INTEGRATION OF FIRST-PRINCIPLES MODEL WITH NEURAL NETWORKS AND HISTORICAL DATA

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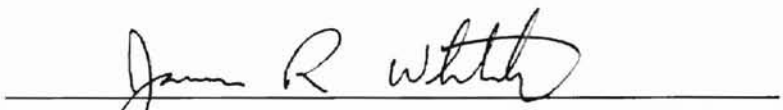

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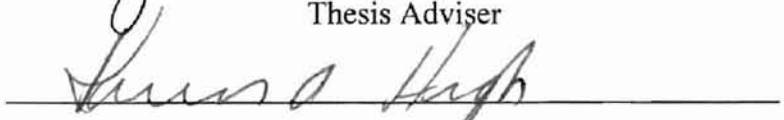

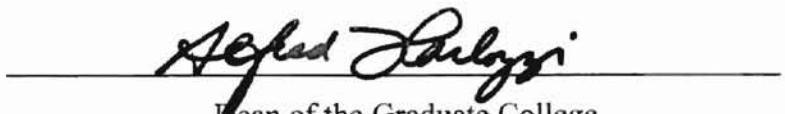

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CHAPTER 1

INTRODUCTION

1.1 Problem Statement

An accurate process model is an essential tool for engineers to improve the process, such as enhancing control system performance, enabling automatic process monitoring and fault detection. But it is always not easy to get an accurate process model.

There are generally two basic types of process models: first-principles and empirical. First-principles models are developed by applying material balance, energy balance and momentum balance, together with thermodynamic and transport relations, etc. The main advantage of using first-principles models is that the resulting model is intended to be generally applicable and rigorous, thus having good interpolation and extrapolation properties. However, the necessary knowledge for a specific system is usually not fully available, so that most of the effort in the modeling strategy is devoted to determining all relevant mechanisms and quantifying these mechanisms correctly. This usually requires an extensive research program (including experiments) which is in conflict with the desire for a short development time of the model.

On the other hand, empirical models, such as a neural network model, are developed by data measured from the actual system that has to be modeled. The main advantage of empirical model development strategy is in the fact that, within a reasonable amount of time, one can obtain a highly accurate mathematical model without detailed

knowledge of the process. However, empirical models are not reliable for extrapolation. Therefore, in the model development phase, the identification experiments should cover the whole application domain of the model to avoid the need for extrapolation during the application of the model. Such a wide application range data that must be available means a time consuming and a money consuming experimental program is needed to obtain the necessary identification data.

This research is to find a suitable combination of first-principles model, empirical (neural networks) model, and historical data, which lead to accurate process model with low cost. Meanwhile, this research is also intended to evaluate the proposed modeling techniques based on the residual errors of the developed model.

1.2 Significance of the study

Practical benefits of the project include:

- *Reduced model development cost.* First, since lots of *a priori* information can be used for model development, the model development process is much easier than that without any *a priori* information. If the final model is first-principles based, since the difficult-to-model parts can be substituted by neural network trained by historical plant data, or, the residual errors in first-principles model can be corrected by neural network, first-principles model need not be rigorously developed. On the other hand, if the final model is neural network based, some *a priori* information, such as process gain, either obtained from personal experience or from not-so-rigorous first-principles model, can be used to train neural networks. The number of data points that required to train neural network can be

greatly reduced. Secondly, since only not-so-rigorous first-principles model need to be developed or fewer experiment data for neural network training, less research program need to be carried out to explore the intrinsic mechanism of the process or less experiment need to be done. Both lead to low cost with less time and money investment.

- *Improved distillation column model.* This research provides attractive distillation process modeling methods that are readily adapted to any distillation column. Improved distillation control based on the proposed model will have a significant impact on reducing energy consumption, improving product quality, and protecting environmental resources.
- *Enhanced student experiment apparatus.* The automated data acquisition and control system built for the distillation column is also available for undergraduate students Unit Operations Lab and Process Control Lab. Students can benefit from the system for the next few years.

1.3 Organization of the thesis

This thesis comprises the following parts: In Chapter 2, the problem background is discussed. In Chapter 3, the hybrid modeling method concept is developed. Hybrid serial approach and hybrid parallel approach is applied to the modeling of experimental distillation column. Chapter 4 addresses the experimental distillation column setup, data collection, detailed modeling methods and the resulting hybrid model qualities. Chapter 5 are the conclusions and recommendations.

CHAPTER 2

PROBLEM BACKGROUND

A first-principles model is derived from first-principles. In Chemical Engineering, first principles refer to material balances, energy balances, momentum balances, together with other properties of the process such as thermodynamic and transport relations. The main advantage of developing a first-principles model lies in the fact that it is more reliable and more accurate than empirical model, provided that all process information is available. However, first-principles model also has its disadvantages. In many cases the equations describing the plant may be inaccurate due to incomplete plant knowledge. Incomplete plant knowledge can lead to both structural and parametric model errors. Structural model errors are characterized by simplified model equations, due to the omission of physical effects. Parametric errors are simply errors in the value of parameters that characterize the behavior of the plant. Parametric errors are caused mainly by insufficient and inaccurate experiment data. For example, in a Continuous Stirred Tank Reactor (CSTR) process, the reaction rate is usually determined by lab scale experiment. If the reaction rate measured from experiment is inaccurate, the first-principles model that uses this reaction rate parameter will have parametric error. In other cases the plant itself or the environment will change over time, thus making the equations and noise characteristics time-dependent.

On the other hand, empirical models describe input-output relations solely on the basis of the measured data. The advantage of developing the empirical model is that it is

easy to construct, as long as enough experiment or historical data are available. But, the internal structures and parameters of empirical model can not be interpreted in terms of physical effects or plant parameters. Moreover, empirical models can only be applied within the operating regime for which they have been identified, thus having unreliable extrapolation capability. Examples of empirical models are NARMAX models (Chen and Billings, 1989) and neural networks (Chen, Billings and Grant, 1990).

Another model type – hybrid model is just attracting lots of researchers. Since both first-principles model and empirical model have their advantages and disadvantages, as mentioned before, researchers are investigating how to incorporate the two model's advantages and overcome the disadvantages. This lead to the creation of the third type of model - hybrid model. Depending on the starting point of the modeling phase, the hybrid modeling method is divided into two directions. If the model development starts with first-principles model, and some difficult-to-model parts of the first-principles model are substituted by empirical model, or outputs of first-principles model are corrected by residual errors predicted by empirical model, semi-mechanistic model is built. If the model development starts with empirical model, and some *a priori* knowledge is incorporated into the empirical model, gray-box model is built.

Neural network model is one class of the generally adopted empirical models. Neural network model is proved to be a powerful tool for representing complex nonlinear processes (Narendra and Parthasarathy, 1990; Pollard, Broussard, Garrison and San, 1992; Su and McAvoy, 1992; Simutis, Havlik, Dors and Lubbert, 1993; van Can, te Braake, Hellinga, Krijgsman, Verbruggen, Huyben and Heijnen, 1995). Therefore, the

empirical model part of our proposed modeling techniques is restricted to neural networks.

2.1 Semi-mechanistic model

Semi-mechanistic model is also denoted as "hybrid model" in some literature, which had a narrower meaning than that we discussed before. According to Thompson and Kramer (1994), there are two types of semi-mechanistic models. One type is called "serial approach," which uses neural networks to model unknown parameters in first principles model. The other is called "parallel approach", in which neural network is used to compensate errors between the real process outputs and first principles models outputs. These two methods will be discussed individually.

2.1.1 Serial Approach

The serial approach is to use a neural network to model unknown parameters (usually those parameters which are difficult to obtain or contain uncertainties) in the first principles model. The structure is shown in Fig. 2.1. Process inputs are supplied to both first-principles model and neural network model. The outputs of neural network model are the unknown parameters of first-principles model. First-principles model calculates the model output by applying first-principles rules, along with the parameters predicted from neural network model.

Psichogios and Ungar (1992) first proposed this idea in 1992. They applied this hybrid model scheme to a simulated fed-batch bioreactor. Neural network model was

used for estimating bacterial growth rate with a standard 3 layer feed forward neural network trained with Back Propagation (BP) algorithm. Simulation results indicated an excellent prediction and satisfactory adaptation for noisy data. For all cases studied, hybrid serial model was better than the equivalent empirical model, based on the interpolation and extrapolation capabilities, easiness for analysis and interpretation, and number of training examples.

Serial approach has applications in many different areas, such as biochemical engineering (Psichogios and Ungar, 1992; Dors, Simutis and Lubbert, 1995; Geeraderd, Herremans, Cenens and Vanimpe, 1998; van Can, te Braake, Hellinga, Luyben and Heijnen, 1997; van Can, Tebraake, Dubbelman, Hellinga, Luyben and Heijnen, 1998; Fu and Barford, 1996; Schubert, Simutis, Dors, Havlik and Lubbert, 1994; Thompson and Kramer, 1994; de Azevedo, Dahm and Oliveira, 1997; Prion, Latrille and Rene, 1997: bioengineering (Tan, Li, Gawthrop and Glidle, 1997), chemical engineering (te Braake, van Can and Verbruggen, 1998; Cubillos and Lima, 1998; van Can, Hellinga, Luyben, Heijnen and te Braake, 1996; Wilson and Zorzetto, 1997; Tulleken, 1991), environmental engineering (Conlin, Peel and Montague, 1997), metallurgical engineering (Reuter and van Deventer, 1991; Reuter, Van Deventer and Van Der Walt, 1993; Cubillos and Lima, 1997; Cubillos and Lima, 1998; Cubillos, Alvarez, Pinto and Lima, 1996), thermal engineering (Guo, Shen, Li and Zhao, 1997), power engineering (Alessandri and Parisini, 1997; Lo, Peng, Macqueen, Ekwue and Cheng, 1997), semi-conductor industry (Nami, Misman, Erbil and May, 1997) and paper industry (Funkquist, 1997; Funkquist, 1997; Allison, Isaksson and Karlstrom, 1997).

