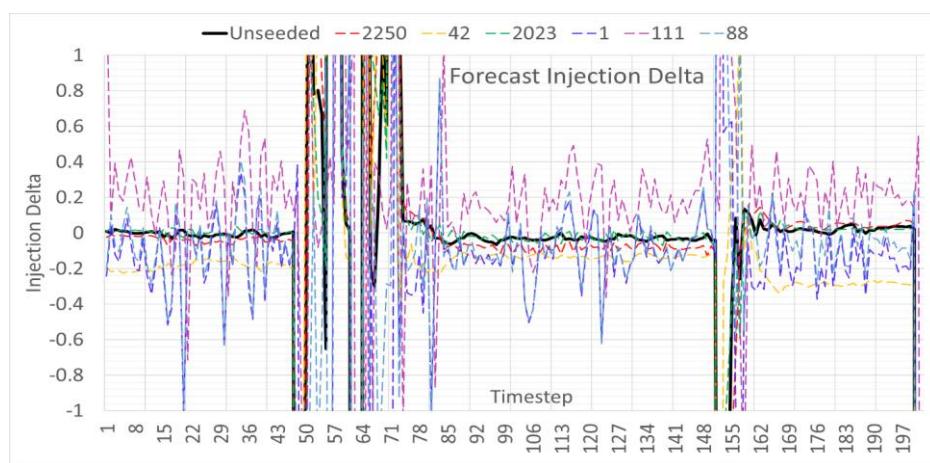
506 We observe that while all runs can predict the anomalies, the signature of the minor differences varies
 507 between seed values (Table 6). We also observe that the RMSE and R2 values on the validation set all lie
 508 within a small range ($\pm 10\%$ or up to 0.2 psi absolute) of the unseeded value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

510

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

<u>Variables</u>	<u>Run 1</u> <u>(Base Case)</u>	<u>Run 2</u>	<u>Run 3</u>	<u>Run 4</u>	<u>Run 5</u>	<u>Run 6</u>	<u>Run 7</u>
Seed Value (SV)	Unseeded	2250	42	2023	1	111	88444
Val RMSE	1.793	1.55	1.69	1.69	1.64	1.87	1.701.87
Val R2	0.770.83	0.82	0.78	0.78	0.79	0.73	0.780.73

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

515

516 *Evaluation against the “Hold-out” Data*

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

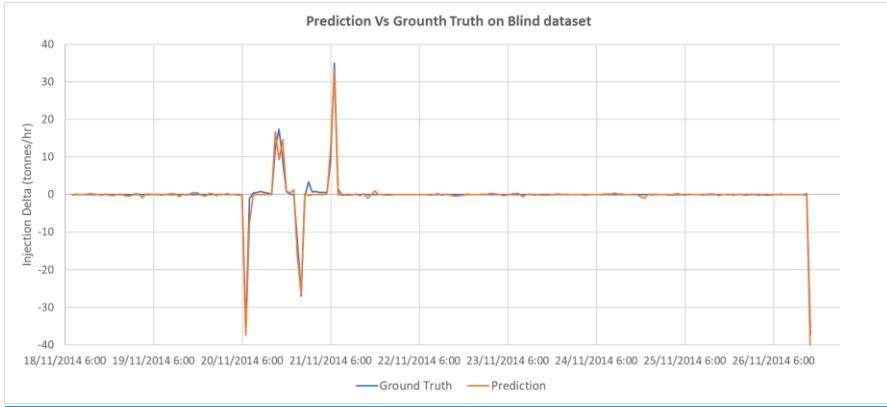
519
520 Figure 8 shows the results of this test, where our model has successfully predicated the presence of four
521 anomalies in the injection rates. When we plot this prediction against what the actual injection rates were (our
522 “ground truth” data), we observe a near perfect overlap in results.

523 shows the model inputs and prediction on the “hold out” dataset. The result shows that there are four
524 anomalies in the predicted injection deltas.

525
526 When correlated back to the input dataset, we observe that for the negative injection deltas, there are
527 corresponding decreases in injection pressure implying a decreased CO₂ injection rate.

528
529 The prediction data also shows corresponding increase in injection pressure during positive injection deltas,
530 implying an increased injection rate. Corresponding changes can also be seen on the other inputs such as
531 temperature and CO₂ vent rate.

532
533 The fact that our model can predict these anomalies using measured sensor data is encouraging; as an
534 operator who is interpreting this result, it would be prudent to firstly ask if these injection deltas are expected.
535 If they are not, then it behoves the operator to investigate/ monitor the well to determine what sort of remedial
536 action should be taken.



