TECHNICAL MEMORANDUM

PROCESS MODELING FOR THE REFINING AND PETROCHEMICAL INDUSTRIES USING ABDUCTIVE NETWORKS

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SUMMARY

This Technical Memorandum proposes the use of abductive network machine learning techniques in modeling chemical processes in the refining and petrochemical industries for monitoring and control purposes. Machine learning models developed using actual process data easily incorporate process nonlinearities and provide better dynamic performance compared to traditional theoretical and empirical models. Fast predication of the process output from the model avoids the long delays and high cost associated with laboratory analysis or online analyzers. Comparison of predicted and actual outputs allows early detection of process drifts, equipment malfunction, deterioration of product quality, etc. The proposed machine learning technique offers a number of advantages compared to neural networks models used recently for this purpose. These include simplified and automated model synthesis requiring less user intervention, and analytical input-output relationships that automatically highlight significant input parameters and give better insight into the modeled process.

The work proposed should be of benefit to Saudi ARAMCO in the area of petroleum refining and the processing of petrochemicals. The technique promises many advantages in terms of better process understanding and optimization, improved product quality, and enhanced plant efficiency. The approach can lead to real savings in terms of reduced operation cost and improved plant availability.

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SECTION 1 INTRODUCTION

Modeling of industrial processes is a useful tool for improving plant efficiency, safety, and profitability. With an adequate model for the process at hand, it can be used offline to reveal the most important factors affecting product quality and yield, and to explore more profitable ways to run the process through a series of simulation and optimization steps to achieve optimal operating conditions subject to given process constraints. Deployed online, the model can provide early detection of process problems and determine optimum set-points that maximize profit. Process models provide fast 'virtual' measurements of product quality parameters in real time, thus avoiding the long delays and high costs associated with analytical testing or online analyzers, and allowing speedy control actions that maintain quality on target. Continuous monitoring of plant operation and comparison of measured and predicted quantities allow the detection of shifts in plant or sensor performance; thus allowing early diagnosis and correction of problems. This, in turn, improves plant availability and averts costly shutdowns.

Traditional process model techniques include theoretical first principle models. These rely on knowledge of the physics of the process. However, industrial chemical processes are quite complex and highly nonlinear and therefore are difficult to describe accurately in terms of a theoretical model. With empirical models, a form for the model relationship is assumed and experimental data are used to estimate the model coefficients; e.g. by regression analysis. Model development is expensive and time consuming. It also involves considerable user intervention which renders it unsuitable for frequent model updating to accommodate changes in process conditions.

Modern computational intelligence and machine learning modeling approaches promise solutions to many of the problems encountered with conventional modeling techniques. This memorandum proposes the use of an abductive network machine learning method that has proved effective in a number of similar applications.

SECTION 2 OBJECTIVES

We propose the application of abductive network machine learning to the important area of process modeling in the refining and petrochemical industries. The technique promises many advantages in terms of better process understanding and optimization, improved product quality, and enhanced plant efficiency.

SECTION 3 DISCUSSION OF THE PROBLEM

3.1. Description of the Problem

System identification and modeling are fundamental requirements in process engineering; with applications in process monitoring, control, and optimization, product classification and quality control, and fault detection and diagnostics. For example, a manual laboratory analysis to determine product quality parameters may take up to several hours, and is therefore not suitable for online use. Although hardware online analyzers may be available, they are expensive and require frequent and costly maintenance. Also, their response times of up to 20 minutes may degrade performance of the control system. Process modeling can provide a virtual, software-

based alternative that is faster and less expensive. With this approach, a model is developed that estimates the parameter to be determined from a number of process variables that are easier and faster to measure.

Mathematical modeling based on theoretical knowledge of the process has been used in the form of traditional linear or first principles models (FPM). However, many industrial chemical processes are highly nonlinear and are often difficult to describe exactly in terms of mass balances and thermodynamic. The FPM models are often complex and it is difficult to update them to take into account operational changes. In practical applications, FPM models require significant tuning by highly skilled and experienced staff. The tuning could take several hours during which the state of the process could have changed significantly, thus invalidating the model for use online [1].

With empirical process modeling [2], a model is chosen a priori, based on intuition or on some theoretical analysis. A set of simulated or measured process data is used to estimate the coefficients of the model using multiple regression analysis, and to validate the model. In many cases, constructing such models is made difficult by the need to make assumptions about the physics, components, and parameters of the model and their interactions, which may not be valid. Model development requires considerable user intervention, which makes it difficult to update the model dynamically to incorporate changes in the process and the setup.

A recent trend in handling such difficult problems has been to resort to artificial intelligence and machine learning techniques such as neural networks, fuzzy logic, and genetic algorithms. The techniques range from knowledge-based approaches in the form of expert systems to data-driven methods such as neural networks. Expert systems have been used to model some industrial processes using rules derived from knowledge gained by human experts [3]. However, processes are often influenced by hundreds of variables in such complex and interactive ways that are difficult to model in a reasonably sized knowledge base. It is often the case that the process is not fully understood and therefore we lack human expert knowledge on the subject. On the other hand, neural network approaches depend primarily on experimental input-output data on the process, which are usually readily available in large quantities. With this approach, a model for the phenomenon considered is automatically developed through training on an adequate number of solved examples. Once synthesized, the model can be used to perform fast predictions of outputs corresponding to new cases previously unseen during training. The method offers a number of advantages over conventional approaches, including increased tolerance to noise, reduced need for knowledge on the modeled phenomenon, and the relative ease of updating the model. In the last few years, neural networks have been applied to a range of process control tasks [4-19], often outperforming other traditional modeling methods and leading to significant improvements in yield, quality, and profitability [4].

