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Hybrid Mechanistic-Neural Network Modeling of Chemical Processes: Application to Crude Oil Distillation

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Abstract This paper discusses the application of hybrid mechanistic-neural network modeling approach to chemical engineering processes. The main features, advantages and disadvantages of the mechanistic, conventional neural network and the hybrid models have been highlighted. Various configurations/coupling arrangements for the application of hybrid mechanistic-neural network modeling to chemical processes are presented. In all the reported applications, the hybrid models predicted and extrapolated the processes better than either the mechanistic model or the neural network model, and have been shown to offer advantages over these conventional modeling approaches, in modeling poorly understood or complex processes. The application of the hybrid mechanistic-neural network modeling to the atmospheric distillation column of an existing crude oil refinery, and a suitable hybrid configuration for implementation is also presented. This approach can be used to improve the accuracy of predictions from shortcut distillation models when applied to existing columns.

Keywords Mechanistic model, Neural network model, Hybrid modeling, Atmospheric distillation column, Model configuration

1. Introduction

Engineering processes are usually complex; hence a simple change in one of the variables may result in complex and non-linear changes in other variables. This complex situation can be handled diligently by gaining an insight into a particular process using process models. A process model being a simplified mathematical representation of those aspects of an actual process that are being investigated [1].

A model is a functional relationship between the process variables that describes the process behaviour, and explains the way the dependent variables respond to changes in the independent variables.

Process models are required for the grassroots design of chemical processes; retrofit design of existing plants; operation of process plants; process control; process plant simulation (i.e. investigating the dynamics and steady state behaviour of the plant under various conditions) and process optimization. They can be classified as mechanistic or statistical models. Mechanistic models are derived from first principles, based on the knowledge of the underlying physical laws which govern the operation of the process. While statistical models are functions which seek to approximate the unknown relationships that exist in a process by relying on the observed information and experience regarding the system.

Hence, the mechanistic modeling approach is applied when the underlying mechanisms in a process are well understood and the system is well specified. On the other hand, when a system is poorly understood or not understood at all, or when the task of obtaining a mathematical model is difficult, or the resulting mathematical model is too complicated, then a statistical modeling approach may be applied [2].

2. Mechanistic Models

Mechanistic models are theoretical models that are derived from basic conservation laws (e.g. conservation of mass, energy and momentum), or mathematical correlations relating the variables of the process. They are usually built on certain simplifying assumptions. The accuracy and complexity of the model depend on the process modeled and the simplifying assumptions used in deriving the model. Mechanistic models are widely applied in the chemical process industry.

A major advantage of using a mechanistic model is that the conservation laws ensure that the model output remains within the feasible region of the process. However, a good knowledge of and a proper specification of the process is required. The physical and chemical laws governing many chemical engineering systems are complex and are not usually well understood. Hence, many mechanistic models are at best fair approximations of the real processes. However, mechanistic models derived for well understood non-complex processes are usually sufficiently accurate for most engineering applications.

3. Statistical Models

Statistical models are function approximators which represent the relationships between variables of a process in a simple manner [3]. They approximate the unknown functional relationship in a process by relying entirely on experimentally gathered information from the system. Hence, the drawbacks of these models are that they are only valid for specific equipment within an experimental domain where the parameters are determined [4] and are only applicable to existing systems (i.e. they cannot be applied to grassroots design). These models are concerned only with the dependence of outputs on the inputs of the process, and ignore the interior structure of the process. They are useful when the process to be modeled is large, complex, poorly understood, or when the scope of application does not require extensive mechanistic models ([3]; [1]).In general the development of statistical models involves data acquisition, regression and model validation.

The artificial neural network (ANN) which falls under this category of models has been widely applied in all fields of research in recent times. The simplicity of their implementation makes them appropriate for modeling various complex non-linear dynamic processes ([5]; [1]). ANN has the ability to recognize patterns and relationships in historical data and subsequently make inferences concerning new data. Although many neural network architecture and algorithms exist, the most commonly used is the feed forward backward propagation (FFBP) algorithm.