539
540
541 [Figure 8: Input \(blue line\) and prediction \(red line\) on blind “hold out” dataset](#)

541 Discussion & Recommendations

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

546
547 Secondly, exploring alternative methods for outlier removal, and implementing advanced techniques to
548 identify and handle outliers effectively will improve the model's ability to identify genuine anomalies, while
549 minimizing false positives.

550
551 Thirdly, the workflow of the model can be improved to reduce runtime. This optimization involves running
552 multiple sets of model ensembles, and aggregating their outputs to obtain a more “generalised” model.
553 Generalising the model can further enhance performance and provide more reliability when it comes to
554 anomaly detection.

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

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561 Conclusion

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

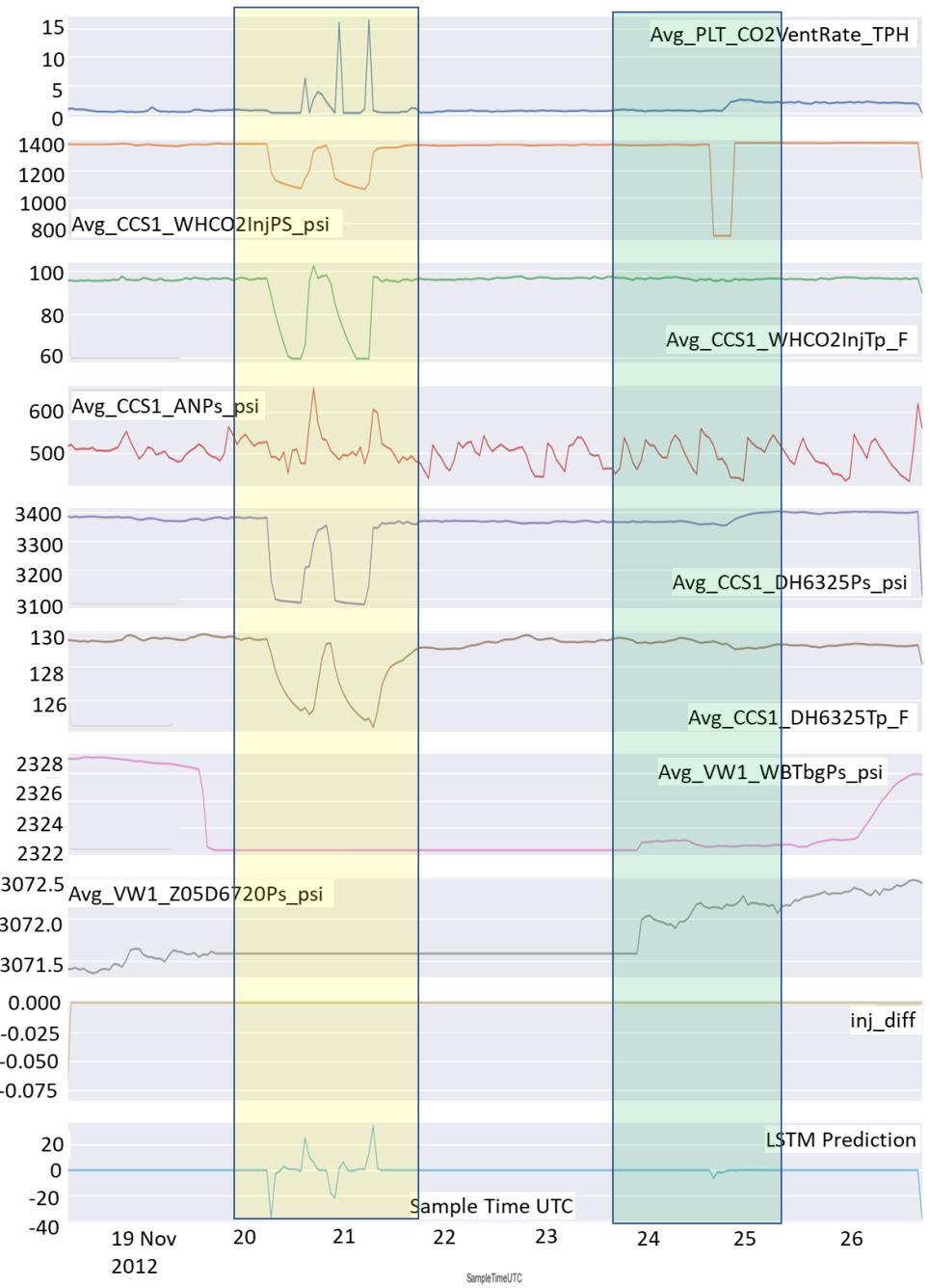
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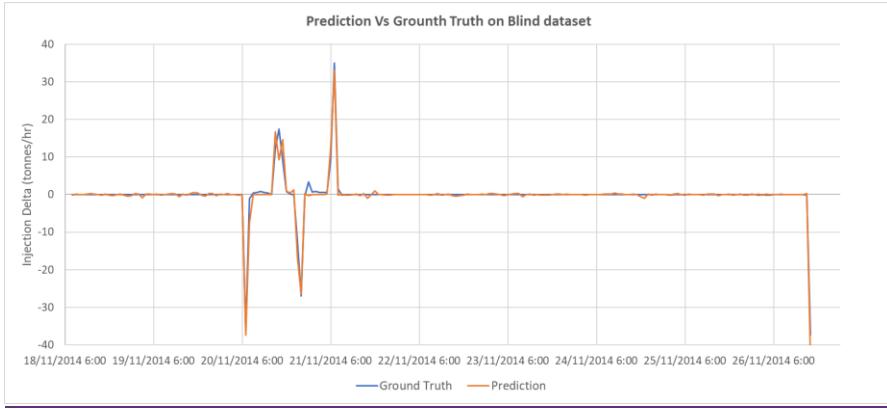
566
567 In this work, we demonstrated how an LSTM based machine learning model has been developed and
568 implemented to predict injection deltas of active CO₂ injection. We demonstrate that our predicted models do
569 well based on RMSE and R2 scores against both the training and validation data sets. Our model was able to
570 predict both large and small anomalies, and we demonstrated that the model is sufficiently generalised for this
571 single input data source.