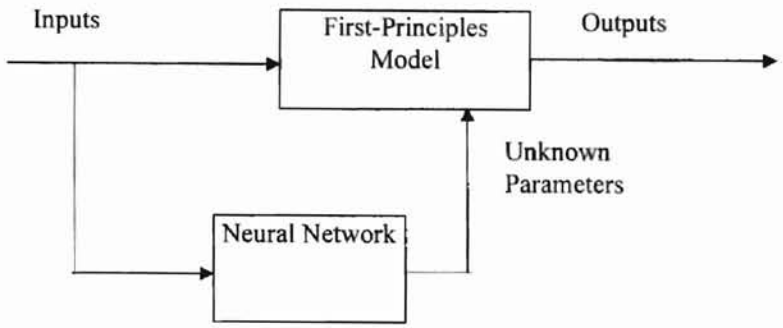

Fig. 2.1 Serial Approach Model Structure

(Neural network is used to model unknown parameters in first-principles model)

Perhaps because serial approach was first generated in the biochemical community (Psichogios and Ungar, 1992), lots of applications were reported in this area. Dors et al. (Dors, Simutis and Lubbert, 1995) applied serial approach to model the repeated fed-batch production of a recombinant therapeutic protein from mammalian cells. Data used to build the model were from the real process. Results showed the model can well predict the process. But no comparison was made between this serial hybrid modeling method and other modeling methods.

Other applications were: modeling of bacterial growth in chilled food products (Geeraderd, Herremans, Cenens and Vanimpe, 1998); pH effects on the enzymatic conversion of penicillin G (van Can, te Braake, Hellinga, Luyben and Heijnen, 1997; van Can, Tebraake, Dubbelman, Hellinga, Luyben and Heijnen, 1998); cell metabolism (Fu and Barford, 1996); fed-batch yeast cultivation (Schubert, Simutis, Dors, Havlik and Lubbert, 1994); fed-batch penicillin fermentation (Thompson and Kramer, 1994); baker's

yeast production in a fed-batch fermenter (de Azevedo, Dahm and Oliveira, 1997); crossflow microfiltration (Prion, Latrille and Rene, 1997); a neutron intensity control system used in bioengineering (Tan, Li, Gawthrop and Glidle, 1997).

In the field of chemical engineering, serial approach also has some applications. te Braake et al. (te Braake, van Can and Verbruggen, 1998) applied serial approach to the modeling of a first order exothermic reaction. All the known parts of the process were based on first principles, and the remaining unknown parts were modeled by neural network model. The comparison showed that for this particular example, both prediction and extrapolation capability of semi-mechanistic modeling technique (specifically, serial approach) outperformed the straightforward nonlinear black-box model. Results were based on simulation.

Other applications were Continuous Stirred Tank Reactor (CSTR) (Cubillos and Lima, 1998), pressure vessel (van Can, Hellinga, Luyben, Heijnen and te Braake, 1996), pilot scale process involving three tanks in series (Wilson and Zorzetto, 1997), and linearized chemical reactor model (Tulleken, 1991).

In environmental engineering, serial approach was used to model the filter pressure drop. Conlin et al. (Conlin, Peel and Montague, 1997) reported that serial approach was better than empirical model on modeling the first stage filter pressure drop in water treatment process. Rate of reaction was predicted by neural network, and then supplied to first-principles model. Concerning model prediction accuracy, results showed that serial approach was much better than empirical model (neural network and polynomial), and was better than parallel approach.

In metallurgical engineering, serial application also has lots of applications, although the applications were still on simulation stage. Reuter et al. (Reuter and van Deventer, 1991; Reuter, Van Deventer and Van Der Walt, 1993) implicitly proposed this strategy to model a series of metallurgy and mineral processes described by kinetic terms. The serial approach in this paper was called Generalized Neural-Net Rate Equation (GNNRE). Neural network was used to estimate the kinetic parameters, which together with conservation equations to construct the generalized model. The GNNRE is process-independent and was applied to simulate adsorption and reduction processes (Reuter and van Deventer, 1991), flotation, leaching and precipitation processes (Reuter, Van Deventer and Van Der Walt, 1993). The leaching and precipitation processes were also validated by industrial kinetic data. The deficiency of this paper is the model validation. Without specific training algorithm dealing with over-parameterization, the number of training data sets from industrial kinetic data was smaller than that of adjustable parameters in neural network, thus making the generalization unreliable.

Other applications were a rougher flotation process (Cubillos and Lima, 1997; Cubillos and Lima, 1998), a direct flow rotary dryer and a batch fluidized bed dryer (Cubillos, Alvarez, Pinto and Lima, 1996).

In thermal engineering, Guo et al. (Guo, Shen, Li and Zhao, 1997) applied serial approach to model coal gasification process. Neural network was used to identify a parameter for the overall reactivity of char named "Active Char Ratio (ACR)". The hybrid serial model was trained with experiment data for two coals and gave good performance.

In power engineering, there are also some applications. Alessandri and Parisini (Alessandri and Parisini, 1997) modeled a section of an actual 320 MW power plant. First, all the known parts were modeled by first principles model. Secondly, neural networks modeled all unknown parts. Thirdly, a stochastic method, Smoothed Simultaneous Perturbation Stochastic Approximation (SPSA), was used to identify the first-principles model parameters. Simulation results showed this was an effective method.

Another application is to use a hybrid counter-propagation neural network and Ward-type equivalent (the equivalent concept as "first-principles model") approach for power system network reduction (Lo, Peng, Macqueen, Ekwue and Cheng, 1997). Test results demonstrated that the serial approach was very efficient and highly accurate compared to the external system equivalent.

In semiconductor industry application, Nami et al. (Nami, Misman, Erbil and May, 1997) showed an example in Metal-Organic Chemical Vapor Deposition (MOCVD). Serial approach was applied to the model that characterizes the MOCVD of titanium dioxide (T_iO_2) films through the measurement of deposition rate over a range of deposition conditions. Neural network predicted outputs - diffusion coefficient, activation energy, and a pre-exponential factor related to the molecular "attempt rate" of the growth process, were fed into the physical deposition rate expression, then the predicted deposition rate was computed. Data for training the neural network were from real experiment.

In paper industry, reports showed that serial modeling approach was applied to a continuous digester (Funkquist, 1997; Funkquist, 1997) and a Thermal Mechanical Pulping (TMP) refiner (Allison, Isaksson and Karlstrom, 1997).

Lindskog and Ljung (Lindskog and Ljung, 1994) reported the SEMI software tool for semi-mechanistic modeling. In SEMI, *Maple* and *Matlab*, which were running as separate processes, provide the symbolic and numerical services. These processes were invoked via a Graphical User Interface (GUI).

2.1.2 Parallel Approach

Parallel approach is the use of neural network to predict residual errors in first-principles model. The structure is shown in Fig. 2.2. Process inputs are supplied to both first principles model and neural network model. The outputs of the neural network are the residual errors of first-principles model. First-principles model outputs and neural network outputs are added together as the hybrid model outputs.

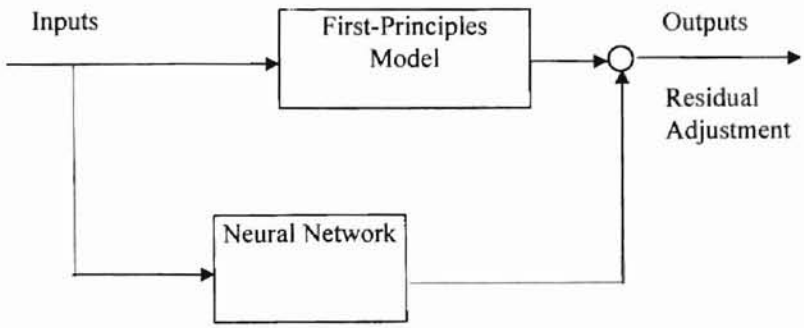

Fig. 2.2 Parallel Approach Model Structure

(Neural network is used to compensate first-principles model prediction error)

Parallel approach was first proposed by Kramer et al. (Kramer, Thompson and Bhagat, 1992) in 1992. A radial basis function neural network was trained to learn the residuals of the default model (a terminology used by Kramer et al. (Kramer, Thompson and Bhagat, 1992), which is equivalent to "first-principles model"), the output of the hybrid parallel model was the sum of the output of default model and the output of neural network model. The network contribution to the output would be small if either the data conform to the default model (in which case there was no residual for the neural network to model), or upon extrapolation. The approach was applied to a CSTR simulation problem. Later in 1994, the same research group published a well-known paper (Thompson and Kramer, 1994) in 1994. The modeling method was applied to a fed-batch penicillin fermentation process. The process state variables were supplied to both default (first-principles) model and a Radial Basis Function Network (RBFN). RBFN output was added to the default model output to predict specific rates. The specific rates were then supplied to an output (first-principles) model to get new state variables. In this paper, parallel approach was combined with the serial approach to reach a better model prediction.

Cote et al. (Cote, Grandjean, Lessard and Thibault, 1995) applied the parallel approach to improve the accuracy of an existing first-principles model of the activated sludge process. Neural network models successfully predicted the remaining errors of the optimized first-principles model. Pettersson et al. (Pettersson, Gutman, Bohlin and Nilsson, 1997) treated residual error of first-principles model as disturbance. Instead of using neural network, a stochastic model, extended Kalman filter, was used to model the disturbance. The approach was tested on a bending stiffness model for paper-board

manufacturing. One other application was the simulation study of a pH-neutralization tank (Johansen and Foss, 1992)

Applying parallel approach alone to a process modeling seems not so attractive as the serial approach according to some researcher. van Can et. al (van Can, Hellinga, Luyben, Heijnen and te Braake, 1996) compared different modeling methods. A pressure vessel modeling using real-time experimental data was carried out. Four approaches were used: neural network model, serial approach with polynomial function as parameter prediction tool, serial approach with neural network as parameter prediction tool, and parallel approach. Based on extrapolation property, parallel approach showed no advantage over neural network model. Both parallel approach and neural network model were much worse than the serial approach. Conlin et al. (Conlin, Peel and Montague, 1997) also reported the same conclusion on the modeling of pressure drop in water treatment.