3.3. Proposed Approach

We propose using the alternative machine learning approach of abductive network [20] for modeling refining and petrochemical industrial processes. This approach has been successfully used at CAPS in a variety of applications, including weather forecasting [21,22], nuclear spectroscopy [23,24], online monitoring of machine vibrations [25], forecasting of energy consumption [26], and medical informatics [27,28]. The technique automatically avoids over-fitting using a criterion for penalizing complexity [20] without requiring a dedicated validation data set; thus leaving more training data for use in actual model synthesis. Compared to neural networks, the method offers the advantages of faster training and more automated and faster

model development requiring little or no user intervention. Automating and speeding up model synthesis makes it easier to update the model dynamically to accommodate changes in the process conditions. With the resulting model represented as a hierarchy of polynomial expressions, analytical relationships thus derived can be compared with previously obtained empirical models to gain better insight into the process modeled and the rules governing plant behavior. This proposal aims at using abductive network machine learning for modeling refining and petrochemical processes for monitoring, quality control, and diagnostics purposes.

A database consisting of an adequate number of solved examples will be used to develop and evaluate the model. This data are usually available as historical process data collected by the plant's distributed control system (DCS). The data should include measured process inputs, which are relevant to the output parameters to be modeled, as well as the values of the output parameters as determined from laboratory analysis or online analyzers. The synthesized model is then evaluated on a subset of the data reserved for this purpose and not used previously for training. The model is validated through examining its performance on this evaluation data set. The proven model can then be put to actual use in predicting process output and can be integrated in the plant's monitoring and control system. Work involves coordination with the client in identifying a suitable application area, preparing the required data bases, performing data pre-processing to ensure good quality of the training and evaluation data, as well as in model integration. Performance will be compared with conventional models that may exist for the process.

SECTION 4 STATEMENT OF WORK

The proposed work includes the following tasks:

4.1. Problem Identification

Identify a suitable application area that is of interest to the client. Depending on the application, it may be adequate to use already existing historical input-output process data for building and evaluating the required model. Tasks 2 and 3 are required if this is not the case and experimental data need to be collected especially for this purpose.

Neural networks have been used to model processes and implement software-based analyzers for a variety of applications in the hydrocarbon processing industry. Examples include:

a. Developing a soft (virtual, inferential) sensor for predicting the 90% distillation point of the fluidized catalytic cracking unit (FCCU) naphtha [5]. This replaces existing hardware online analyzers for determining the naphtha end-point, which are expensive, unreliable, and have severe maintenance problems.

b. Online estimation of the LPG propane weathering point based on column operating conditions and online chromatographs [6].

c. Modeling of side stream qualities in a crude distillation plant, such as 90% distillation point, flash point, freeze point, and cloud point [7].

d. Modeling of gasoline blending octane numbers [7].

e. Modeling of asphalt penetration number from isoviscosity analyzer results and the density of the crude feedstock. [7].

f. Prediction of yield and RON for a semi regenerative catalytic reforming unit [7].

g. Modeling of product quality at the output of a hydro cracking process fractionator. The study included constructing models for the jet fuel endpoint and diesel fuel pour point [8].

h. Monitoring of reformulated gasoline (RFG) emissions from a refinery [9].

i. Continuous emission monitoring of NOx, SO2, and CO contents in the exhaust gases of furnaces and boilers for early predictive maintenance and improved safety [6].

j. Online monitoring of frationator side stream properties in a refiner. This allowed direct control of the light cycle gasoline oil (LCGO) 90% point to maximize the yield [10].

k. Estimating gasoline octane number (ON). In this study, the ON was modeled in terms of the feed quality, reactor beds inlet temperatures, catalyst activity, and plant throughput [11].

l. Estimating naphtha splitter product qualities. Based on the predicted output, the heavy fraction, rich in naphthenic, is sent to the catalytic reformer while the light fraction is directed to the isomerization plant [11].

m. Estimating product composition in a high-purity distillation column [12].

n. Modeling and optimization of a Synthol gas loop process for manufacturing liquid fuels from hydrocarbon gas feedstock [1].

o. Predicting polymer quality parameters from secondary measurements taken near the reactor [13].

p. Identification and control of distillation column process [14,15].

q. Estimating reactive impurities and reactor fouling during early stages of batch polymerization [16].