572
573 The model can detect anomalies which operators can use when determining which wells to inspect for
574 potential leaks, especially in scenarios where multiple wells are used for injection. By passing the measured
575 data through the model, one can determine at which well containment breach location downhole losses were
576 observed during the injection process. The model can also help engineers to perform computational based de-
577 risking of geological formations, by understanding how changing certain storage parameters impacts CO₂
578 containment. The model will also aid in the understanding of the injection process and optimising well
579 operations and costs, reducing the reliance on periodic (or ad-hoc depending on operator budget) tests like
580 well annulus pressures, casing tests, and use of cased hole reservoir saturation tools.

582 The primary objective of this model is to detect anomalies and alert operators to closely inspect the wells
583 for potential leaks. This predictive capability becomes especially valuable in scenarios where multiple wells
584 are in operation, as it eliminates the need for additional operators, thereby reducing operational costs. We also
585 recommended a series of improvements and model enhancements in this paper which would increase the
586 machine learning model's predictive ability, potentially providing operators with timely alerts for potential
587 leaks while optimizing operational efficiency and cost-effectiveness.

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Figure 8: Input and prediction on “hold out” dataset

Nomenclature

GHG	greenhouse gas
CO ₂	carbon dioxide
CH ₄	methane
N ₂ O	nitrous oxide
EPA	Environmental Protection Agency
CCUS	Carbon Capture Utilisation and Storage
EOR	Enhanced Oil Recovery
Δ	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

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DCA	decline curve analysis	
q_i	initial rate (bbls/day)	
D_i	initial decline rate (units)	
b	degree of curvature of the line	
AI	artificial intelligence	
LSTM	Long Short-Term Memory	
IBDP	Illinois Basin <u>—</u> 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	
R^2	coefficient of determination	
lr	Learning Rate	
ADAM	Adaptive Moment Estimation	
<u>Z score</u>	<u>a statistical measurement describing a value to the mean of a group of values</u>	
<u>CCS1_ANPs_psig</u>	<u>CCS1 annulus pressure in psi</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>CCS1_DHPs_psig</u>	<u>CCS1 downhole pressure in psi</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>CCS1_DHTp_F</u>	<u>CCS1 downhole temperature in Deg F</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>CCS1_WHCO2InjPs_psi</u>	<u>CCS1 wellhead pressure in psi</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>CCS1_WHCO2InjTp_F</u>	<u>CCS1 wellhead temperature in Deg F</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>PLT_CO2InjRate_TPH</u>	<u>CO2 injection rate in tonnes per hour</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>PLT_CO2VentRate_TPH</u>	<u>CO2 vent rate in tonnes per hour</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>VW1_ANPs_psig</u>	<u>Validation well (VW1) annulus pressure in psi</u>	Formatted: Font: (Default) Times New Roman, 12 pt
<u>VW1_PTbgPs_psig</u>	<u>VW1 tubing pressure in psi</u>	Formatted: Font: (Default) Times New Roman, 12 pt

