Numerical modelling studies of CO_2 storage in deep saline aquifers using artificial intelligence methods

Abstract

Sustainable Development Scenarios developed by the International Energy Agency (IEA), which outline the path to achieving long-term climate goals, assumes that carbon capture, utilization and storage (CCUS) technologies will play an important role in reducing CO_2 emissions in the industrial and energy sectors. In accordance with the so-called CCS Directive on the geological storage of carbon dioxide in the European Union within the territory of the EU member states, the selection of a suitable underground geological formation for permanent CO_2 storage must be preceded by a detailed characterisation and assessment of the potential storage reservoir and the surrounding rock formation. The characterisation of the dynamic behaviour of carbon dioxide stored in the geological formation is a crucial step in the assessment of a potential CO_2 reservoir. Dynamic modelling involves a series of simulations of the CO_2 injection process into the storage site using a three-dimensional static geological model of the rock formation. The results of numerical simulations, determining the estimated CO_2 storage capacities in geological structures, are a key element in the decision-making process when considering the implementation of CCS projects on an industrial scale.

Numerical modelling is widely used in reservoir engineering and is used, among others, for optimizing production and forecasting reservoir efficiency, adjusting and calibrating the reservoir model based on actual data, as well as for developing uncertainty analysis and risk assessment. Managing reservoirs and solving issues related to oil and gas engineering often require significant time investment, substantial computational power and associated costs. Numerical simulations are complex and time-consuming processes that utilize iterative procedures to replicate the reservoir conditions present in the analysed geological structure and to model the anticipated technological processes. Therefore, an increasingly common approach is surrogate modelling that employs elements of artificial intelligence, which allows for obtaining approximate operational parameters of reservoirs with significantly reduced labour input.

The possibilities for applying machine learning (ML) algorithms in CCUS technologies are diverse and encompass nearly all stages of CCUS development processes. One such challenge is the widespread use of machine learning methods to assist in conducting complex and time-consuming numerical simulations of the design and optimization processes for carbon dioxide storage in geological structures.

The research process of this work included the following stages:

- analysis of scientific and technical literature regarding the current state of knowledge on CCUS technologies and the development and classification of artificial intelligence systems, including the fundamentals of constructing artificial neural networks, which represent one of the main research directions in artificial intelligence development;
- construction of numerical reservoir models in the region of three selected structures of the Upper Silesian Coal Basin (USCB);
- sensitivity analysis of the simulation model along with determining the impact of key model parameters on the CO_2 storage process;
- development of a surrogate model based on artificial neural networks.

I developed dynamic simulation models based on regional static models of actual reservoir structures from selected areas of the Upper Silesian Coal Basin (USCB). Based on multiple reservoir simulations in the numerical model of Dębowiec layers, I generated output data necessary for developing the surrogate model. As a result of the sensitivity analysis of the simulation model of Dębowiec layers, aimed at reducing the dimensionality of the dataset, I identified the input data of the Dębowiec layers model that had the greatest impact on the simulation results for the selected objective function.

The development an appropriately representative database is one of the most important stages in the construction of a surrogate reservoir model based on artificial intelligence methods. For this purpose, a dataset of individual variants of the numerical model was generated, consisting of 150 simulations covering forecasts for 25 years of carbon dioxide injection into the rock mass. I prepared the complete set of simulation results, intended for training, validation, and testing of the neural network, using Petrel software (Schlumberger). To create a set of 150 approximation models of the analysed reservoir representative of the assumed model parameters, I employed statistical sampling of the input data space using the Latin Hypercube Sampling (LHS) method.

As a result of the analyses performed regarding the selection and optimization of the artificial neural network (ANN) structure, in the final version of the ANN-based predictive model, I applied a two-layer feedforward neural network with a hidden layer containing 5 neurons that utilize the hyperbolic tangent activation function. In the output layer, I used a linear activation function. I analysed various training variants of the network using available error backpropagation algorithms. The best results were obtained using the Bayesian Regularization algorithm, which is a modification of the Levenberg-Marquardt algorithm.

As part of testing the surrogate reservoir model, I compared the CO_2 injection results generated using the artificial neural network with the values defining the total amount of carbon dioxide injected into the rock mass in the numerical reservoir model. The results of the tests confirmed the reliability of the surrogate reservoir model built based on the artificial neural network. The obtained value of the coefficient of determination for the basic training data set in variant no. 1 is $R^2 = 0.9995$. The maximum value of relative error for the basic training data set does not exceed 2.89%, while in the additional testing data set (blind testing samples), this value is equal to 2.09%.

In this doctoral thesis, I determined the effectiveness of the geological CO_2 storage process in deep saline aquifers using artificial intelligence methods. I showed that the use of a surrogate model, which has previously undergone training, testing, and validation, can significantly reduce the effort involved in developing time-consuming numerical simulations of geological CO_2 storage at the initial stage of the CCS project.