Neural networks have been successfully used to model many chemical process systems including wastewater treatment ([6]; [7]; [8]; [9]) and crude oil distillation ([10]; [11]; [12]; [13]; [14]; [15]). The developed ANN models were all reported to accurately predict the modeled processes. However, neural network models have been criticized for a lack of dependence on physical relationships between the variables of the process, and a poor capacity for extrapolation [5].

4. Hybrid Mechanistic-Neural Network Modeling

4.1. Hybrid modeling

Hybrid models are process models which combine the beneficial features of two or more modeling techniques. They have been shown to be superior to any of the component models in describing the modeled process. Hybrid models are usually structured to overcome challenges encountered by use of conventional modeling methods.

Hybrid mechanistic-ANN modeling approaches have proven to be potentially very efficient in obtaining more accurate process dynamics of complex non-linear processes. This is so because the mechanistic component of the hybrid model can specify the basic dynamics of the relevant process variables, while the neural network component accounts for the unknown and non-linear parts of the process not captured by the mechanistic model ([16]; [5]; [17]; [18]).

Such hybrid models have been successfully applied to fermentation processes, wastewater treatments and particulate systems. Charef et al [16], modeled baker yeast production in a fed-batch fermenter, and reported that the hybrid model approximated the process better than the conventional ANN model. Rivera et al [19], also modeled the continuous production of bioethanol. The ANN component of the model was used to model the microbial specific growth rate, and the hybrid model was reported to describe the simulation data well. Thompson & Kramer [20], modeled the cell biomass and secondary metabolites in a fed-batch penicillin fermentation. They observed that the values predicted by the hybrid models were more consistent with the reality than those from conventional neural network, and that the hybrid model gave better extrapolation. The fermentation in a fed-batch reactor was also modeled by [18]. In the hybrid configuration, ANN was used to model the cell growth rate, while the mechanistic model was derived from mass balances on the reacting species. The hybrid model was reported to give better predictions than the ANN, was unaffected by the data size, and gave better interpolation and extrapolation.

A coke wastewater treatment process was modeled by [5], using a parallel hybrid configuration. The hybrid model was reported to give better predictions of the process than the mechanistic model. Lee et al [17], also modeled coke plant wastewater treatment by both the parallel and serial hybrid approaches. The two hybrid models performed better than the mechanistic and the ANN models in predicting the process. It was also reported that the parallel hybrid configurationgave better performance than the serial model, and also required comparatively limited amount of data. The successful application of hybrid models in the modeling of particulate systems subjected to shearing has also been reported by [21].

4.2. Configuration/Structure of Mechanistic-ANN Models

4.2.1. Semiparametric Configurations

(i) Serial configurations

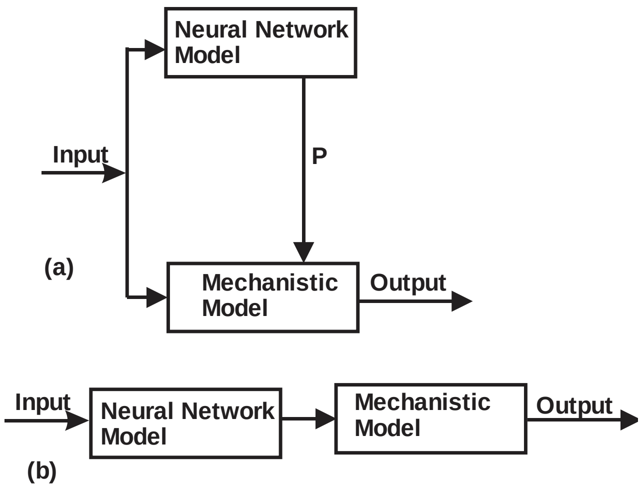

Figure 1: Serial hybrid configurations

In Figure 1(a), the ANN component receives inputs (process variables), and provides an estimate of the current parameter values, which is fed as input to the mechanistic model, which then produces the output values of the process variables [18]. In the case of Figure 1(b), the ANN estimates intermediate variables which are fed to the mechanistic model for the process variables output ([20]; [16]).

