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From neural network to neuro-fuzzy modeling: applications to the carbon dioxide capture process

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Abstract

Research on improving efficiency of the amine-based post combustion carbon dioxide (CO_2) capture process has been ongoing during the past decade. A good understanding of the intricate relationships among parameters involved in the CO_2 capture process is important for process optimization. The objective of this study is to uncover relationships among the significant parameters impacting CO_2 production by modeling the historical real-time process data. The data were collected from the amine-based post combustion CO_2 capture process at the International Test Centre of CO_2 Capture (ITC) located in Regina, Saskatchewan of Canada.

Relevant literature review and opinions from the experienced engineers of the ITC CO_2 capture plant suggested that the four parameters of reboiler heat duty, lean loading, CO_2 absorption efficiency and CO_2 production rate are the key parameters for assessing efficiency of the process. The eight process parameters that influence these four consequent or output parameters were identified as the conditional or input parameters. In this study, two artificial intelligence techniques were applied for modeling the relationships among the conditional and consequent parameters: (1) artificial neural network combined with sensitivity analysis and (2) neuro-fuzzy modeling. The results from the two modeling processes were compared, and it was observed that the neuro-fuzzy modeling technique was able to achieve on average higher accuracies than the combined approach of neural network modeling and sensitivity analysis.

Keywords: artificial neural network; neuro-fuzzy modeling; post combustion CO_2 capture process

1. Introduction

Combustion of fossil fuels in power generation and in various industrial processes have produced large amount of carbon dioxide, which is responsible for global warming and adverse environmental impacts such as rising sea levels, flooding of coastal cities, and severe drought conditions in inland regions. One of the mitigation strategies of the post combustion CO_2 capture technology is commonly adopted for reducing industrial CO_2 emissions. The primary objective of the research conducted on the CO_2 capture process system is to improve its efficiency. This requires a good understanding of the intricate relationships among parameters involved in the CO_2 capture process. The objective of this research is to study the nature of relationships among the key parameters using the approaches of data modeling and analysis. The data used in our modeling study is the operational data collected in 2003-2006

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from the amine-based post combustion CO_2 capture process system at the International Test Centre for CO_2 Capture (ITC) located in Regina, Saskatchewan of Canada.

The past research findings [1][2][3] indicate that the most significant parameters used to evaluate efficiency of the CO_2 capture process system include heat duty, CO_2 production rate, CO_2 lean loading, and CO_2 absorption efficiency. Therefore, they are defined as the consequent or output parameters in our study. Based on the opinions of the experienced operators of the CO_2 capture process system, eight other process parameters which have direct influence on the four consequent parameters were defined as the conditional or input parameters. Two different techniques were applied to model the relationships among the consequent and conditional parameters: (1) neural network modeling combined with sensitivity analysis and (2) neuro-fuzzy modeling. In the first approach, four neural network models that included the eight conditional parameters and the four consequent parameters were developed. Since some of the conditional parameters do not have significant influence on the consequent parameters, they were removed to simplify the models. Then, sensitivity analysis was applied on the developed models to explicate the conditional parameters' precise influences on the consequent parameters. The experts of the CO_2 capture domain validated the sensitivity analysis results. A second round of neural network modeling was conducted with the refined parameter sets, and the accuracies of the developed models were compared to those of the original models. In the second approach, the method of adaptive-network-based fuzzy inference system (ANFIS) was adopted to develop fuzzy inference systems that can represent the relationships between the conditional parameters and each consequent parameter. The neural networks within the ANFIS method learned from the given data to generate the appropriate membership functions and rules for the fuzzy inference system.

The prediction accuracies of the models from the two approaches were compared, and the neuro-fuzzy models showed on average higher prediction accuracies. Also, the developed fuzzy inference systems serve as a knowledge repository, which helps to illustrate the nature of the relationships among the process parameters. This paper describes the modeling and analysis procedures, and discusses the results from the two different approaches.