There were not so many applications reported using parallel approach as those using serial approach.

2.2 Gray-box model

Gray-box modeling strategy starts with the building of a empirical model (neural network is one of the most popular empirical model), *a priori* knowledge is then incorporated into the building of the model. The model development can be divided into two phases, design phase and training phase. In each of the phase, a priori knowledge can be incorporated to make the model more accurate.

Design Phase

In design phase, it is necessary to know the type and structure of the neural network. For example, the following questions must be answered.

1) Is the process continuous or discrete? The answer to this question lead to the selection of a continuous-type network or discrete-type network.
2) Is the process dynamic or static? The answer to this question lead to the selection of a dynamic-type network or static-type network. Some intrinsically static network can also be used to model dynamic process by treating delayed process inputs as different neural network inputs.
3) How many input variables and output variables are required for the process? The answer to this question lead to the determination of the number of input nodes and output nodes of the neural network.

These questions seem trivial, but they are important *a priori* knowledge to determine the type and structure of the neural network.

Dimopoulos and Kambhampati (Dimopoulos and Kambhampati, 1998) proposed a method to determine the number of minimum neurons required for Dynamic Recurrent Neural Networks. The authors used relative order of systems as *a priori* knowledge to specify network topology before training, thus greatly reducing the training effort. Another application (Schender and Agarwal, 1991) is to adopt state space concept into neural network structure.

Training Phase

In the training phase, there is much information that can be treated as *a priori* knowledge for network training. Examples are process stability (Tulleken, 1993; Craddock, Kambhampati, Tham and Warwick, 1998), constraints on the model parameters or variables (Joerding and Meador, 1991), the smoothness of the system behavior (MacKay, 1992; Foresee and Hagan, 1997), and derivatives of process variables at certain points (Tulleken, 1993; Lampinen and Selonen, 1995; Kosanovich, Gurumoorthy, Sinzinger and Piovoso, 1996; Hartman, 1998).

Train neural networks to model the process with only sparse plant data is a very practical issue in the real world. In such situations, a priori information must be incorporated to generate "pseudo data". The derivative information of process variables at certain points can be used as *a priori* information. The derivatives not only can serve to generate "pseudo data," but also the derivatives can make the trained neural networks comply with *a priori* rules (Martinez and Wilson, 1998).

Lampinen and Selonen(Lampinen and Selonen, 1995) used inaccurate derivative information to train 3 layer feed forward neural networks. A revised Back Propagation (BP) algorithm was derived and used to train the neural network. Simulation results showed that this network had a better representation of the system than a standard 3 Layer feed forward neural network trained with traditional BP algorithm.

Kosanovich et al. (Kosanovich, Gurumoorthy, Sinzinger and Piovoso, 1996) proposed to use information from first-principles model, which designated as "time rate of change of the error", along with the training data, to train feed forward neural network.

The simulation results for a chaotic process showed that such trained neural network had better performance than conventional network.

Lee and Oh (Lee and Oh, 1997) took "Jacobian of mapping", which is similar to derivative information, as *a priori* knowledge of the system. Neural network learning was the hybridization of the error back propagation and the Jacobian learning. The method showed good performance in accelerating the learning speed and improving generalization. From simulation, results showed that using the Jacobian synthesized from noise-corrupted data could accelerate learning speed.

Although the idea is still under development, Pavilion Technologies Inc. (Hartman, 1998) applied gain-constrained training into its product *Process Insights*® and has already filed a patent on this idea. Whether or not this idea is already mature enough on the stage of commercialization, only Pavilion can show the results now, if any.

Instead of using neural network as the black-box part in gray-box modeling, stochastic method is also frequently reported. Tulleken (Tulleken, 1991; Tulleken, 1993) proposed a bayesian approach. Given a prior distribution, associated with the physical knowledge (process stability, sign of stationary gains, etc.) and data likelihood, a posterior distribution was constructed. Explicit solutions were given for special cases of Gaussian likelihood and *a priori*, which is uniformly or piece-wise linearly distributed on a linearly constrained gray-box model class. Simulation was applied to the kinetic parameter estimation of a continuous and a batch reactor model in (Tulleken, 1991). Simulation results to a distillation process showed (Tulleken, 1993) the advantage of the constrained estimates under realistic experiment conditions. Considerable variance can be reduced at the cost of a somewhat larger bias.

Sadegh et al. (Sadegh, Melgaard, Madsen and Holst, 1994) used probability distribution function in system parameters as prior partial information for optimal experiment design. A continuous time physical model of the heat dynamics of a building was considered and the results showed that performing an optimal experiment corresponding to a Maximum A Posteriori (MAP) estimation results in a considerable reduction of the experimental length.

Bohlin and Graebe (Bohlin and Braebe, 1994) reviewed the strategy for stochastic gray-box identification and surveyed experiences and lessons of applying it to a number of industrial processes. The industrial processes applied were yeast production (Fan, 1990), rinsing of strip steel (Sohlberg, 1991; Bohlin, 1994), mould level control (Graebe and Bohlin, 1992; Graebe and Goodwin, 1992), recovery boiler(Bohlin, 1993), pulp digester (Funkquist, 1993; Funkquist, 1997a; Funkquist, 1997b). A tool kit, IdKit, and a user's shell, IKUS, was developed and reported.

2.3 Summary

Recently, combination of *a priori* knowledge with black-box modeling techniques is gaining considerable interest. However, there are still lots of issues need to be considered. First, most applications are still in simulation stage. The very limited cases of industrial application were very simple process. No complicated process such as distillation column has been the subject. Secondly, all the reported applications were case studies. No systematic modeling method is developed that can be applied to almost all processes. Thirdly, no criteria are developed to guide the modeling, to tell under

which conditions which model can and is best to be developed. This research is intended to do further investigation, applying the modeling method to distillation column.

CHAPTER 3

CONCEPT DEVELOPMENT

In order to develop accurate process model with least amount of time and money, one need to maximize the usage of available prior information of the process. If most of the mechanisms of the process are known, a model starting from physical mechanism very likely to be developed. Then the unknown mechanism can be empirically correlated by additional experimental data. On the other hand, if little of the mechanism of the process is known, but rich process history data are available, a gray box model is likely to be developed. The ideal situation is that one does not need to do any experiment and use all the available prior information to create a process model.

This chapter comprises three parts: first, the hybrid model development strategy is proposed. Secondly, hybrid serial modeling method is applied to experimental distillation column. Thirdly, hybrid parallel modeling method is applied to model the same experimental distillation column. Lastly, model evaluation criteria are developed to evaluate the model.

3.1 Hybrid Modeling Method Development Strategy

At the very first step, a model developer must make it clear that which kind of model needs to be built to meet the requirement of the model. For example, if the model is to be used in an on-line control application, a dynamic model is necessary. In control applications, accurate one step ahead prediction may be the defining performance criteria.

On the other hand, if the model is to be used in a plant-wise optimization purpose, then a simpler, lumped model for individual process units is enough. In optimization, accurate steady-state prediction may be the most important to address.

The second step is the prior knowledge analysis. Prior knowledge is knowledge about the process that exists prior to the synthesis of the model. The prior knowledge includes hard constraints and soft constraints imposed on the process by first principles or design considerations, historical plant data and much more.

The "hard" or "soft" constraints depend on their precedence with respect to the data. Hard constraints must be strictly obeyed. Examples of hard constraints are valve openings, which is limited from 0% to 100%; tank levels, which is limited from zero to the height of the tank; safety limits, such as the limit of pressure of a tank; product quality needs, such as the sterility, purity limits.

On the other hand, "soft" constraints are those that "preferably" to be obeyed. For example, process response under step change preferably is first order plus dead time, with small time constant and dead time. Model preferably can be extrapolated beyond the training data set. Model is also desired to have some qualitative behavior such as smoothness.

Historical plant data are important prior knowledge. Plant data reflect the intrinsic material and energy balance, physical restrictions due to equipment limitations, and real process behavior, etc. But plant data in most chemical processes are corrupted by measurement noise and calibration error. In addition, because the processes usually work on some certain set point, the all-range process behaviors are usually unavailable.

When applying prior knowledge to the modeling process, in most cases it is difficult to meet all the requirement of the process. Some compromise must be made. The relationship between "hard" constraints, "soft" constraints and historical data is that "hard" constraints should take precedence over historical plant data, and historical plant data should take precedence over "soft" constraints.

The third step is to select a starting point to develop the model. The ultimate purpose of research is to reveal the intrinsic mechanism of the process. One should incorporate as much physical mechanism in the model as possible. This logically lead to the conclusion: If first principles model is possible, then develop the first principles model. But if only partial mechanism is available, depend on how much the priori knowledge is available, a hybrid serial model or hybrid parallel model can be developed. At a worse situation, if only some intuitive knowledge, such as process gains at certain points, process smoothness, is available, one can only develop a gray box model. The worst situation is that one know nothing about the process, but only some input-output data are available, the only choice is to develop a empirical model.

If only small amount of experiment work is enough for empirical model fitting, semi-mechanistic model is likely to be developed. Furthermore, hybrid serial model is likely to be developed if most mechanism of the process are known, and model coefficients are unknown but can be estimated from process variables. If in some region, parts of the mechanism are unknown, but historical data are available to do the correlation, hybrid parallel model is likely to be developed.

On the contrary, if little mechanism of the model is known, and rich plant history data are available, gray box model is likely to be developed. If only sparse plant data are

available, some technique like gain constraint training method may be employed to fill the data gap.

The last step is to develop the model. Since most of the work is done in the first three steps, this step is only a routine work that needs to be done.