<u>VW1_PTbgTp_F</u>	<u>VW1 tubing temperature in Deg F</u>	Formatted
<u>VW1_Z01D7061Ps_psi</u>	<u>VW1 Zone01 pressure (7061 ft) in psi</u>	Formatted
<u>VW1_Z01D7061Tp_F</u>	<u>VW1 Zone01 temperature (7061 ft) in Deg F</u>	Formatted
<u>VW1_Z02D6982Ps_psi</u>	<u>VW1 Zone02 pressure (6982 ft) in psi</u>	Formatted
<u>VW1_Z02D6982Tp_F</u>	<u>VW1 Zone02 temperature (6982 ft) in Deg F</u>	Formatted
<u>VW1_Z03D6945Ps_psi</u>	<u>VW1 Zone03 pressure (6945 ft) in psi</u>	Formatted
<u>VW1_Z03D6945Tp_F</u>	<u>VW1 Zone03 temperature (6945 ft) in Deg F</u>	Formatted
<u>VW1_Z04D6837Ps_psi</u>	<u>VW1 Zone04 pressure (6837 ft) in psi</u>	Formatted
<u>VW1_Z04D6837Tp_F</u>	<u>VW1 Zone04 temperature (6837 ft) in Deg F</u>	Formatted
<u>VW1_Z05D6720Ps_psi</u>	<u>VW1 Zone05 pressure (6720 ft) in psi</u>	Formatted
<u>VW1_Z05D6720Tp_F</u>	<u>VW1 Zone05 temperature (6720 ft) in Deg F</u>	Formatted
<u>VW1_Z06D6632Ps_psi</u>	<u>VW1 Zone06 pressure (6632 ft) in psi</u>	Formatted
<u>VW1_Z06D6632Tp_F</u>	<u>VW1 Zone06 temperature (6632 ft) in Deg F</u>	Formatted
<u>VW1_Z07D6416Ps_psi</u>	<u>VW1 Zone07 pressure (6416 ft) in psi</u>	Formatted
<u>VW1_Z07D6416Tp_F</u>	<u>VW1 Zone07 temperature (6416 ft) in Deg F</u>	Formatted
<u>VW1_Z08D5840Ps_psi</u>	<u>VW1 Zone08 pressure (5840 ft) in psi</u>	Formatted
<u>VW1_Z08D5840Tp_F</u>	<u>VW1 Zone08 temperature (5840 ft) in Deg F</u>	Formatted
<u>VW1_Z0910D5482Ps_psi</u>	<u>VW1 Zone0910 pressure (5482 ft) in psi</u>	Formatted
<u>VW1_Z0910D5482Tp_F</u>	<u>VW1 Zone0910 temperature (5482 ft) in Deg F</u>	Formatted
<u>VW1_Z09D5653Ps_psi</u>	<u>VW1 Zone09 pressure (5653 ft) in psi</u>	Formatted
<u>VW1_Z09D5653Tp_F</u>	<u>VW1 Zone09 temperature (5653 ft) in Deg F</u>	Formatted
<u>VW1_Z10D5001Ps_psi</u>	<u>VW1 Zone10 pressure (5001 ft) in psi</u>	Formatted
<u>VW1_Z10D5001Tp_F</u>	<u>VW1 Zone10 temperature (5001 ft) in Deg F</u>	Formatted
<u>VW1_Z11D4917Ps_psi</u>	<u>VW1 Zone11 pressure (4917 ft) in psi</u>	Formatted
<u>VW1_Z11D4917Tp_F</u>	<u>VW1 Zone11 temperature (4917 ft) in Deg F</u>	Formatted
<u>inj_diff</u>	<u>difference in the injection rate (IR) at time t and time (t-1) in psi</u>	Formatted

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Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

Munish Kumar:

Conceptualization, Methodology, Software, Data Curation, Formal analysis, Writing - Review & Editing, Supervision, Project administration

Kannappan Swaminathan:

Software, Formal analysis, Formal analysis, Writing – Editing, Resources, Data Curation, Writing - Original Draft, Visualization