In the serial configurations generally, the hybrid model output is forced to be consistent with the mechanistic model, hence the model has guaranteed output behaviour (i.e. only feasible model outputs are generated). The draw back in this arrangement is that the ANN component has no physical structure.

(ii) Parallel Configurations

In the configuration in Figure 2(a), the mechanistic model serves as a guide to the neural network model. The mechanistic model imposes structure to the ANN component. The outputs of the ANN and mechanistic models are combined to give the total model output ([5]; [20]). The output behaviour of an arrangement such as the one in Figure 2(a), may not be guaranteed.While in Figure 2(b), mechanistic model compensates for sparse data, and improves extrapolation, while the ANN component compensates for the uncertainty of the default model. The mechanistic output model on the other hand enforces equality constraint on the output [20]. In general, parallel configurations are less sensitive to the size of data sets.

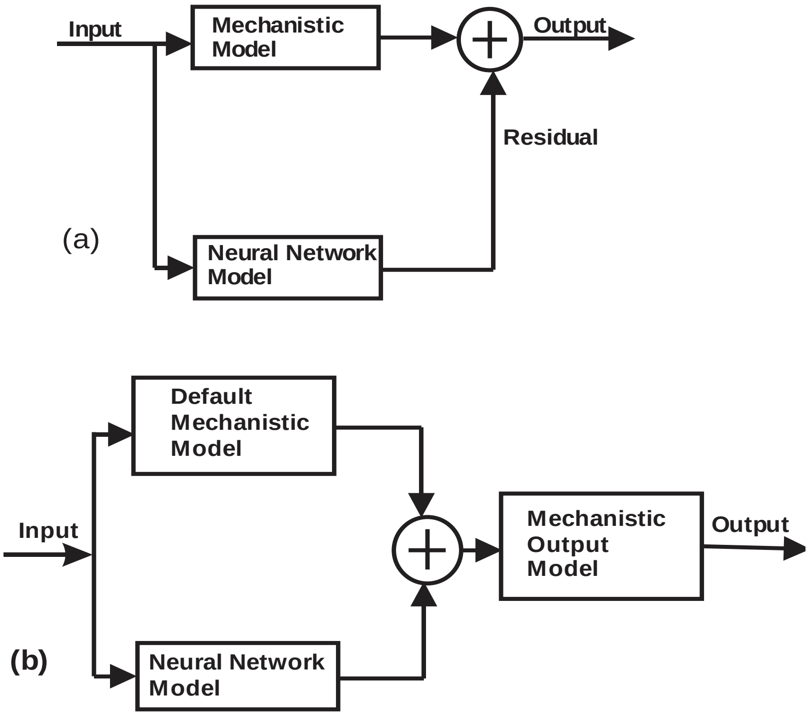

Figure 2: Parallel hybrid configurations

4.2.2. Modular Configurations

This approach involves the construction of interconnected neural network models depending on the topological and functional structure of the process. The process model is decomposed into groups of related variables. Instead of a single large network in which every input affects every output, a sub-network is constructed for each process unit, the individual results are then combined to give the model output [20].

In modular hybrid configurations, the modules may be arranged either serially or in parallel. The main feature of the serial arrangement is the sequential processing of data in which one module processes data and extracts process variables information that are fed to the next module. For parallel arrangements, the modules operate in parallel either on some common data or different data, but combine their results for an overall output. Parallel arrangements offer the capability of using feedback of information from the output of one module into the input of another, resulting in better control of the system. In general, modular designs are easier to train and interpret, but lack physical structure and may give output behaviour that is not guaranteed.