3.2 Hybrid Serial Modeling Method

Hybrid serial model has better prediction over first-principles model. The reason lies in the fact that neural network can use all influencing variables, thus leading to better parameter prediction capacity. In distillation column modeling, column efficiency is difficult to model by first-principles model, while it can be inferred from process operating conditions. Neural network can be used as the mapping between process variables and column efficiency.

As the schematic diagram shown in Fig. 3.1, serial approach is a hybrid model, which consists of two sub-models, i.e., neural network model and first-principles model. Neural network model is used to predict overall column efficiency. All trays are assumed to have the same Murphree vapor phase efficiency, which equals to the overall column efficiency. Neural network model inputs are process variables that can determine the tray efficiency, such as feed flow rate, feed composition, feed preheat temperature, reflux flow rate, reboiler temperature and top tray temperature. The final inputs to the neural network should be determined by trial and error, only the variables that have close correlation to the output are selected. Neural network model output is the overall column efficiency.

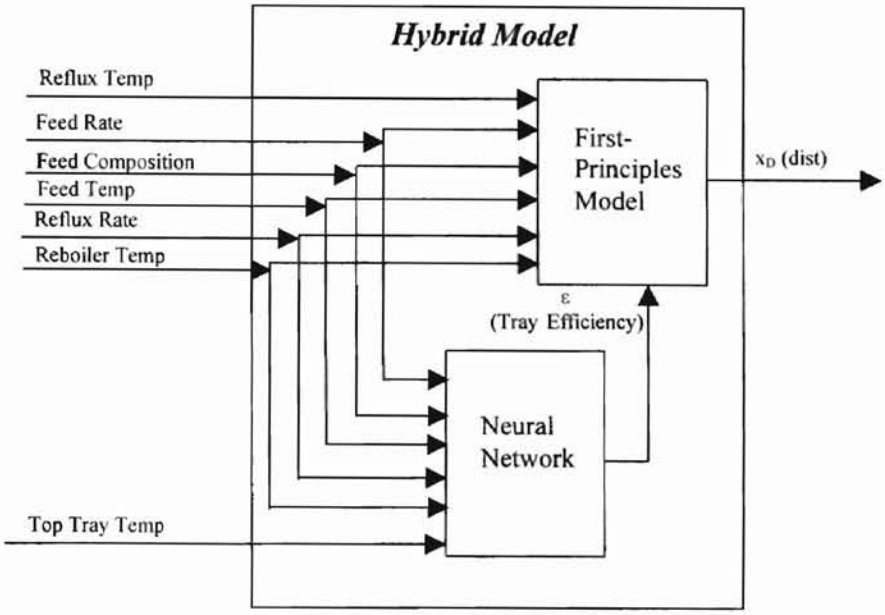

Fig. 3.1 Distillation Column Model Structure in Serial Approach

(Neural network is used to model tray efficiency)

A standard feed forward neural network is applied. The neural network consists of one input layer, one hidden layer and one output layer. The proposed training algorithm is Levenberg-Marquardt with bayesian regularization (Foresee and Hagan, 1997), which requires fewer experimental data points while still overcoming the overfitting problem. Bayesian regularization ensures smoothness in the output of the neural network. Optimum number of hidden neurons can be determined as follows: Train neural network with 1, 2, ... hidden neurons, record the effective number of parameters in each neural network, which is automatically reported in the training results. Starting from a neural network with n hidden neurons, all the neural networks with n+1, n+2, ... hidden neurons will have the same number of effective number of parameters. Choose

the neural network with n hidden neurons as the one that to be used in hybrid serial modeling. The experiment data need to cover the whole operating range in order to avoid neural network extrapolation. Otherwise neural network need to do extrapolation, which is totally unreliable.

First-principles model takes reflux temperature, feed flow rate, feed composition, reflux flow rate and reboiler temperature as principal inputs, and predicted overall column tray efficiency from neural network model as secondary input. First principles model applies material balance, energy balance, thermodynamics, etc., to calculate distillate composition, which is the outputs for both first principles model and hybrid serial model.

Bottom composition is also a candidate output for the hybrid serial modeling, but distillate composition is preferred. The value of bottom composition are mostly in the range of 0 - 10 mol% MeOH, and the value of distillate composition are mostly in the range of 60 - 90 mol% MeOH. If the absolute measurement error for composition remains the same, the relative error for distillate composition would be much less than that for bottom composition.

3.3 Hybrid Parallel Modeling Method

Hybrid parallel model has the possibility of reducing the mathematical model size by allowing a somehow larger modeling error because of the unaccounted process mechanism. The model error is later corrected by neural network. When this approach applies to distillation column modeling, first principles model part can be assumed working at fixed column efficiency, although the actual process works at varied column

efficiency. The induced error can be corrected by neural network part of the model. The neural network corrects not only the error induced by column efficiency, but also various other first-principles modeling errors.

As the schematic diagram shown in Fig. 3.2, parallel approach is also a hybrid model, which consists of two sub-models, i.e., neural network model and first-principles model. The proposed parallel approach is a variation of the parallel approach discussed previously, in which neural network does not exactly have the same inputs as first principles model has.

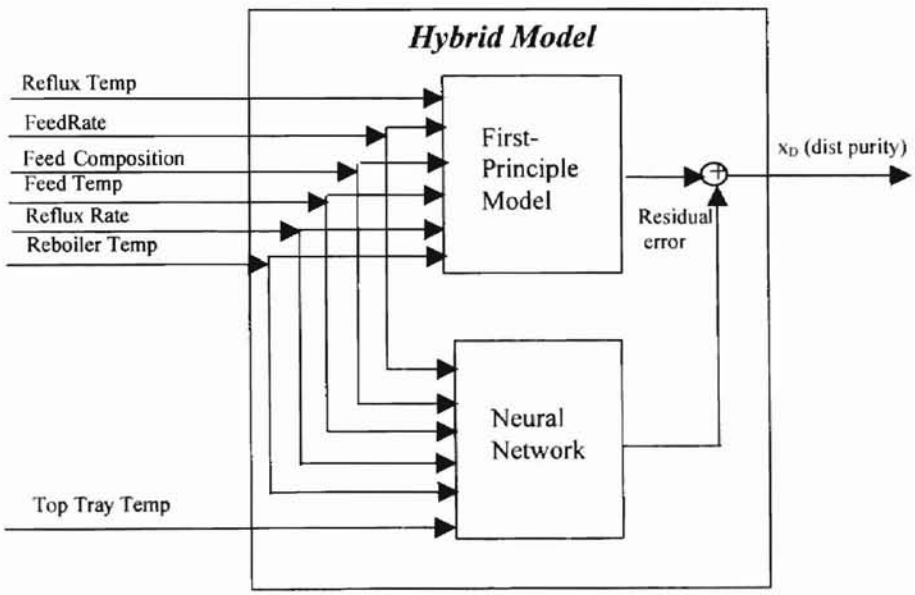

Fig. 3.2 Distillation Column Model Structure in Parallel Approach

(Neural network is used to compensate first-principles model prediction error)

First-principles model takes reflux temperature, feed flow rate, feed composition, feed temperature, reflux rate and reboiler temperature as inputs, then first principles

(material balance, energy balance, thermodynamics relationships, etc) are applied to calculate distillate composition, which is the first principles model output. Neural network model takes process variables, such as feed flow rate, feed composition, feed temperature, reflux rate, reboiler temperature and top tray temperature, as inputs. The final inputs to the neural network is determined by trial and error, only the variables that have close correlation to the output is selected. Neural network model serves for error correction to first-principles model, since first-principles model outputs have errors comparing to the actual process outputs. Neural network model output (residuals) is then added to first principles model output (distillate composition). The sums serve as the hybrid model output. A standard feed forward neural network is used. The neural network structure and training algorithm is the same as that used in hybrid serial model, that is, one input layer, one hidden layer and one output layer, training algorithm is Levenberg-Marquardt with bayesian regularization.

3.4 Model Evaluation

The distillation column can be viewed as a stochastic process. A stochastic process consists of two parts: one is the deterministic part, which is predictable. The other is the random part, which is unpredictable. A well-modeled stochastic process model should include all the predictable factors, and leave the unpredictable factors as residual error, i.e. noise. If the residual errors are biased noise, then the noise part contains something that is predictable, and the model has to be improved. The residual error mean value should be zero. Also, the residual errors in a well-modeled stochastic

process should only contain white noise, i.e., "a sequence of independent (identically distributed) random variables with a certain probability density function" (Ljung, 1999).

There are several ways to test the whiteness of the noise. One common way is the auto-correlation method (Box, Jenkins and Reinsel, 1994). One can visually tell whether the residuals are white or not from plots of auto-correlation function. A more rigorous way is to use χ^2 test (Ljung, 1999). In this research, only the auto-correlation test was used.

For auto correlation method, if infinite number of data points are available, the normalized auto correlation function for white noise equals to 1.0 at lag k=0, i.e., no lag. At all other points, auto correlation function equals to 0. In reality, since only limited amount of data is available, the auto correlation function is only close to 0 at lag $k \neq 0$.

The data can be arranged in experiment sequence, provided that the experiment is planned in such a way that adjacent experiment data points are close to each other in the multi-dimensional process variable space.

The residual error auto correlation function at lag k can be expressed as:

$$\rho_k = \frac{E[(e_t - \mu)(e_{t+k} - \mu)]}{\sqrt{E[(e_t - \mu)^2]E[(e_{t+k} - \mu)^2]}} \tag{3-1}$$

Where ρ_k – auto correlation function at lag k.

e_t, e_{t+k} – residual error at time instant t and t+k, respectively.

μ – mean value of e_t.

E[ ] – mathematical expectation of the random variable(s) in the bracket. $E[e_t] = \mu$.