2. Literature Review

2.1 Amine-based CO_2 capture domain

The amine-based CO_2 capture process at the ITC primarily involves two stages: firstly, the amine solvent absorbs CO_2 from the flue gas under high temperature; secondly, the CO_2 is separated from the amine solvent. The regenerated solvent is returned to the process for further CO_2 capture, and the pure CO_2 stream will be used for other industrial purposes or vented into the atmosphere. The details of the process can be found in Zhou et al [4]. Based on a literature review of the CO_2 capture process, the following four parameters are used for evaluating the process efficiency and plant performance: (1) CO_2 production rate, which reflects the amount of wet CO_2 extracted from the flue gas and the amine solvent, (2) heat duty, which shows the amount of heat required for amine solvent regeneration, (3) CO_2 absorption efficiency, which reflects the amount of the CO_2 extracted from the flue gas in the absorption phase, and (4) lean loading, which reflects the amount of CO_2 contained in the regenerated amine solvent. They are defined as consequent parameters in our modeling study.

2.2 Artificial Neural Network (ANN) and Sensitivity Analysis (SA)

As a data processing system, an artificial neural network (ANN) accepts the known parameters as inputs and exports outputs, which represent the target parameters. During the process of neural network training or learning, a set of data including inputs and desired outputs are provided to the network model. Based on different learning algorithms, the neural network is constructed by fitting itself to the training data to "learn" to predict the unknown outputs.

Sensitivity analysis (SA) is the study of how the variation or uncertainty in the output of a mathematical model can be apportioned, qualitatively or quantitatively, to different sources of variation in the input of a model [5]. The sensitivity analysis (SA) method helps to reveal the uncertainties associated with the model parameters so that the input parameters can be more optimally selected. This is especially applicable when the studied process is not well understood, in which case combining sensitivity analysis with the ANN approach can extract useful information about the relationships among the model inputs and outputs [6].

2.3 Neuro-Fuzzy Technology and ANFIS

The neuro-fuzzy technology combines ANN and fuzzy logic. It effectively integrates the learning capability of neural networks into the development process of a fuzzy inference system. That is, it helps to determine the membership functions and fuzzy rules through learning from the data using the neural network. In this way, the accuracy of modeling by the fuzzy system can be greatly enhanced. Due to the different connections between ANN and the fuzzy system, a number of neuro-fuzzy models can be found in the relevant literature [7][8][9][10][11]. The adaptive-network-based fuzzy inference system (ANFIS) discussed by Jang [12][13] was a Sugeno type fuzzy inference system implemented in the framework of an adaptive neural network with supervised learning capability. It has been widely adopted in many real world applications and all achieved high accuracies [14][15][16][17]; this system has been adopted in our study [18].

3. Neural Network Modeling combined with Sensitivity Analysis

The first stage of the data analysis process that involved the combined approach includes the following four steps: (1) construct the ANN models using the original parameter sets, (2) perform sensitivity analysis on the modeling results from step 1 and tentatively remove insignificant conditional variables, (3) validate the refined models with the experts, and (4) apply the refined ANN models to the data again.

3.1 Construction of the ANN models

The four consequent variables are defined as output layer units in the ANN and the eight conditional variables that influence the consequent variables are defined as input layer units. The feed-forward back-propagation neural network was adopted for its simplicity and maturity. The model includes only one hidden layer, since this is deemed to be sufficient for modeling the problem.

3.2 ANN Modeling with Original Parameter Sets

The ANN models were constructed using Weka version 3.4.12 (trademark of Weka), which is a data mining software in Java. Four different prediction models that relate the eight conditional variables with each of the predicted or consequent variables were developed. The models for predicting CO_2 production rate, heat duty, absorption efficiency, and lean loading respectively have accuracies of 99.9%, 92.9%, 94.7%, and 88.4%.