4.3. Advantages imposed by the Hybrid Mechanistic-ANN Modeling Approach

When a mechanistic model is combined with a universal function estimator such as a neural network model, the hybrid approach confers the following advantages on the process model;

- (i) The mechanistic component improves the ANN model predictions when trained on sparse and noisy process plant data.
- (ii) The mechanistic model controls the extrapolation of the hybrid model in the regions of input space that lack training data, resulting in better extrapolation capacity.
- (iii) The mechanistic component enforces equality constraints that ensure that the model does not operate outside the feasible region of the system, i.e. the model is forced to give only feasible solutions.
- (iv) The mechanistic model introduces structure to the ANN model, and makes the hybrid model easier to interpret and analyse.

(v) The ANN component compensates for the inaccuracy in the mechanistic model, arising from simplifying assumptions, poor specification of the process, inadequate understanding of the underlying processes and inherent non-linearity in the process due to complex interactions among process variables.

5. Application of Hybrid Modeling to Crude Oil Distillation Columns

The two mechanistic modeling approaches employed in distillation modeling are the rigorous methods and the shortcut (simplified) methods. The choice of which approach to apply depends on the information to be provided by the model, the ease of developing, implementing and validating the model, as well as the use to which the model would be put [3]. The shortcut distillation models relate the feed and compositions to the number of stages employed without considering the profile across the length of the column, unlike the rigorous models which involve stage-by-stage calculations. Hence, the shortcut models which are more robust and quicker to solve are more suitable to combine with a neural network in a hybrid modeling approach.

In crude oil distillation which involves complex column interactions, the application of shortcut models would require the decomposition of the complex column into a sequence of simple columns. The shortcut model can then be applied to each simple column in a sequential manner, since the shortcut models are derived for simple columns with one top product and one bottom product ([3]; [22]). The decomposition of a typical atmospheric crude distillation column into a sequence of indirect simple columns is shown in Figure 3.

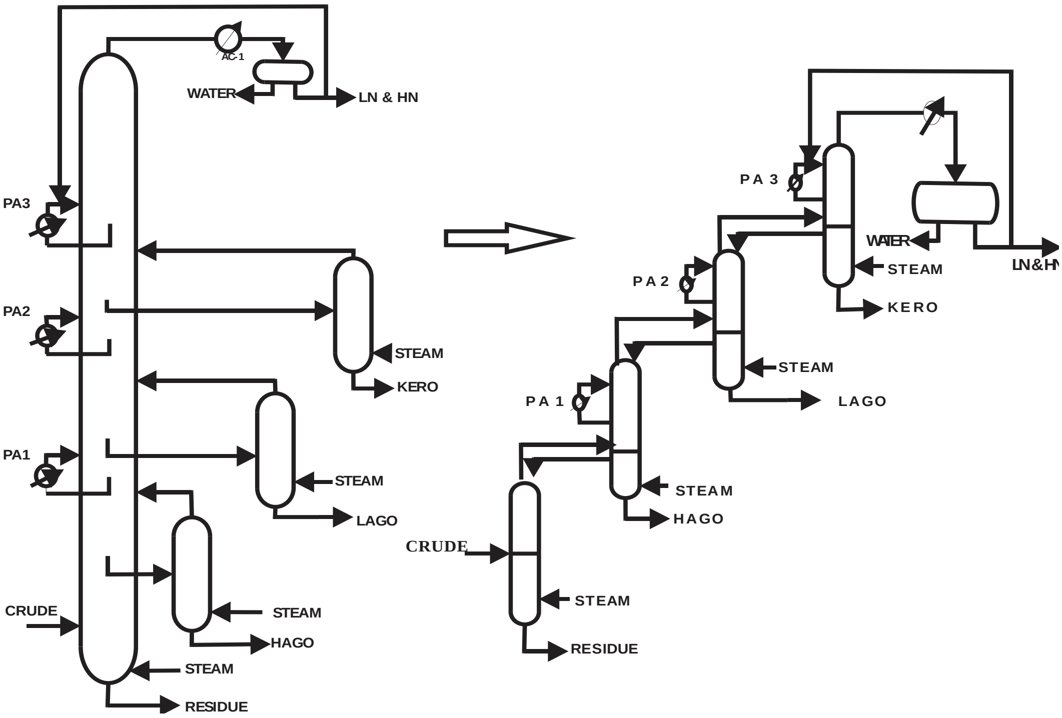

Figure 3: The decomposition of complex atmospheric crude distillation column into a sequence of simple columns