μ can be estimated from the data set by

$$\hat{\mu} = \frac{1}{N}\sum_{t=1}^{N} e_t \tag{3-2}$$

ρ_k can be estimated from the data set (Box, Jenkins and Reinsel, 1994) by

$$\hat{\rho}_k = \frac{c_k}{c_0} \tag{3-3}$$

where

$$c_k = \frac{1}{N}\sum_{t=1}^{N-k}(e_t - \hat{\mu})(e_{t+k} - \hat{\mu}) \tag{3-4}$$

$\hat{\mu}$ and $\hat{\rho}$ are the estimate of mean and auto correlation function, respectively. N is the total number of points.

In this research, residual errors are the difference between experiment distillate composition and hybrid model predicted distillate composition.

CHAPTER IV

EXPERIMENT RESULTS

The application of semi-mechanistic model (hybrid serial model and hybrid parallel model) and gray box model reported in the literature was restricted to either simulation studies or simple processes. The applicability of the modeling strategies to complex process is still under investigation. In this chapter, the proposed methods are applied to model distillation column.

Distillation column modeling is a challenging problem for both testing the proposed modeling methods and for practical reasons. The difficulty of distillation column modeling provides a good example for testing the modeling methods. As we know, distillation column is a complex chemical process, which has complex characteristics including severe non-linearity, large dead-time, interactions, and subjection to many constraints and disturbances.

For practical reasons, accurate distillation column model is always needed. Distillation is the most important separation technique in chemical process industries around the world and constitutes a significant fraction of chemical plant capital investment. The operating costs of distillation columns are often a major part of the total operating costs of many chemical plants. Within the U. S., there was an estimated 40,000 columns which consumed approximately 3% of the total all-purpose energy usage (Humphrey, Seibert, and Koort, 1991). Improved distillation control based on more accurate model can have a significant impact on reducing energy consumption,

improving product quality, and protecting environmental resources. Hence, accurate distillation column model is necessary.

This chapter is organized as follows: Section 1 introduces the experimental distillation column setup, including column instrumentation, Data acquisition and control system, and interfacing program development. Section 2 is the step by step hybrid serial modeling method and the resulting model performance. Section 3 is the step by step method for hybrid parallel modeling and the resulting model performance. Section 4 shows the model evaluation results.

4.1 Experimental System

4.1.1 Experimental Setup

Figure 4.1 depicts the experimental distillation column in Unit Operations Lab of the School of Chemical Engineering, Oklahoma State University. The column consisted of 6 sieve trays, one direct heated reboiler and one total condenser. Feed was pumped (P-1) from Feed Tank (TK-1), electrically preheated (E-1) and then fed into the column. Reboiler (E-3) was also electrically heated. Bottom product was cooled through bottom cooler (E-2) before flowed to bottom product tank (TK-2). Vapor from the top tray was first condensed (E-1) before flowed to reflux drum (D-1). Part of the condensate overflowed to distillate tank. Part of the liquid was pumped (P-2) back to the column as reflux. An electric heater preheated the reflux before it was fed back to the column. Water from municipal water supply pipeline was used as coolant. Cooling water was first used in the condenser (E-1) to condense the vapor, and later was fed into bottom

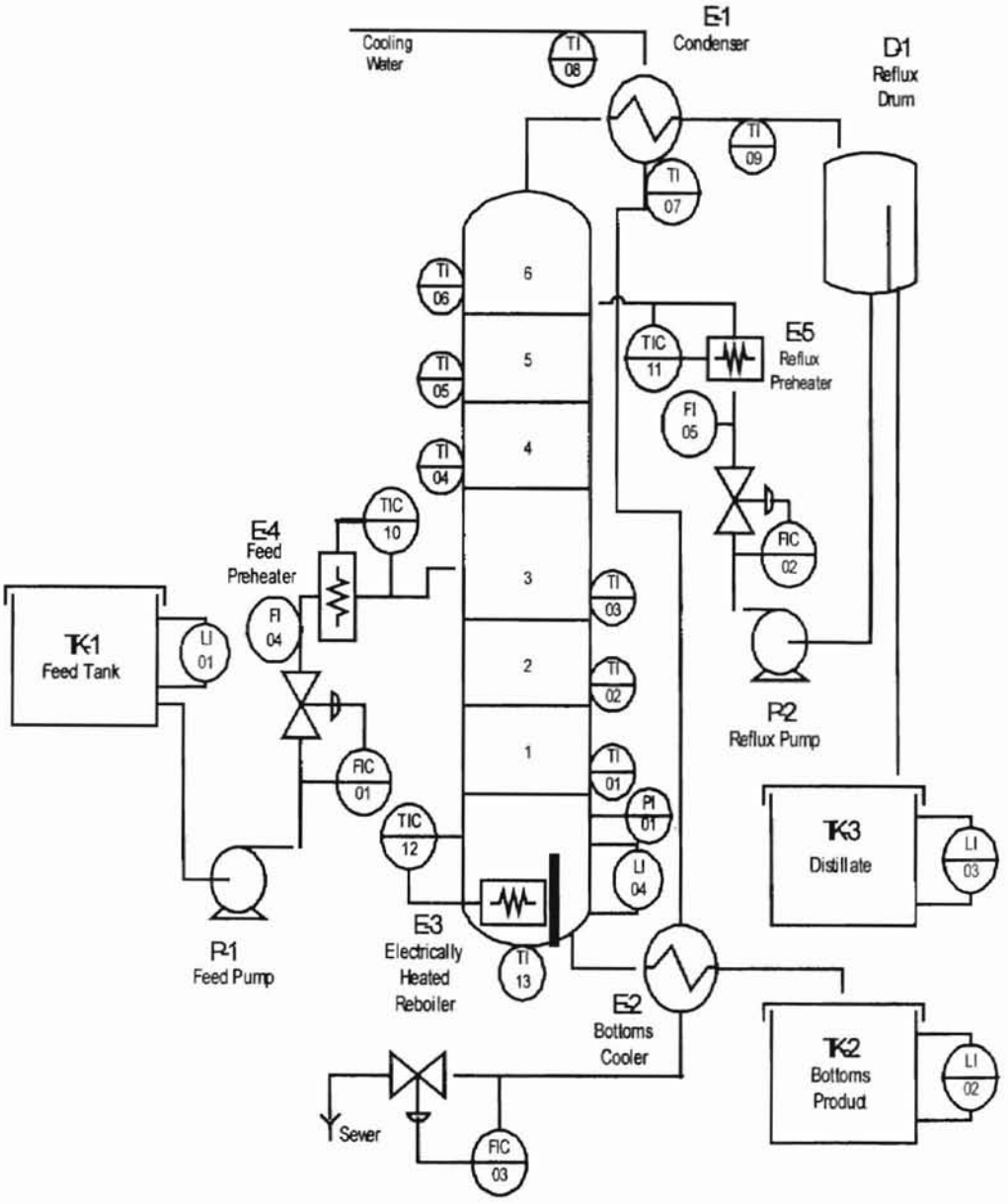

Fig 4.1 Instrumentation Diagram of Experimental Distillation Column

cooler (E-2) to lower the bottom product before the bottom product went to bottom product storage tank (TK-2).

4.1.2 Instrumentation

There were totally 13 temperature measurement points. Each tray temperature was measured (TI-01, TI-02, TI-03, TI-04, TI-05 and TI-06). Cooling water temperatures were measured before it entered the condenser (TI-08) and after it left the condenser (TI-07). Condensate temperature (TI-09) out of the condenser was measured. Feed temperature (TIC-10) after the preheater was measured, and controlled through SCR. Reflux temperature (TIC-11) after the preheater was measured, and controlled through SCR. Reboiler temperature (TIC-12) was measured, and controlled through SCR. All the above temperatures were measured by type K thermocouples. All the temperatures were also indicated in the computer and recorded in an ASCII-format logging file.

There was also a local temperature indicator directly mounted on the reboiler to measure the reboiler temperature (TI-13).

Feed flow rate (FIC-01), reflux flow rate (FIC-02) and cooling water flow rate (FIC-03) were measured and controlled. The measurement devices were Differential Pressure (DP) cells (the integration of orifice meter and pressure transducer). All the above flow rates were controlled by control valves. All the above flow rates were also indicated in the computer and recorded in an ASCII-format logging file.

Feed flow rate (FI-04) and reflux flow rate (FI-05) were also indicated by two rotameters, respectively.

Four liquid levels were measured: feed tank (LI-01), bottom product tank (LI-02), distillate tank (LI-03), reboiler level (LI-04). All measured levels were indicated in the computer and recorded in an ASCII-format logging file.

Only one pressure point, the reboiler pressure (PI-01), was measured and indicated in the computer. At the same time, the value was recorded in an ASCII-format logging file.

Methanol compositions (feed composition, bottom product composition and distillate composition) were sampled at steady state and measured off-line by refractormeter.

All other necessary process variables were inferred from the above measured variables. Distillate flow rate was calculated from the distillate tank level change in 5 minutes intervals, the cross sectional area of the tank and the density of the liquid. Bottom product flow rate was calculated by the same method.

Fig. 4.2 and Fig. 4.3 shows the front view and back view of the distillation column, respectively. From Fig. 4.2, one can see the 6-sieve-tray distillation column, reboiler at the bottom and condenser at the top.

From Fig. 4.3, one can see SCR (Silicon Rectifier) at the up-front position, feed flow rate transducer and feed valve at the middle-back position, feed pump at the bottom-front position, and feed tank at the bottom-back position.

