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Modelling of a Post-combustion CO₂ Capture Process Using Neural Networks

Fei Li¹, Jie Zhang¹*, Eni Oko², Meihong Wang²

¹School of Chemical Engineering and Advanced Materials, Newcastle University, Newcastle upon Tyne NE1 7RU, U.K.
e-mail: jie.zhang@newcastle.ac.uk
²School of Engineering, University of Hull, Hull HU6 7RX, U.K.

Abstract

This paper presents a study of modelling post-combustion CO₂ capture process using bootstrap aggregated neural networks. The neural network models predict CO₂ capture rate and CO₂ capture level using the following variables as model inputs: inlet flue gas flow rate, CO₂ concentration in inlet flue gas, pressure of flue gas, temperature of flue gas, lean solvent flow rate, MEA concentration and temperature of lean solvent. In order to enhance model accuracy and reliability, multiple feedforward neural network models are developed from bootstrap re-sampling replications of the original training data and are combined. Bootstrap aggregated model can offer more accurate predictions than a single neural network, as well as provide model prediction confidence bounds. Simulated CO₂ capture process operation data from gPROMS simulation are used to build and verify neural network models. Both neural network static and dynamic models are developed and they offer accurate predictions on unseen validation data. The developed neural network models can then be used in the optimisation of the CO₂ capture process.

Keywords: CO₂ capture; chemical absorption; neural networks; data-driven modelling.

1 Introduction

Post-combustion CO₂ capture for fossil fuel-fired power plants is attracting more attention as a result of the large amounts of existing fossil fuel-fired power plants and no significant changes to equipment configurations required [1]. For the efficient design and operation of a post-combustion CO₂ capture plant, process optimisation is required. Process optimisation requires reliable and efficient process models. Different modelling technologies, such as first principle models and statistical models, have been studied to investigate the post-combustion
carbon capture process efficiency. Previous studies showed that the establishment of first principle models is very time consuming and requires extensive knowledge of the underlying physics of the process. Numerical optimisation typically requires thousands of function evaluations. Evaluation of a detailed first principle model is typically computationally very demanding. To overcome this problem, neural network models can be developed from process operational data and used in plant optimization [2]. Neural network models can be developed very quickly from process data and their evaluation is much less computationally demanding compared with a first principle model. Conventional neural networks sometimes suffer from poor generalisation performance due to the limitations in training data and training algorithms. More advanced neural network modelling methods should be utilised [3-6]. This paper uses bootstrap aggregated neural networks to build data-driven models for a CO₂ capture chemical absorption process with solvents.

The paper is organised as follows. Section 2 presents an overview of CO₂ capture processes. Section 3 presents bootstrap aggregated neural networks. Modelling of a CO₂ capture process using bootstrap aggregated neural networks and results and discussions are detailed in Section 4. Both steady state and dynamic models are developed. Section 5 draws some concluding remarks.

2 An overview of CO₂ capture processes

2.1 Post-combustion CO₂ capture via chemical absorption

Post-combustion CO₂ capture process removes CO₂ emission after the combustion of fossil fuel in a combustor. It can be retrofitted to existing fossil fuel-fired power plants for CO₂ capture. Several separation technologies can be employed in this process and they include adsorption, physical absorption, chemical absorption, cryogenics separation and membrane absorption [1]. Among these methods, chemical absorption is found to be most suitable for CO₂ capture from fossil fuel-fired power plants industrial flue gas due to the high selectivity and final pure CO₂ stream [1].

As shown in Figure 1, CO₂ capture plant with chemical absorption mainly consists of two packed columns, namely absorber and stripper columns. The flue gas from power plant is fed into the bottom of absorber and contacted counter-currently with lean amine solvent from the top side. The lean amine solvent chemically reacts and absorbs CO₂ in the flue gas. Then the
treated gas stream with lower CO₂ concentration leaves from the top of absorber. The amine solution with more CO₂ (now rich amine), coming from the bottom of absorber, is pumped to the stripper after preheating in cross heat exchanger. In the stripper, the rich amine solution is regenerated by heating via a reboiler \[7\]. The reboiler energy is often provided by low-pressure steam from the steam cycle of the power plant causes large energy consumption. The vapour that results from heating the rich amine is richer in CO₂ than the left over liquid phase (lean amine). The vapour is cooled in a condenser followed by flash separation. The vapour from the flash separator, mostly CO₂ (up to 99%) is compressed and transported to storage sites while the liquid phase from the flash separator is refluxed back to the stripper. Finally, the lean amine is cooled in cross heat exchanger by exchanging heat with rich amine and then pumped back to the absorber.