3.3 Sensitivity Analysis

We hypothesized that not all the conditional parameters contribute significant influences on the target consequent outputs. However, the experienced engineers of the CO_2 capture process system who initially selected the conditional parameters could not specify each parameter's precise and measurable influence on the consequent parameters. Therefore, sensitivity analysis was performed to unravel the precise relationships among the conditional parameters and the consequent outputs to reveal the relative significances among the input parameter(s) in predicting the output values. The equation and variable perturbation methods of sensitivity analysis were implemented in Weka version 3.4.12 (trademark of Weka). Table 1 shows the SA results on the CO_2 production rate model. It can be observed that the parameters of (1) absorber in gas actual flow, (2) input absorber fluid CO_2 gas, (3) absorber TK440 off gas flow, (4) lean amine to absorber flow rate and (5) reboiler pressure have very low sensitivities compared to the other independent or input parameters according to both methods. Therefore, these parameters can potentially be removed to simplify the model. Similar analysis was conducted on the other three prediction models for heat duty, lean loading and absorption efficiency.

Table 1 Sensitivity Analysis Results on Production Rate (FI-700) Model

Parameter Name	Sensitivity #1 (Equation Method)	Sensitivity #2 (Variable Perturbation)
Absorber in gas actual flow (tonnes/day)	1.8611	0.0037226
Input Absorber fluid CO2 gas (CO2%)	-0.96393	0.0017973
Absorber TK440 off gas flow (1000 m3/day)	-0.90355	-1.11E-05
Lean Amine to absorber flow rate (kg/m)	-0.18434	-3.98E-04
Reboiler Pressure (kpa)	4.78588	0.0091487
Pressure of steam entered reboiler (kpa)	-55.0173	-0.1008869
Steam from reboiler flow rate (kg/h)	934.078	1.7669448
Amine Concentratiion	0.48322	1.767934
Heat Duty	-652.923	0.4619202

3.4 Expert Validation and Model Reformulation

The ITC experts validated the results generated from the SA during an interview. By combining the SA results and experts' opinion, the reformulated model for CO_2 production rate was developed and the refined conditional parameters are shown in the last column of Table 2. The prediction accuracies of the original and refined ANN models are listed in the last row of Table 2. It can be seen that the accuracy of the refined model (0.999) is the same as that of the original model (0.999). Hence, the refined model is able to predict CO_2 production as well as the original model even after two conditional parameters were eliminated. Similar analysis was conducted on the other three prediction models for heat duty, lean loading and absorption efficiency. Since the predictive accuracies of the new models were high, the refined sets of parameters were considered complete and reliable. Hence, the refined sets were adopted in the neuro-fuzzy modeling.

Table 2 Production rate model before and after model refinement

	ANN model with All parameters	Refined ANN model based on expertise and SA results
Absorber in gas actual flow factored for concentration	X	X
Flow rate of flue gas into absorber	X	
CO2 concentration of flue gas into absorber	X	
Amine solvent circulation rate	X	X
Pressure of reboiler	X	X
Pressure of inlet steam of reboiler	X	X
Flow rate of outlet steam of reboiler	X	X
Amine concentration	X	X
Heat Duty	X	X
Correlation coefficient (R)	0.999	0.999

4. Neuro-Fuzzy modeling

A weakness of the ANN approach is that it does not explicate the nature of relationships among the parameters of the process, and the neuro-fuzzy modeling approach was applied to address this weakness. The ANFIS model is used to develop fuzzy inference systems which interpret the interrelationships among the parameters by learning from the dataset of historical operating data from ITC.

4.1 Architecture and Learning Algorithm of ANFIS

An ANFIS consists of nodes connected through the directional links, and each node performs a particular function on the incoming signal. Some of the nodes are adaptive and contain a set of parameters. The output of the adaptive nodes depends on these parameters, whose values can be changed during the learning process based on the given training data so as to minimize a prescribed error measure [12][13][14]. The hybrid learning algorithm, combining the back-propagation gradient descent method and the least squares estimate (LSE), is used as learning rules of the adaptive networks.