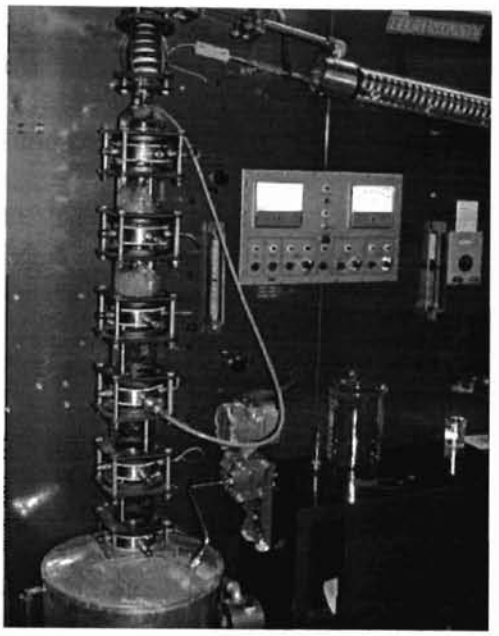

Fig 4.2 Front View of Distillation Column

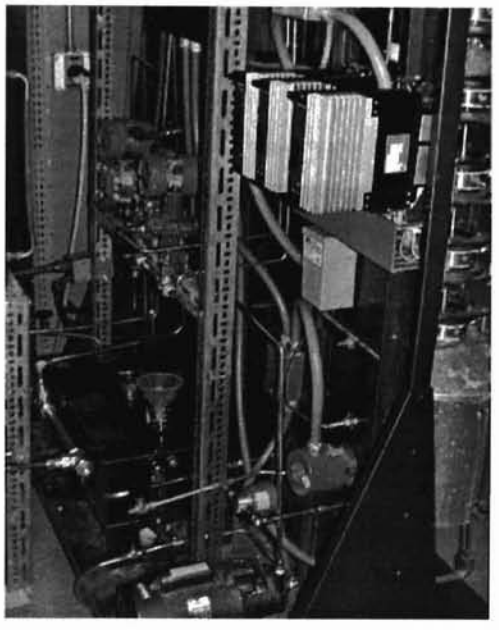

Fig 4.3 Back View of Distillation Column

4.1.3 Data acquisition and control system (Camile Products, LLC, 1997, 1998)

Camile 2200 hardware, along with Camile TG 3.7 software, was selected to meet the specific data acquisition and control needs of this research.

Camile 2200 is a nine-slot Camile chassis with an optional integrated PC (not installed for this application). In this application, 6 boards were installed. One controller board (PN 564) was to perform control action calculation and scheduling data collection and transmission. One terminator board (PN 554) was installed to minimize system noise by damping resonant frequencies in the bus. One network communication board (PN 565) was used to communicate with the host PC. One thermocouple board (PN 525) was for thermocouple inputs signals. One analog input board (PN 525AI) was for analog input signals (flow rates, levels, and pressure). One analog output board (PN 522) was for analog output signals (to control valves, SCRs).

Fig. 4.4 shows the front view of the Camile 2200 unit with board installed.

Fig. 4.4 Camile 2200 (with boards installed)

A network communication board (PN 566) was installed in host computer to communicate with camile box.

Camile TG 3.7 software was installed in a host PC, which was used to configure the process, perform control, programming user interface, data logging, and data retrieval.

Fig 4.5 shows the computer screen while the experiment was running. The computer can be configured to display trends of any process sampled variables. The scale can be as small as millisecond, or as large as days.

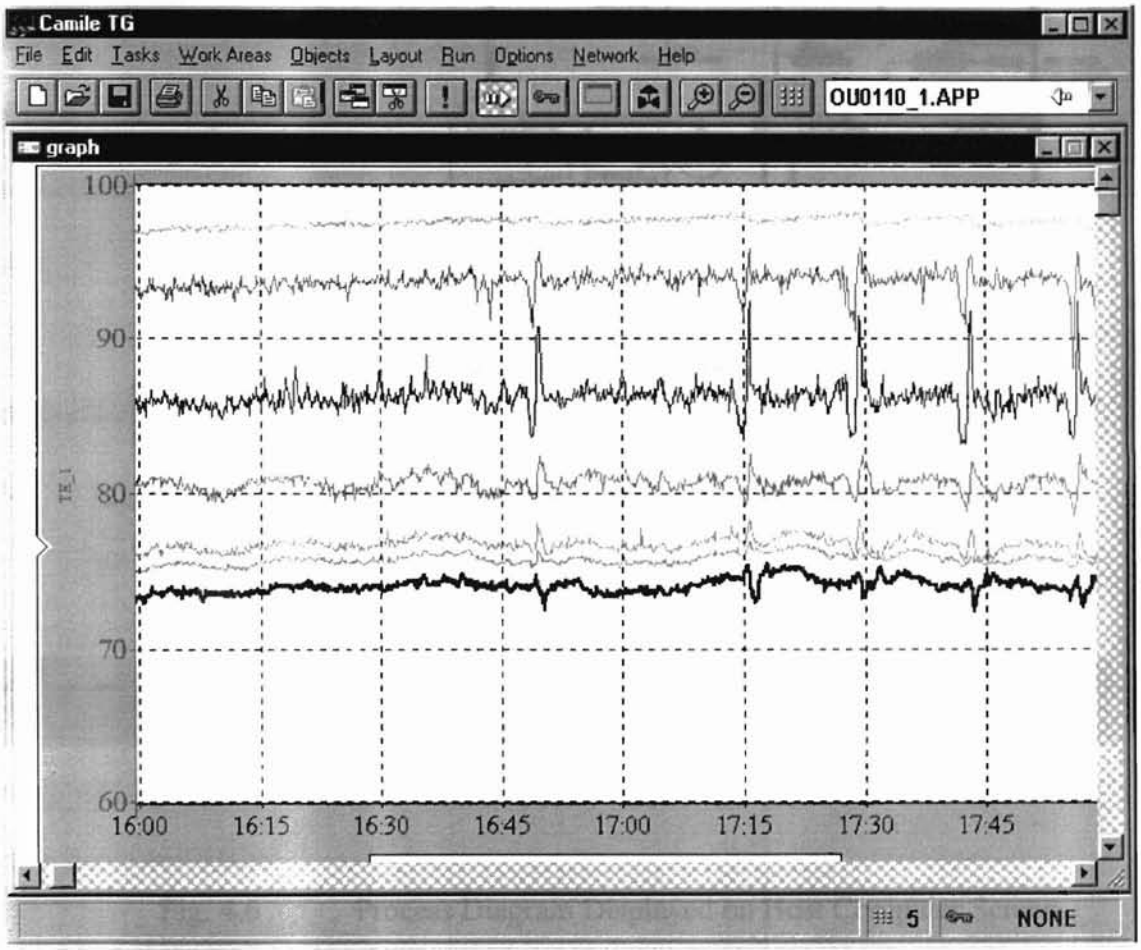

Fig. 4.5 Trends of Process Variables Displayed on Host Computer Screen

Figure 4.6 is the graphical configuration of the process. The graphical interface provides the flow sheet for the process.

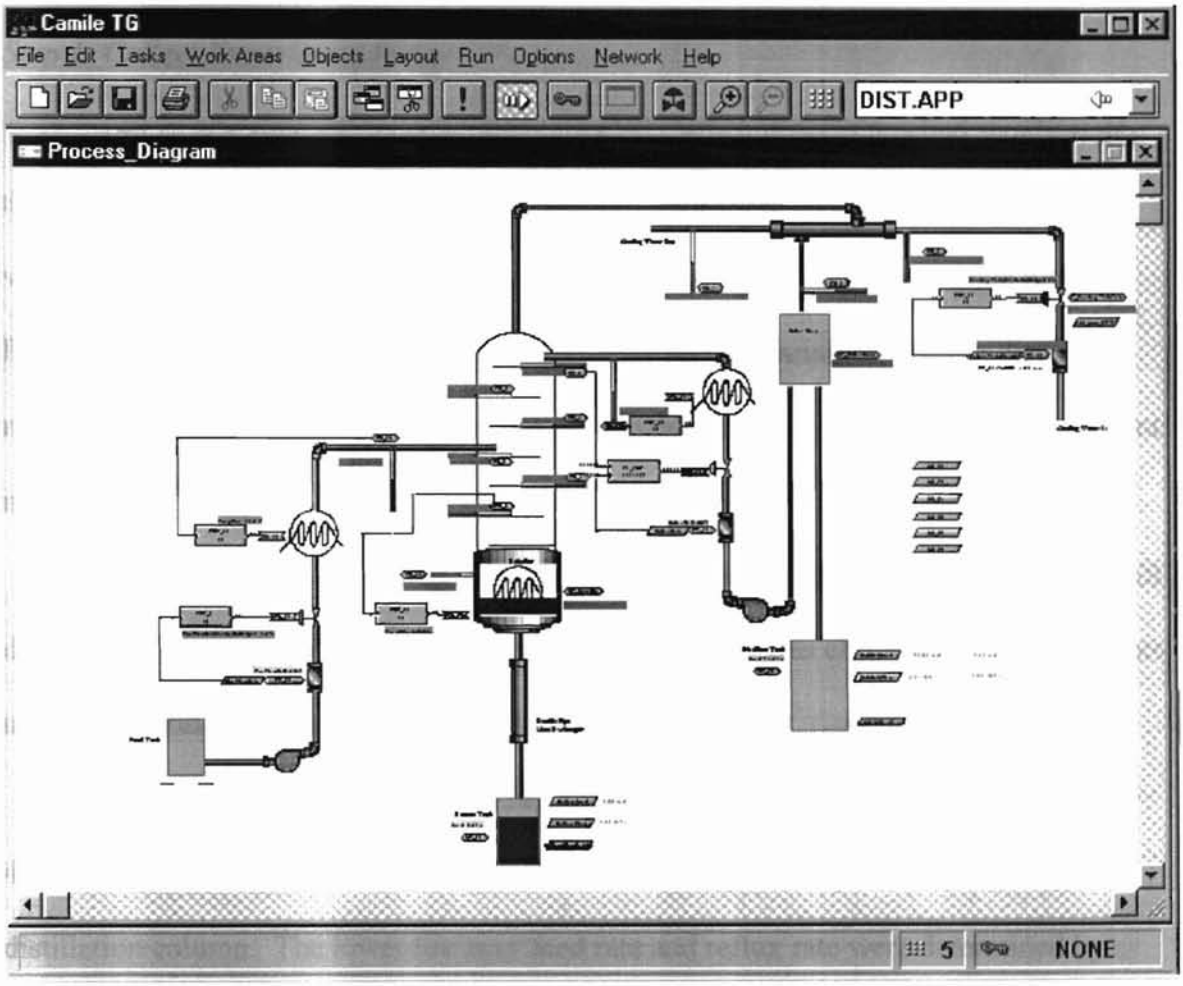

Fig. 4.6 Process Diagram Displayed on Host Computer Screen

4.2 Hybrid Serial Modeling Method

4.2.1 Modeling procedure

The modeling of distillation column can be described in the following 5 steps.