A significant portion of operation cost of CO₂ capture with chemical absorption is the energy requirement. In order to make CO₂ capture economically viable, the process operation should be optimised to identify the best process operating conditions such as temperature and pressure in absorber, stripper, reboiler and condenser. A reliable model is essential for carrying out the optimisation tasks.

### 2.2 Review of previous studies in modelling post-combustion CO₂ capture

Post-combustion CO₂ capture with chemical solvent is a reactive absorption involving simultaneous phenomena. One is mass transfer of CO₂ from the bulk vapour to the liquid solvent and the other is chemical reaction between CO₂ and the solvent. As stated in \[8\], mass transfer rate contributes a lot to reactive absorption design. The relationship between mass transport and reaction rate will determine where the species can react, such as in the bulk phase, or in the bulk and interfacial regions, or purely in the interfacial layers.

Mass transfer rates between the vapour and liquid phase can be described using different theories, namely two-film theory and penetration theory among others \[1\]. Two-film theory is however more commonly used due to its simplicity and ease of application. In two-film theory, the liquid and vapour phases are both assumed to consist of two regions; bulk and film region. The effects of heat and mass transfer resistances are taken into account only in the laminar film regions. In penetration theory on the other hand, it is assumed that the
The exposure time affects mass transfer coefficient significantly because it can imply the effects of hydrodynamic properties of the system.

In Pintola and Meisen [9], a steady-state model was developed for the absorber. This assumes a rate-based mass transfer with an enhancement factor to estimate the actual absorption rate. The study emphasized that the variation of enhancement along the absorber column is important for model prediction. The evaporation and condensation of water, the variations in physical properties and heat of chemical reaction all play a vital role to provide reliable model prediction. On the other hand, most CO₂ absorption took place in the bottom of the absorber. In the work of Alatiqi et al. [10], a further steady-state model involving integrated absorber and stripper columns was developed. The model is similarly rate-based with different enhancement factors to estimate absorption and desorption rates. In the work of Abu-Zahra et al. [11], a steady-state model was implemented in Aspen Plus® using RADFRAC columns, to study the effects of chemical reaction and mass transfer on the absorption process.

However, steady-state models are not particularly helpful to understand the impact of the post-combustion capture plant on the operability of the power plant. For instance, what is the response of post-combustion capture plant when the power plant is operating with a varying load? Will flooding occur during transient conditions, such as start-up and shutdown procedures? Therefore, a dynamic model is necessary to answer these questions. In Lawal et al. [12], a dynamic model of absorber was developed using equilibrium-based approach in Aspen Plus® and rate-based mass transfer in gPROMS®. They showed that the rated-based approach gives better prediction than the equilibrium-based approach. Kvamsdal et al. [13] also developed a dynamic model for an absorption column in gPROMS using rate-based mass transfer approach. In this study, an enhancement factor is used to account for the impact of chemical reactions. In Ziaii et al. [14], a dynamic model of stripper was created in Aspen Custom Modeller (ACM) by using rate-based approach. Two operating strategies were carried out in this study: reducing reboiler steam rate with and without adjusting the rich solvent rate. By implementing the ratio of rich solvent rate to steam rate control, the lean loading and temperature remains constant, as well as less response time for the system. The rate-based dynamic model of the amine regeneration unit was also developed in Mores et al.
[7], with an enhancement factor to represent the influence of the reactions on the CO$_2$ mass transfer.

However, these studies only looked at the individual unit (either absorber or stripper). Due to the coupling effect between two columns linked together with a recycle loop, analysis of the stand-alone columns is insufficient to understand the dynamics of the complete post-combustion CO$_2$ capture process. Therefore, further studies are necessary to investigate the performance of the complete recycling process through dynamic models. Lawal et al. [15] carried out a study to compare the accuracy of dynamic models for stand-alone columns and integrated columns using gPROMS®. The rate-based models assumed all reactions attained equilibrium. The absorber and stripper units were linked together with heat exchanger. The results showed that the integrated model predicted the temperature profile better than stand-alone models. In Lawal et al. [16], a rate-based model was developed to analyse two dynamic cases, including reducing power plant loading and increasing capture level set point to 95%. They summarized that the CO$_2$ capture plant had a slower response than power plant. They further explored how capture level affects the power plant loading and difficulties to achieve a steady power plant output quickly.

