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## MACHINE-LEARNING PREDICTIONS CO<sub>2</sub> SOLUBILITY AND RESIDUAL TRAPPING INDEXES

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Ongoing human activities that emit carbon dioxide (CO<sub>2</sub>) into the atmosphere cause severe air pollution that leads to complex changes in the climate, which poses threats to human life and ecosystems. Geological CO<sub>2</sub> storage (GCS) is seen as a promising solution to address this environmental issue by removing some of the CO<sub>2</sub> emissions. To ensure the success of GCS projects, it is crucial to understand the efficiency of CO<sub>2</sub> solubility and residual trapping in saline aquifers. There are different strategies to reduce CO<sub>2</sub> emissions, including carbon capture and storage (CCS) and carbon capture utilization and storage (CCUS). The distinction between CCS and CCUS is based on the final destination of the captured CO<sub>2</sub>. In CCUS, the captured CO<sub>2</sub> is used to enhance oil production and provide long-term carbon storage. On the other hand, underground CCS only focuses on storage efficiency in target formations [1,2]. To predict the solubility trapping index (STI) and residual trapping index (RTI) of CO<sub>2</sub> in saline aquifers, this study employs four robust machine learning (ML) and deep learning (DL) algorithms.

### Data collection and description.

To construct reliable ML or DL models for predicting CO<sub>2</sub> trapping indexes in potential storage reservoir formations, a large and trustworthy database is required. In this study, 6811 simulation records pertaining to CO<sub>2</sub> residual and solubility trapping indexes were compiled from published sources [1].

### Methodology.

To predict STI and RTI accurately, four different machine learning and deep learning models - Extreme Learning Machine (ELM), Least Square Support Vector Machine (LSSVM), General Regression Neural Network (GRNN), and Convolutional Neural Network (CNN) were used on a dataset of 6811 simulation records from published studies. To evaluate the performance of the models, statistical error metrics such as Root Mean Squared Error (RMSE), Coefficient of Determination (R<sup>2</sup>), and Average Absolute Relative Error (AARE) were used along with score and robustness analyses. The dataset was divided into training and testing subsets, and each model was evaluated based on its ability to predict CO<sub>2</sub> STI and RTI. A sensitivity analysis was conducted, and it was found that the most consistent results were obtained when the data records were split into 80 % training and 20 % testing subsets. The workflow for developing the models and predicting STI and RTI based on eight input variables is described in Figure.

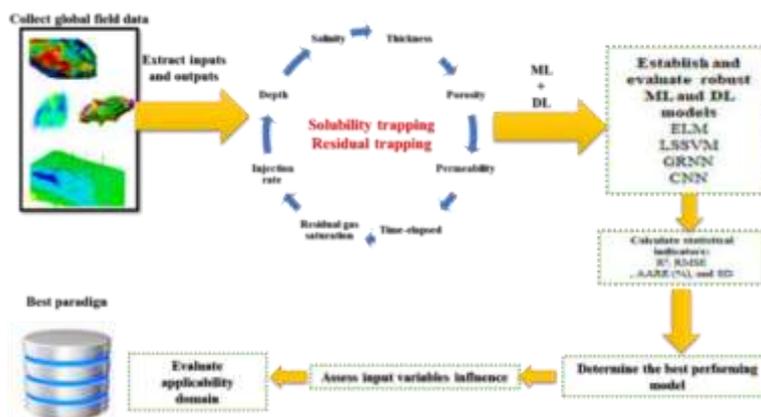


Fig. Schematic diagram of the implemented workflow for developing, evaluating, and comparing the ML and DL models for STI and RTI prediction. Reproduced with permission from [1]

Table presents the R<sup>2</sup>, RMSE, and AARE values for each model's predictions of STI and RTI with respect to the testing and training subsets and for the trained model applied to the complete dataset. The best performing LSSVM model, considering results for the complete dataset, yielded the most dependable STI and RTI predictions. It delivered AARE, RMSE, and R<sup>2</sup> values of 1.1583 %, 0.0043, and 0.9985, respectively, for STI, and 1.3886 %, 0.0105, and 0.9965, respectively, for RTI.

According to the RMSE and AARE (%) values obtained by the models in predicting the STI and RTI, the models are ranked in the following order: LSSVM (best) < GRNN < ELM < CNN (worst).

Table

Statistical error metrics for the STI and RTI predictions made by the ML and DL models considering the training and testing subsets and the complete (Total) dataset. The table was reproduced with permission from [1]

Targeted variable	Model	Error metrics	Data subset		
			Training	Testing	Total
STI	ELM	R <sup>2</sup>	0.9829	0.9824	0.9826
		RMSE	0.0149	0.0171	0.0153
		AARE (%)	3.6208	3.8569	3.6683
	GRNN	R <sup>2</sup>	0.9995	0.9930	0.9981
		RMSE	0.0022	0.0098	0.0048
		AARE (%)	0.0740	1.5479	0.3689
	LSSVM *	R <sup>2</sup>	0.9996	0.9943	0.9985
		RMSE	0.0020	0.0088	0.0043
		AARE (%)	1.1124	1.3417	1.1583
	CNN	R <sup>2</sup>	0.9696	0.9648	0.9685
		RMSE	0.0217	0.0251	0.0225
		AARE (%)	13.645	9.6011	12.836
RTI	ELM	R <sup>2</sup>	0.9962	0.9804	0.9953
		RMSE	0.0051	0.0253	0.0122
		AARE (%)	1.2371	6.0177	2.1938
	GRNN	R <sup>2</sup>	0.9993	0.9824	0.9959
		RMSE	0.0045	0.0242	0.0114
		AARE (%)	0.1075	2.1755	0.5214
	LSSVM *	R <sup>2</sup>	0.9994	0.9853	0.9965
		RMSE	0.0041	0.0219	0.0105
		AARE (%)	0.7529	3.9294	1.3886
	CNN	R <sup>2</sup>	0.9632	0.9559	0.9617
		RMSE	0.0370	0.0409	0.0378
		AARE (%)	9.1038	9.0903	9.1011

(\*) represents the best-performing model

To predict solubility trapping index (STI) and residual trapping index (RTI) accurately in saline aquifers, a prediction methodology using three machine learning models (ELM, GRNN, and LSSVM) and one deep learning model (CNN) was developed. The methodology was evaluated using a dataset of 6811 simulation records that had eight geologically relevant input variables, such as depth, salinity, porosity, thickness, permeability, injection rate, residual gas saturation, and time elapsed. The performance of the models was evaluated using statistical error metrics such as Root Mean Squared Error (RMSE) and Coefficient of Determination (R<sup>2</sup>), and score and robustness analyses were conducted.

The results showed that the LSSVM model outperformed the other three models in terms of predicting both STI and RTI, with RMSE and R<sup>2</sup> values of 0.00043 and 0.9985 for STI, and 0.0105 and 0.9965 for RTI, respectively. The score analysis also ranked LSSVM as the best performing model, followed by GRNN, ELM, and CNN. Additionally, the robustness analysis showed that the LSSVM model was the least influenced by white noise, making it the most robust of the four models.

Overall, the prediction methodology using LSSVM, GRNN, ELM, and CNN models was found to be effective in accurately predicting STI and RTI in saline aquifers based on the eight geologically relevant input variables.

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