4.2 Data Division

After filtering the data as discussed in Section 3, there are altogether 10422 tuples of data that remained. The set of parameter data was then divided into three subsets for neuro-fuzzy modeling: (1) a training dataset for training the ANFIS to learn information about the input-output mappings, (2) a checking dataset used together with the training dataset in the learning process to prevent model overfitting, and (3) a testing dataset used for model validation to check the generalization capability of the developed fuzzy inference system. There is no overlap or duplicate data sample among these three datasets, i.e., no data sample can exist in more than one dataset.

4.3 ANFIS Modeling

The training process was independently conducted for each consequent parameter and four fuzzy inference systems were developed. Each fuzzy inference system consists of one output and the set of input conditional variables previously refined by the process of SA and expert validation. The procedures and results of ANFIS modeling is discussed as follows.

4.3.1 Initialization of Membership Functions of Variables

The first step in developing the fuzzy inference system involves determining the types and number of membership functions for the input and output variables for ANFIS so as to initialize the fuzzy inference system. Take for example the parameter of CO_2 concentration in flue gas into absorber (AIT-203), its operating range can be divided into three regions, which can be linguistically described as “high”, “medium”, “low”, according to the experienced operators. Therefore, the initialized membership function of AIT-203 includes three subsets, which are respectively defined by the three linguistic variables.

The details of membership functions of all six input variables for modeling heat duty are listed in Table 3. The Gaussian function was selected to be the form of the membership function, and the center and width of each membership function were initialized by ANFIS. These parameters associated with the membership functions will be adjusted during the training process.

Table 3 Input Membership Functions for heat duty

Input Parameters	Number of MF	Linguistic Variables
CO_2 concentration of flue gas into absorber (AIT-203)	3	High, Medium, Low
Amine solvent circulation rate (FT-600)	3	Fast, Medium, Slow
Pressure of inlet steam of reboiler (PT-103A)	3	High, Medium, Low
Flow rate of outlet steam of reboiler (FT-103C)	3	Fast, Medium, Slow
Amine concentration	3	High, Medium, Low
Absorption efficiency	3	High, Medium, Low

4.3.2 Generation of Fuzzy Inference System

Grid partitioning was used for initializing the fuzzy inference system. The entire input space is partitioned into fuzzy subspaces based on the dimension of input variables and the number of membership functions associated with each input variable. Each rule is activated only in a particular subspace [12]. Hence, the number of rules is equal to the number of the fuzzy subspaces. Take for example the parameter of heat duty, since the numbers of membership functions associated with the six input variables are all three, our 6-dimensional input space can be partitioned into 3^6 =729 subspaces, which determines that the fuzzy inference system for heat duty will contain 729 rules. For CO_2 production rate, lean loading, and absorption efficiency, the rule bases of the fuzzy inference system contain 648, 729, and 576 rules respectively, based on the algorithm of grid partitioning.

4.3.3 Result: Fuzzy Inference System

In our study, a fuzzy inference system was developed after the training process was completed, i.e., the membership functions of the input variables were adjusted and the rules were generated. The structure of a sample inference system for heat duty is shown in Figure 1.