All these simulation models, relating to chemical, fluid mechanic and thermodynamic laws, require extensive knowledge of the underlying physics of the process. Even though they can provide advanced features such as customizing component models for the application in hand, there is still a limitation to carry out complicated simulations. For instance, it is difficult to identify which underlying theory and assumption result in the rising uncertainties of the simulation model. In addition, the solution of these simulators is very complex and time consuming. Thus, data-driven “black-box” models should be employed as an alternative to first principle models. In Zhou et al. [17], a model of the relationship between critical parameters in post-combustion carbon capture was developed by applying multiple regression. However, it is unable to represent the non-linear relationships among the parameters and the selection of input variables strongly relies on the experts’ knowledge. Zhou et al. [18] compared three modelling approaches: statistical model, artificial neural network (ANN) model combined with sensitivity analysis (SA), and neuro-fuzzy model. Sipocz et al. [19] has developed ANN model with sensitivity analysis for a chemical absorption process, by exploring the relationships between inputs and outputs from data set of integrated post-combustion CO$_2$ capture process. However, some previous studies pointed out
the disadvantages of single ANN model, such as over-fitting of the training data and poor
generalisation performance [20]. The combination of different neural network models would
overcome the mentioned shortcomings, thereby increasing the prediction accuracy [21, 22].
Bootstrap aggregated neural network [22] is used in this study to model the post-combustion
CO₂ capture with chemical absorption.

3 Bootstrap aggregated neural networks

Due to the limitations in training data and training algorithms, it is generally not possible to
obtain a perfect neural network model. For example, neural network training might be
trapped in a poor local minimum or the trained network might over fit noise in the training
data. Several techniques have been developed to improve neural network generalisation
capability, such as regularisation [23], early stopping [24], Bayesian learning [25], training
with both dynamic and static process data [26], and combining multiple networks [27-29]. In
training with regularisation, the magnitude of network weights is introduced as a penalty term
in the neural network training objective function with the purpose of avoiding unnecessarily
large network weights which usually leads to poor generalisation. In training with early
stopping, neural network performance on the testing data is continuously monitored during
the training process and the training process is terminated when the neural network prediction
errors on the testing data start to increase. Among these techniques, combining multiple
networks has been shown to be a very promising approach to improving model predictions on
unseen data.

Figure 2 shows a bootstrap aggregated neural network model [22], where several neural
network models are developed to model the same relationship and are then combined. These
individual networks can be multilayer feedforward neural networks, radial basis function
networks, or recurrent neural networks. In this study, the individual networks are single
hidden layer feedforward networks. In order for the combined network to give accurate
predictions, the individual networks should be different. These individual networks are
trained on bootstrap replications of the original training data [30]. These individual networks
can have different number of hidden neurons and their training start from different sets of
initial weights. Instead of selecting a “best” single neural network model among these
individual networks, these individual neural networks are combined together to improve
model accuracy and robustness. The terminology “bootstrap aggregation” is originated from “bagging predictors” introduced by Breiman in [31]. The overall output of the aggregated neural network is a weighted combination of the individual neural network outputs:

\[ f(X) = \sum_{i=1}^{n} w_i f_i(X) \]  \hspace{1cm} (1)

where \( f(X) \) is the aggregated neural network predictor, \( f_i(X) \) is the \( i \)th neural network, \( w_i \) is the aggregating weight for combining the \( i \)th neural network, \( n \) is the number of neural networks to be combined, and \( X \) is a vector of neural network inputs. Since the individual neural networks are highly correlated, appropriate aggregating weights could be obtained through principal component regression [29]. Instead of using constant aggregating weights, the aggregating weights can also dynamically change with the model inputs [32, 33].