The derivation of shortcut distillation models are usually based on some limiting assumptions, which affect the accuracy of the models such as, constant relative volatilities across a section of column, equilibrium column stages, and that the separation is occurring between two primary key components [23]. The deviations from reality, arising from these simplifying assumptions, and the unknown and non-linear parts of the process not captured by the shortcut model can be modeled by a neural network component.

A parallel hybrid configuration such as Figure 4, in which the shortcut model specifies the basic dynamics of the process variables, while the ANN model is used to model the residuals (i.e. the difference between actual plant data and the predicted values from the shortcut model), can be applied in this case as the modeling strategy [5]. The output from the shortcut model is then summed up with the output from the ANN model to give the hybrid model output. This approach relies on the understanding that the residuals contain the unknown information regarding the process that the shortcut model has not captured.

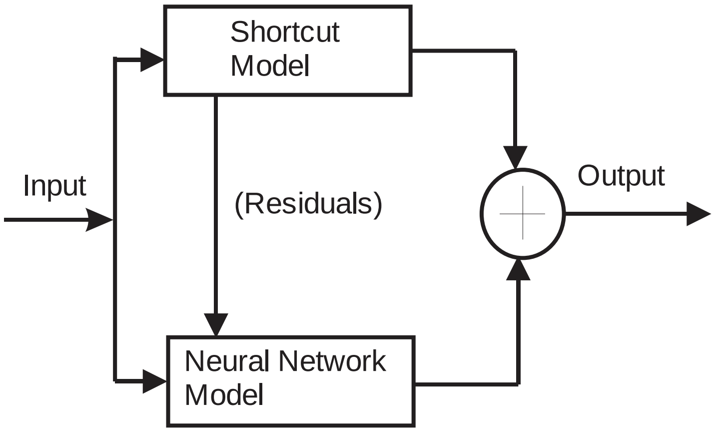

Figure 4: Configuration of Parallel Hybrid Mechanistic-ANN Distillation Model

There are two possible approaches to implementing this hybrid model on the decomposed columns. One approach is to apply the hybrid model to each column sequentially beginning from the first column to the last. The other approach is to first apply the shortcut model to the sequence of simple columns, followed by the ANN modeling of the residuals. The former approach is modular in nature, and may only capture interactions occurring between the variables in a particular decomposed column. On the other hand, the later approach can capture the interactions occurring between all the variables of the atmospheric column.

6. Conclusions

Hybrid mechanistic-ANN modeling approach has been successfully used to model many chemical engineering processes. The hybrid models generally predict the processes better than either the mechanistic or the conventional ANN models, and also give better extrapolation. They offer advantages over these two conventional modeling approaches. The semi parametric hybrid configurations give model output behaviours that are guaranteed, while modular configurations are easier to implement. This modeling approach is however applicable only to existing plants, since historical data of the process is required to build the neural network component of the hybrid model.

Hybrid mechanistic-ANN modeling approaches have been shown to be effective in modeling poorly understood or complex processes, and are expected to find wider application in many more complex processes such as the crude oil distillation in an existing refinery atmospheric column where this could be used to improve the accuracy of predictions from shortcut distillation models. A parallel hybrid configuration, in which a suitable shortcut model is sequentially applied to the decomposed columns of an atmospheric distillation column, while a neural network component is used to model the residuals, would better capture all the interactions between the variables of the crude distillation column.

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