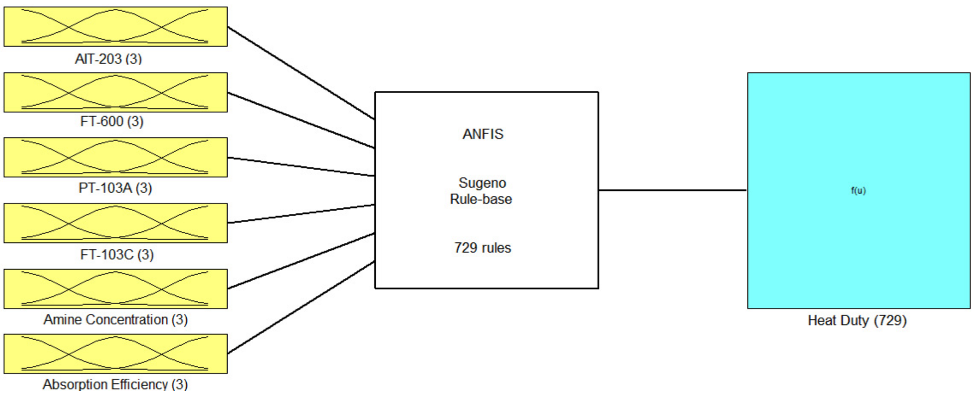

Figure 1 Structure of inference system for heat duty

The six input variables all contain three Gaussian membership functions, as shown in the yellow brackets. Although the membership functions of the input variables were initialized by the ANFIS, the training process changed the parameters of the initial membership functions to optimize their representation of the input and output mappings.

The rule base consists of 729 Sugeno-type rules. The premise part of each rule is a conjunction of linguistic labels of the input variables connected by "AND"; the consequent part is a linear function between the output variable and all the input variables. Assume the six coefficients for the six inputs are α_i, β_i, δ_i, γ_i, ρ_i, λ_i and the constant is ε_i, then the *ith* rule is in the form of:

If CO_2 concentration in flue gas (AIT-203) is A_l, and amine circulation rate (FT-600) is B_l, and pressure of inlet steam of reboiler (PT-103A) is C_l, and steam flow rate (FT-103C) is D_l, and amine concentration is E_l, and absorption efficiency is F_l, then $O_i = \alpha_i \times$ (AIT-203) + $\beta_i \times$ (FT-600) + $\delta_i \times$ (PT-103A) + $\gamma_i \times$ (FT-103C) + $\rho_i \times$ (amine concentration) + $\lambda_i \times$ (absorption efficiency) + ε_i (i = 1, 2....144)

Where A_l, B_l, C_l, D_l, E_l, F_l are the linguistic labels of membership functions for each input variable, and O_i is the output in the *ith* rule.

Since there are 729 rules in the fuzzy inference system for heat duty, there will be 729 output values which are calculated using the 729 linear functions. The final output value is then calculated based on the output value and firing strength of each rule.

The accuracies of the models developed by ANN combined with SA and ANFIS are summarized in Table 4. The accuracies of the fuzzy inference systems for CO_2 production rate, reboiler heat duty, and CO_2 absorption efficiency are all over or close to 95%. Besides CO_2 production rate, the ANFIS models for heat duty, lean loading and absorption efficiency all have higher accuracies then the ANN models. Therefore, we conclude that the fuzzy inference systems for modeling the relationships among the process parameters give highly satisfactory performance.

Table 4 Comparison of accuracies between ANN with SA and ANFIS modeling

Fuzzy Inference Systems	Accuracy from ANN with SA	Accuracy from ANFIS
Heat Duty	90.2%	95.0%
CO_2 Production Rate	99.9%	96.0%
Lean Loading	85.1%	92.3%
Absorption Efficiency	92.0%	95.8%

6. Conclusion and Discussions

In this study, two artificial intelligence techniques were applied for modeling the relationships among the conditional and consequent parameters of the CO_2 capture process: (1) ANN combined with SA and (2) ANFIS modeling. The first approach allowed us to identify and refine the significant conditional parameter sets, thereby simplifying the input parameter set and the modeling process. To address the weakness of the ANN model being a "black-box", the neuro-fuzzy modeling approach was adopted. The neuro-fuzzy approach combines interpretability of the fuzzy inference system and the learning ability of the ANN approach. Therefore, the fuzzy inference systems developed could serve as a knowledge repository, which helps to illustrate the nature of the relationships among the process parameters. Also, the neuro-fuzzy modeling technique achieved on average higher prediction accuracies than the approach of combined ANN modeling and SA.

In the future, other relationships among the process parameters will be studied and the method of ANFIS will be applied to an expanded parameter set in an effort towards a more comprehensive explication of relationships among a larger set of the process parameters of the CO_2 capture process. The membership functions and rules developed using the ANFIS method can also serve as a knowledge base that will become the basis for optimization studies of the CO_2 capture process system.

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