The reason that combining multiple models can improve model prediction accuracy is illustrated by Perrone and Cooper [34]. Suppose that \( N \) independent predictors are combined, then the combined predictor can reduce the mean squared prediction errors by a factor of \( N \). Let the error of the \( i \)th model \( f_i(x) \) be \( \varepsilon_i = f(x) - f_i(x) \), where \( f(x) \) is the true function to be approximated, the mean square error can be written as:

\[ \text{MSE}[f_i] = E[\varepsilon_i^2] \]  \hspace{1cm} (2)

The average mean square error is therefore

\[ \overline{\text{MSE}} = \frac{1}{N} \sum_{i=1}^{N} E[\varepsilon_i^2] \]  \hspace{1cm} (3)

If the \( N \) models are combined through simple averaging, then

\[ f_{AV}(x) = \frac{1}{N} \sum_{i=1}^{N} f_i(x) = f(x) - \frac{1}{N} \sum_{i=1}^{N} \varepsilon_i(x) \]  \hspace{1cm} (4)

If we assume that the \( \varepsilon_i(x) \) are mutually independent with zero mean, then the mean square error for \( f_{AV}(x) \) can be calculated as:

\[ \text{MSE}[f_{AV}] = E[(\frac{1}{N} \sum_{i=1}^{N} \varepsilon_i)^2] = \frac{1}{N^2} E[\sum_{i=1}^{N} \varepsilon_i^2] + \frac{1}{N^2} E[\sum_{i \neq j} \varepsilon_i \varepsilon_j] = \frac{1}{N} \overline{\text{MSE}} + \frac{1}{N^2} \sum_{i \neq j} E[\varepsilon_i] E[\varepsilon_j] \]
It can be seen from Eq(5) that combining $N$ independent model can reduce the mean square error by $N$ times. An implication of this result is that significant improvement in model prediction can be obtained if dissimilar models are combined. Zhang et al. [29] propose using principal component regression to combine neural networks where independent contributions from individual network predictions are combined.

Another advantage of bootstrap aggregated neural network is that model prediction confidence bounds can be calculated from individual network predictions [22]. The standard error of the $i$th predicted value is estimated as

$$\sigma_e = \left( \frac{1}{n-1} \sum_{b=1}^{\sigma} [y(x_i; W^b) - y(x_i; \cdot)]^2 \right)^{1/2} \quad (6)$$

where $y(x_i; \cdot) = \sum_{b=1}^{n} y(x_i; W^b)/n$ and $n$ is the number of neural networks in an aggregated neural network. Assuming that the individual network prediction errors are normally distributed, the 95% prediction confidence bounds can be calculated as $y(x_i; \cdot) \pm 1.96\sigma_e$. A narrower confidence bound, i.e. smaller $\sigma_e$, indicates that the associated model prediction is more reliable. Thus, model prediction associated with a narrow prediction confidence bounds is preferred and is considered to be reliable. On the other hand, model prediction with a wide confidence bound is unreliable and should not be trusted.

4 Modelling of CO$_2$ capture Process

The CO$_2$ capture process considered here is through chemical absorption. A detailed first principle gPROMS dynamic model for absorber was developed in [12] and a gPROMS dynamic model for the whole process was developed in [15]. Simulators for the absorber and the whole process based on the first principle models were developed in gPROMS®. Simulated steady state and dynamic process operation data were generated using the simulators.
4.1 Steady state model for absorber

For the steady state model, only the absorber is modelled. Simulated steady state absorber operation data using first principle model developed in [12] are shown in Figure 3. The process variables selected as model input variables are inlet flue gas flow rate, CO₂ concentration in inlet flue gas, pressure of flue gas, temperature of flue gas, lean solvent flow rate, MEA concentration and temperature of lean solvent. They are shown in plots (a) to (g) respectively in Figure 3. CO₂ capture level, shown in plot (h) in Figure 3, is taken as the model output variable. Considering that steady state data is usually not abundant in practice as a process is usually operated in just a few steady states, a small number of data samples are produced as shown in Figure 3.

The generated steady state data was split into training data (56%), testing data (24%), and unseen validation data (20%). The data were scaled to zero mean and unit variance before they were used for network training. A bootstrap aggregated neural network consisting of 30 individual single hidden layer feedforward networks was developed. For the development of an individual network, a replication of the training and testing datasets was generated through bootstrap re-sampling with replacement [30] and the network was developed on the bootstrap replication. The number of hidden neurons in each neural network was determined through cross validation. A number of neural networks with different numbers of hidden neurons (between 3 and 30) were trained on the training data and tested on the testing data. The network with the lowest mean squared errors (MSE) on the testing data was considered to have the appropriate number of hidden neurons. Each network was trained using the Levenberg-Marquardt optimisation algorithm [35] with regularisation and cross-validation based “early-stopping”.