Step 1: Collect Experiment Data.

148 steady state data points were collected. When process reached steady state, the experiment continued to run for additional 30 minutes in steady state. Process variables were measured every 30 seconds during this 30-minutes steady state period. Process variables (except for liquid level and level related variables, such as distillate rate, bottom rate) were averaged over this 30 minutes time period to reduce measurement noise.

For hybrid serial modeling, 88 data points from the whole data set were used. All data points where column efficiency equals or close to 1.0 was eliminated. The 88 points used for hybrid serial modeling can be found in Appendix E.

The operating limits and operating points of process variables is shown in Table 4.1. Operating limits is the physical limitation of each process variable for this specific distillation column. The lower limits of feed rate and reflux rate were determined by measurement device, which would give large measurement error if the flow rates were below the lower limits.

Manipulated variables were feed rate, feed composition, reflux rate, reboiler duty. Originally, 3 to 5 operating points were selected for each manipulated variable. For example, feed rate was operated at 15, 24 or 30 lbm/hr for each experiment. Theoretically, 3*3*5*3=135 experiment points need to be carried out. In reality, some

points were out of feasible operating region. As the result, those points were eliminated from the experiment. For example, at point where feed rate equals to 30 lbm/hr, feed composition equals to 40%, reboiler duty equals to 60%, reflux rate equals to 80 lbm/hr, because of the high feed flow rate and the low reboiler duty, the distillation column could not operate at this point. In addition, in some operating region, distillate rate was sensitive to one or more of the manipulated variable. When this situation occurred, more experiments were carried out to fill the gaps.

Table 4.1 Operating Limits and Points of Process Variables

(Feed Temperature set to 35 °C, Reflux Temperature set to 50 °C)

Process Variables	Operating Limits	Operating Points
Feed Rate (lbm/hr)	10 – 36	15, 24, 30
Feed Composition (mol% MeOH)	16 – 40	20, 30, 40
Reboiler Duty (% of Full Power)	60-100	60, 70, 80, 90, 100
Reflux Rate (lbm/hr)	10 – 82	15, 40, 80
Distillate Composition (mol% MeOH)	54 – 95	
Bottoms Composition (mol% MeOH)	0 – 28	

Feed and reflux temperatures were originally set to be at 35 °C and 50 °C. In reality, due to the inadequate feed preheater heating capacity, reboiler preheater heating capacity, and cooling water cooling capacity, both feed temperature and reflux

temperature were "out-of-control" in some points. All these points were kept in the experiment data set.

Step 2: Reconcile Data

The characteristics of the experiment distillation column determines that bottom product flow rate and distillate flow rate were measured with least confidence. The training data must agree with overall material balance and component material balance.

Overall material balance:

$$F = D + B \tag{4-1}$$

Component (methanol) material balance:

$$Fx_F = Dx_D + Bx_B \tag{4-2}$$

where

F – feed flow rate (lb/hr)

D – distillate flow rate (lb/hr)

B – bottom product flow rate(lb/hr)

x_F – feed composition (mass% methanol)

x_D – distillate composition (mass% methanol)

x_B – bottom product composition (mass% methanol)

Adjust bottom product flow rate and distillate flow rate to comply with the balance equations. That is, solve α and β in the following equation:

$$F = (D' + \alpha) + (B' + \beta) \tag{4-3}$$

$$Fx_F = (D' + \alpha)x_D + (B' + \beta)x_B \tag{4-4}$$

where

D' – measured distillate flow rate (lb/hr)

B' – measured bottom product flow rate (lb/hr)

The values of α and β tell how much the experiment errors are. The reconciled distillate and bottom product flow rates are

$$D = D' + \alpha \tag{4-5}$$

$$B = B' + \beta \tag{4-6}$$

This step was done in Microsoft Excel. The "equation solver" function in Excel helped in solving balance equations.

Step 3: Run ChemCAD to Determine Column Efficiency.

ChemCAD is one of the most popular commercial simulation software for chemical processes. ChemCAD Simultaneous Correction Distillation Simulation (SCDS) model was served as first-principles model in this research.

ChemCAD inputs were from reconciled data set. The inputs were: feed temperature, feed pressure (14.7 psia), feed methanol flow rate, feed water flow rate (calculated from feed flow rate and feed composition), subcooled delta T (calculated from reflux temperature), reflux flow rate, bottom product flow rate. Other less important inputs were: distillate flow rate, reflux flow rate, top tray temperature, second top tray temperature. All of the less important inputs were just estimated values for convergence purpose. Then over all column efficiency was adjusted to make the ChemCAD predicted distillate composition match experiment distillate composition.

Column efficiencies were adjusted by trial and error to the second significant digit, which were enough to keep difference of the distillate composition from ChemCAD and the distillate composition from experiment less than 0.3 mol% of MeOH (results can be found in Appendix E). Double check again to see if the predicted bottom product composition matches experimental bottom product composition. The difference of the bottom composition from ChemCAD and the bottom composition from experiment is less than 0.6%. In most cases, the difference is less than 0.1%.

Step 4: Train Neural Network to Predict Column Efficiency

Till this step, all the measured process variables and the corresponding tray efficiency were available. The neural network output was the column efficiency. But which variables should be the neural network inputs need to be determined. First, all measured variables were used for training neural network. These variables were: feed flow rate, feed composition, feed temperature, reflux flow rate, reflux temperature, reboiler temperature, tray 1 – tray 6 temperature. Then, reduced the inputs one by one. If the reduced variable made the prediction error significantly large, this variable was then kept as the true neural network input. Otherwise this variable was not used for neural network input. Based on the selection procedure described above, the final inputs to neural network were: feed flow rate, feed composition, feed temperature, reflux rate, bottom product flow rate and top tray temperature.

Experiment data need to be scaled to [-1 1] before used for training. Each variable scaling were based on the following equation:

$$\frac{measured - \min}{\max - \min} = \frac{scaled - (-1)}{1 - (-1)} \tag{4-7}$$

where "max"and "min" were the minimum measured value and maximum measured value, respectively.

All experiment data were divided into training set and test set. Based on the sequence number, the training set include 2/3 of all the data, which included data points 1,2,4,5,7,8, … The test set included 1/3 of all the data, which included data points 3,6,9…

The 3-layer neural network structure is 6-5-1. The input layer consists of 6 nodes. The hidden layer has 5 nodes, each node has hyperbolic tangent sigmoid transfer function. The output layer consists of 1 node with linear transfer function. There are totally 41 adjustable parameters. The neural network was trained by Levenberg-Marquardt algorithm with bayesian regularization (MacKay, 1992; Foresee and Hagan, 1997). The algorithm requires fewer experimental data points for training while overcoming the overfitting problem. Regularization ensures smoothness in the function approximation performed by the neural network. The training was stopped when any of the following criterion was met: value of objective function less than the performance goal (goal set to 0.0), minimum gradient reached (minimum gradient set to 1e-10), maximum epochs reached (maximum epoch set to 2000), maximum time elapsed (maximum time set to infinity), maximum μ reached (maximum μ set to 1e10, μ is a parameter in Levenberg-Marquardt algorithm). Details of the neural network training can be found in Appendix A and B.

Neural network output was then scaled back from [-1 1] to its real range.

Step 5: Test Hybrid Serial Model.

Various tests were taken to show the performance of the hybrid serial model. First, the prediction error of the neural network was examined. Secondly, hybrid serial model predicted distillate composition vs. the true distillate composition was compared to fixed efficiency first-principles model vs. the true distillate composition. Thirdly, the prediction capability between hybrid serial model and fixed efficiency first-principles model was compared. Lastly, in each experiment run, the prediction error between hybrid serial model and fixed efficiency first-principles model was compared.

4.2.2 Experimental results

In hybrid serial modeling, the improved model prediction accuracy over fixed efficiency first-principles model depends heavily on the neural network. As a result, neural network prediction accuracy must be examined. The error (ChemCAD column efficiency minus neural network predicted column efficiency) has a mean of 0.003 and standard deviation of 0.032. It is a nice prediction result. Fig. 4.7 is the plot of neural network predicted efficiency vs. ChemCAD column efficiency. ChemCAD predicted column efficiency is assumed to be the true column efficiency. The closer the diamond point to the diagonal line, the better the neural network prediction is. From the figure, it also shows that neural network gives nice prediction result.

The next step is to test hybrid serial model predicted distillate composition vs. the true distillate composition with fixed efficiency first-principles model predicted distillate composition vs. the true distillate composition. First-principles model was run under fixed column efficiency, which was the average column efficiency of all runs. In this

research, fixed column efficiency was chosen to be 40% (mol % of methanol), which is the average column efficiency for the whole experiment runs. This is the key test to see whether the hybrid model is better than first-principles model or not.