4.2. Data Collection and Experiment Design

Data for model synthesis and evaluation are often taken from available historical data bases containing the process measurements and other relevant information such as laboratory analysis results and quality control reports. If experimental process data are not available and need to be especially collected for use in the project, this part of the work needs to be carried out by the client's process engineers. Data need to be evenly distributed within the space of permissible process input variables. This may require the use of some experimental design (ED) techniques [17] to determine the tests to be conducted, the parameters to be measured, the regions of operation, the size of input changes, and the order of changing multiple inputs to the process [18]. Plant tests are normally conducted continuously over several weeks due to the large time

constants and delays generally associated with chemical processes.

4.3. Data Preprocessing

Data gathered shall be examined to check for completeness and avoid obvious errors. Missing data values should be estimated by interpolation or the whole data row is discarded. Obvious outliers should be removed and data are usually normalized as Z scores of zero mean and unity standard deviation by subtracting the column mean and dividing by the column standard deviation [19]. The opposite operation restores the model output to the original problem space.

4.4. Model Development

Records constituting about 70% of the total data are randomly selected for use in synthesizing an abductive network model that describes the input-output relationship. A model is synthesized for each variable declared as 'output'. The remaining 30% of the data would be reserved for model evaluation.

Abductive network models take the form of layered feed-forward networks of functional elements (nodes) [20]; see Figure 1. Elements in the first layer operate on various combinations of the independent input variables (x's) and the single element in the final layer produces the predicted output for the dependent variable y. Both the element type and the combination of inputs to it from all the previous layers are selected automatically for best prediction performance.

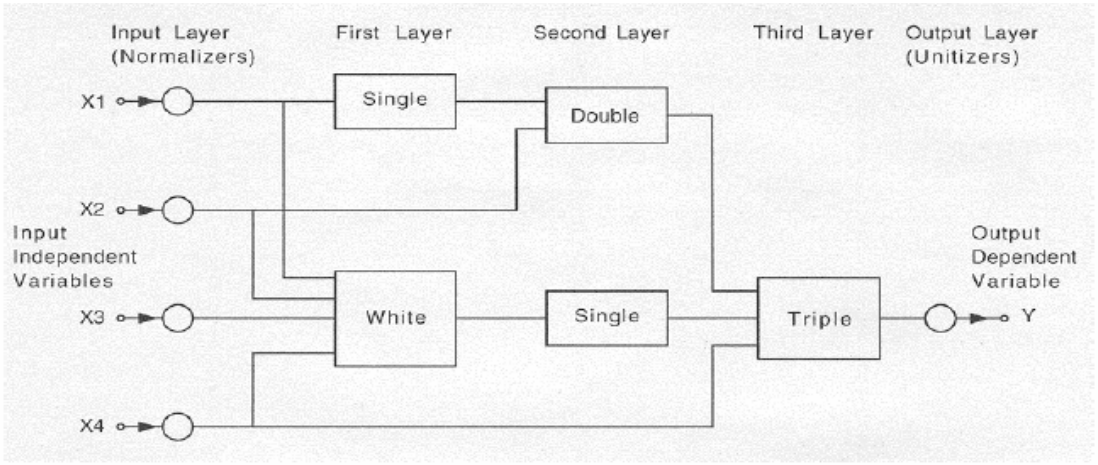

Figure 1. A typical abductive network model showing various types of functional elements

The following main functional elements are supported:

(i) A white element consisting of a constant plus the linear weighted sum of all outputs of the previous layer, i.e.:

"White" Output $= w_0 + w_1x_1 + w_2x_2 + w_3x_3 + ... + w_nx_n$

where x_1, x_2,..., x_n are the inputs to the element and w_0, w_1,..., w_n are the element weights.

(ii) Single, double, and triple elements implementing a 3rd-degree polynomial expression with all possible cross-terms for one, two, and three inputs, respectively; for example,

"Double" Output = $w_0 + w_1x_1 + w_2x_2 + w_3x_1^2 + w_4x_2^2 + w_5x_1x_2 + w_6x_1^3 + w_7x_2^3$

This allows taking into account nonlinear combinations of the input variables automatically as required. Substituting equations of the various functional elements gives a polynomial expression relating the modeled output to the input variables.

4.5. Model Evaluation and Analysis

The resulting model is evaluated on the evaluation set of process data, previously unseen during training. Various procedures for error analysis will be employed. In addition to predicting the modeled output from measured inputs, the resulting abductive network model provides useful information on the modeled relationships. The model automatically selects input parameters that contribute most to the modeled output and can provide simplified analytical expressions for the model relationship that reveal significant input variables and their relative importance. These expressions can be easily imported to other analysis/visualization software packages. With neural networks, this information can only be derived through the inspection of large weight matrices. Derived model relationships will be compared with any empirical relationships that may exist for the process being modeled.

4.6. Model Integration

The resulting model is integrated into the control system of the plant for use as a virtual online software monitor. Explore using the model for applications such as quality control and yield improvement, online product classification, open-loop and closed-loop control, etc. This part of the work requires close cooperation with the client's engineers.

4.7. Performance Assessment

Evaluate the performance of the model in a realistic operating environment for extended durations. Investigate the need for model updating to accommodate long-term drifts in the process conditions. Study the level of acceptance of the new model by the client's work team.

4.8. Documentation

Full documentation will be provided on the data sets used, pre-processing employed, model synthesis, resulting model structures and input-output relationships, and model evaluation analysis.

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