Figure 4 shows the number of hidden neurons in the individual neural networks. It can be seen that the number of hidden neurons vary a lot with different training and testing data sets. This indicate that the “best” neural network structure depends on the model building data and slight variation in the model building data can lead to different neural network structure. The individual networks are then combined through averaging in this study.

Figure 5 shows the MSE values on training and testing data (top) and on unseen validation data (bottom) from the 30 different individual neural networks. It is clearly seen that single neural networks give inconsistent performance on the model building data (training and testing) and validation data.
testing data) and on the unseen validation data. For instance, the 14th and 17th networks are among the few best networks in terms of performance on the model building data, but their performance on the unseen validation data is not among the best. The non-robustness of single neural networks is clearly indicated by the difference in performance of individual neural networks on model building data and unseen validation data.

Figure 6 shows the MSE values on training and testing data (top) and on unseen validation data (bottom) from aggregated neural networks with different numbers of constituent networks. In Figure 6, the first bar in each plot represents the first single neural network shown in Figure 5, the second bar represents combining the first two single neural networks, and the last (30th) bar represents combining all the 30 networks. Figure 6 clearly indicates that the bootstrap aggregated neural networks give consistent performance on the model building data and on the unseen validation data. It can be seen from Figure 6 that as more networks are combined, the MSE values on both model building data and unseen validation data decrease and converge to stable values. Furthermore, bootstrap aggregated neural networks give much more accurate prediction performance than most of the individual networks. This demonstrates that bootstrap aggregated neural networks can give reliable and accurate prediction performance than single neural networks.

Figure 7 shows the actual values, neural network model predictions, and 95% confidence bounds of CO₂ capture level on the unseen validation data. Clearly, the predictions by using aggregated neural networks are close to the actual values. The prediction confidence bounds offer extra information to the process operators on the prediction reliability. A prediction with narrow prediction confidence bounds is considered to be reliable while, on the other hand, a prediction with wide prediction confidence bounds is considered to be unreliable. Figure 7 shows that the model prediction confidence bounds are quite narrow for almost all samples, except for 2nd, 10th, 11th, and 12th samples. Therefore, extra care needs to be taken when using predictions for these samples.

4.2 Dynamic model for the whole process

Dynamic simulation of the whole process was carried out using the first principle model developed in [15] and the simulated process operation data were sampled using a sampling
time of 5s. The generated data were split into training data (56%), testing data (24%), andunseen validation data (20%). The data were scaled to zero mean and unit variance before
they were used for neural network training. Two multi-inputs single output (MISO) first order
dynamic nonlinear models were developed for CO$_2$ capture level and CO$_2$ capture rate using
bootstrap aggregated neural networks. The developed dynamic model is of the following
form:

$$y(t) = f(y(t-1), u_1(t-1), u_2(t-1), \ldots, u_8(t-1))$$  \hspace{1cm} (3)

where $y$ represents CO$_2$ capture level or CO$_2$ capture rate, $u_1$ to $u_8$ are, respectively, inlet gas
flow rate, CO$_2$ concentration in inlet flue gas, inlet gas temperature, inlet gas pressure, MEA
circulation rate, lean loading, lean solution temperature, and reboiler temperature.

Each of the nonlinear dynamic models is developed using a bootstrap aggregated neural
network consisting of 30 individual neural networks. These individual neural networks are
single hidden layer feedforward neural networks. The number of hidden neurons in each
network was determined through cross validation. Each network was trained using the
Levenberg-Marquardt optimisation algorithm [35] with regularisation and cross-validation
based “early-stopping”.

Figure 8 shows the MSE values on model building (training and testing) data (top) and
unseen validation data (bottom) from individual neural networks. It can be seen from Figure
8 that the individual networks give various prediction performance. Furthermore, their
performance on the training and testing data is not consistent with that on the unseen
validation data. For example, network 15 is among the worst performing networks on the
training and testing data. However, it offers the best performance on the unseen data. This
clearly demonstrates the non-robust nature of single neural networks.

Figure 9 shows the MSE values on model building data (top) and unseen validation data
(bottom) from different aggregated neural networks with different number of constituent
neural networks. In Figure 9, the horizontal axes represent the number of individual networks
contained in an aggregated neural network. The first bar in Figure 9 represents the first
individual neural network shown in Figure 8 and second bar in Figure 9 represents combining
the first two individual networks shown in Figure 8. The last bar in Figure 9 represents combining all the 30 neural networks. It can be seen from Figure 9 that bootstrap aggregated neural networks give much more consistent performance on model building data and unseen validation data. The MSE values of aggregated neural networks generally decrease as more networks are combined and converge to stable levels. This occurs in both the model building and unseen validation data sets. In addition to robustness, Figure 9 also indicates that aggregated neural networks give more accurate prediction performance than individual neural networks.

Figure 10 shows the one-step-ahead predictions and multi-step-ahead predictions of CO₂ capture rate using aggregated neural networks. In Figure 10, the solid curve is the actual CO₂ capture rate, the dashed curve is the one-step-ahead prediction, and the dash dotted curve is multi-step-ahead prediction. In calculating one-step-ahead predictions, the measured process output (CO₂ capture level or CO₂ capture rate) at sampling time \( t \) is used as neural network model input to predict the process output at sampling time \( t+1 \). In calculating multi-step-ahead predictions, the neural network model predicted process output at sampling time \( t \) is used as neural network model input to predict the process output at sampling time \( t+1 \). Accurate multi-step-ahead predictions are hence much more difficult to achieve than accurate one-step-ahead predictions because prediction errors at the previous sampling times are introduced in the model inputs and this could further increase the model prediction errors at future sampling times. It can be clearly seen from Figure 10 that the predictions are very close to the actual values, except for a few samples where the CO₂ capture rates are very high or very low. The slightly larger prediction errors at these samples are likely due to the fact that training data is scarce at these extreme operating points. The accurate multi-step-ahead predictions are very encouraging indicating that the model has captured the underlying dynamics of the process. The long range predictions are very accurate till about 90 step-ahead predictions. Such accurate long range predictions are usually more than sufficient for model predictive control and real-time optimisation applications.

The neural network dynamic model for CO₂ capture level is also very accurate as shown in Figure 11. In Figure 11, the solid curve is the actual CO₂ capture level, the dashed curve is the one-step-ahead prediction, and the dash dotted curve is multi-step-ahead prediction. It can be seen from Figure 11 that the long range predictions are accurate until 82-steps-ahead predictions. Again such long prediction horizon is generally adequate for many applications.
such as model predictive control and real-time optimisations, which will be investigated in future studies.

5. Conclusions

The neural network steady state and dynamic models of CO₂ capture rate and CO₂ capture level are developed and they are shown to be able to give accurate predictions. The aggregated neural networks model is found to be a useful tool to model the post-combustion CO₂ capture process and is more accurate and reliable than the traditional neural network models. Bootstrap aggregated neural networks give consistent performance on the model building data and unseen validation data. Furthermore, bootstrap aggregated neural networks can give model prediction confidence bounds, which are very useful measures on the prediction reliability and can be incorporated in the optimisation framework to give reliable optimisation results [36]. Reliable optimisation of the CO₂ capture process using the developed neural network models will be studied in the future.

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References


Figure 1. Simplified process flow diagram of chemical absorption process for post-combustion capture [8]

Figure 2. A bootstrap aggregated neural network
Figure 3. Steady state absorber operation data: (a). inlet flue gas flow rate (kg/s); (b). CO$_2$ concentration in inlet flue gas (mass fraction); (c). pressure of flue gas (Pa); (d). temperature of flue gas (K); (e). lean solvent flow rate (kg/s); (f). MEA concentration (mass fraction); (g). temperature of lean solvent (K); (h). CO$_2$ capture level (%)
Figure 4. Number of hidden neurons in individual neural networks

Figure 5. MSE of CO₂ capture level for individual neural networks
Figure 6. MSE of CO$_2$ capture level for aggregated neural networks

Figure 7. Steady state model predictions for CO$_2$ capture level on unseen validation data
Figure 8. MSE of CO$_2$ capture rate for individual neural networks

Figure 9. MSE of CO$_2$ capture rate for aggregated bootstrap neural networks
Figure 10. Dynamic model prediction of CO₂ capture rate

Figure 11. Dynamic model prediction of CO₂ capture level