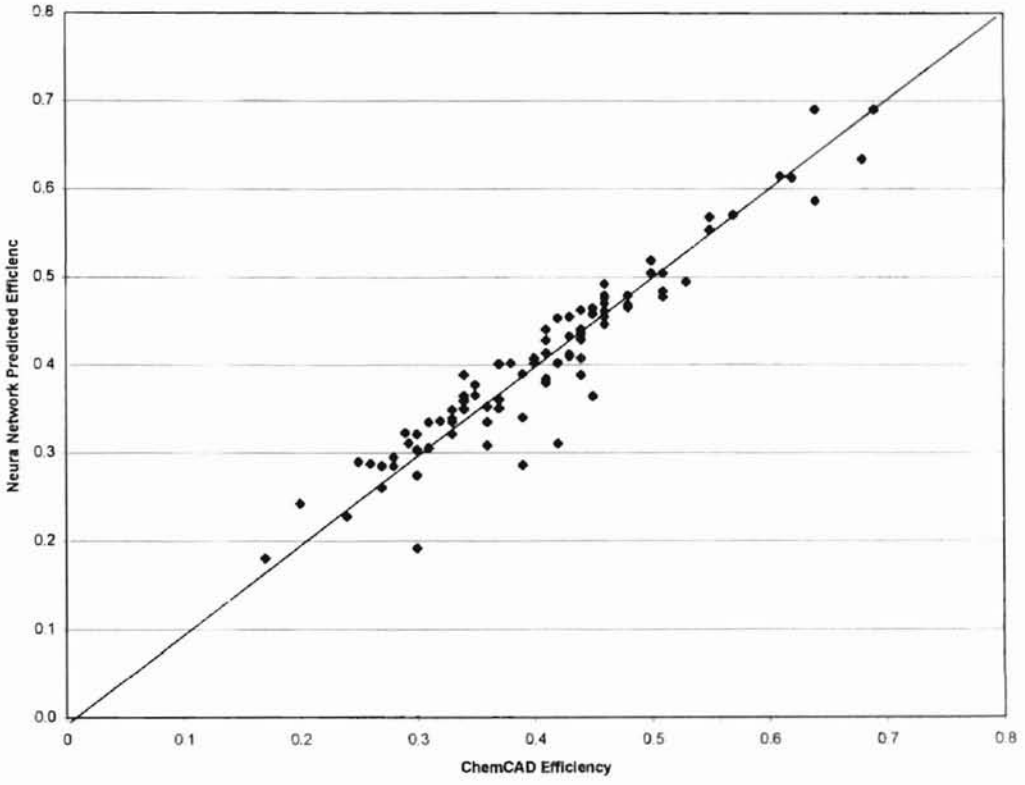

Fig. 4.7 Serial Approach: Neural Network Predicted Column Efficiency vs. ChemCAD Column Efficiency

Table 4.2 shows the prediction error of hybrid serial model and fixed efficiency first-principles model. The average error (mean error) of hybrid serial model is –1.31 mol% MeOH, which is smaller than –1.67 mol% MeOH, mean error of fixed efficiency first principles model. Standard deviation of hybrid serial model is 4.70 mol% MeOH, which is much smaller than 7.88 mol% MeOH, standard deviation of fixed efficiency

first-principles model. Table 4.2 tells that hybrid serial model provides better model prediction accuracy for the distillation column modeling.

Table 4.2 Comparison of Prediction Error between Hybrid Serial Model and Fixed Efficiency First-principles Model (unit: mol% MeOH)

	Hybrid Serial Model	**Fixed Efficiency Model**
Mean Error	-1.31	-1.67
Standard deviation	4.70	7.88

Fig. 4.8 is the model predicted distillate composition vs. actual distillate composition. The circles are the first-principles model predicted distillate composition (at fixed column efficiency) vs. actual distillate composition. The diamonds are the hybrid serial model predicted distillate composition vs. the actual distillate composition. The closer the points to the diagonal line, the better the model prediction accuracy is. Fig. 4.8 tells that hybrid serial model does provide better model prediction accuracy than fixed efficiency first-principles model.

Hybrid serial model takes unmodeled parameter – column efficiency into account, which makes the model able to predict distillate composition at any column efficiency. On the other hand, fixed efficiency first-principles model only takes average column efficiency as its parameter. First-principles model should give good distillate composition prediction if the column runs at that efficiency. But first-principles model would give bad distillate composition prediction if the true column efficiency deviate

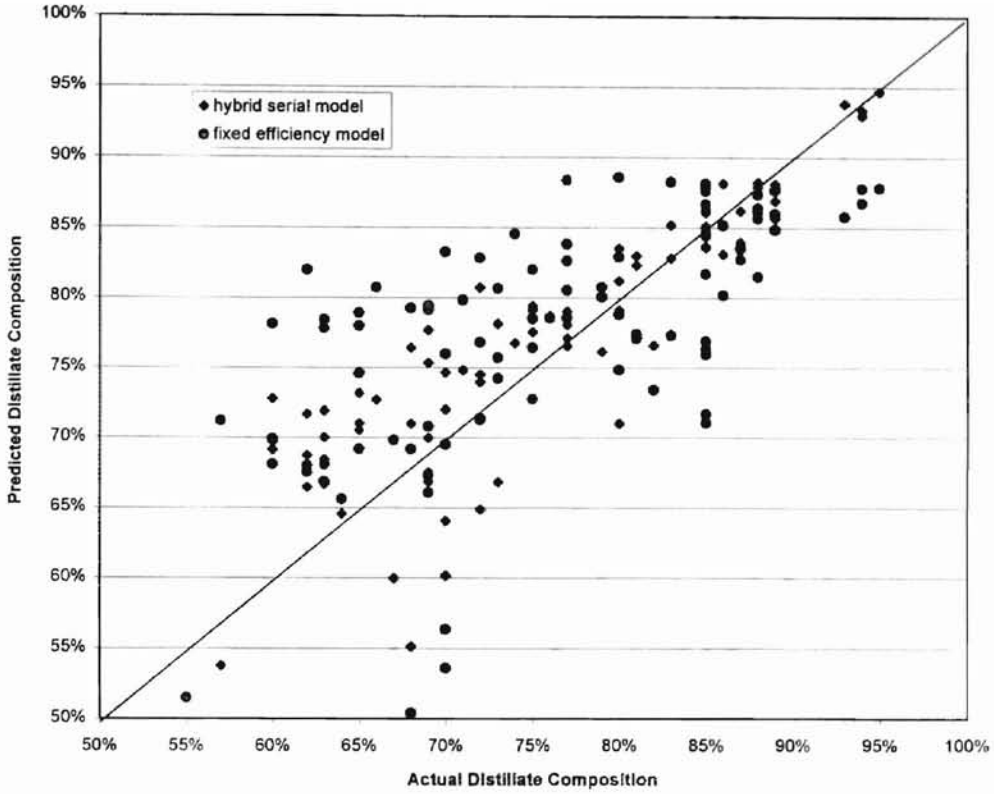

Fig. 4.8 Hybrid Serial Model Predicted Distillate Composition vs. True Distillate Composition

from the average column efficiency. Fig. 4.9 shows this conclusion. Fig. 4.9 is the plot of distillate composition predicted errors vs. column efficiency. The diamonds are the hybrid serial model distillate composition predicted errors vs. column efficiency. The trend line of hybrid serial model is almost flat, with square of correlation coefficient equals to 0.0105. At different column efficiency, hybrid serial model gives statistically the same prediction error. The circles are the first-principles model distillate composition predicted errors vs. column efficiency. The error trend line is skewed, with square of correlation coefficient equals to 0.5951. At low column efficiency, the model predicted

distillate compositions are statistically always lower than the actual distillate compositions. If the actual column efficiency is close to the average column efficiency, which was used by first-principles model all the times, first-principles model gives good prediction of distillate composition. At high column efficiency, the model predicted distillate compositions are statistically always higher than the actual distillate composition.

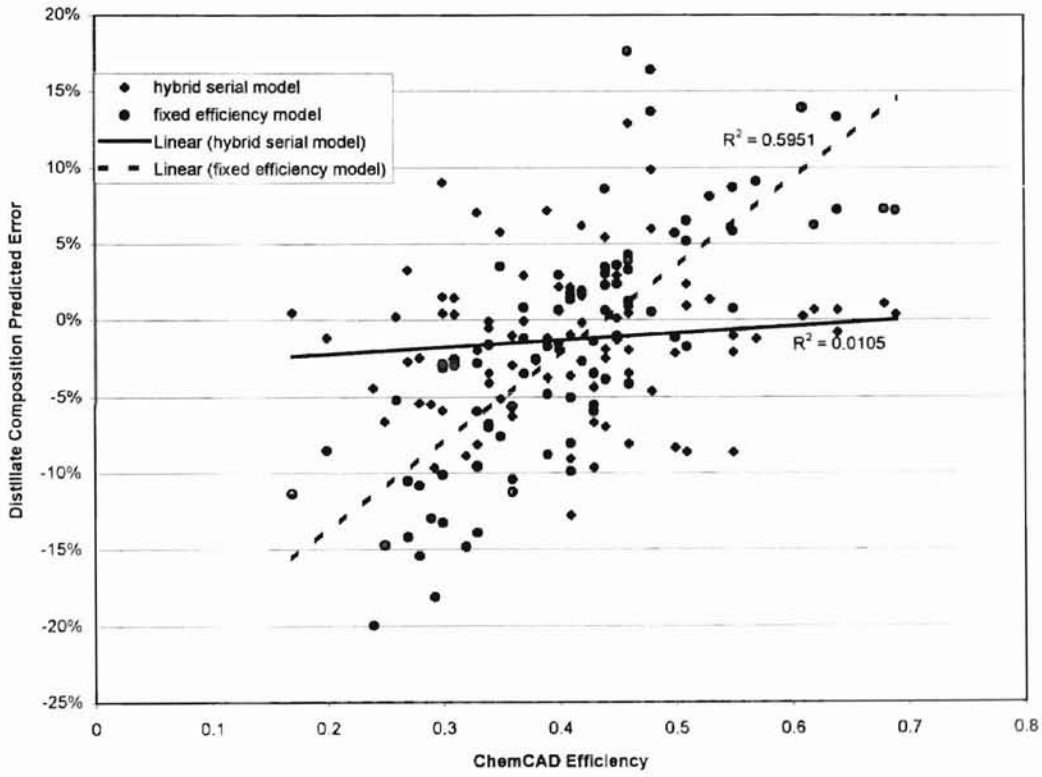

Fig. 4.9 Serial Approach: Distillate Composition Predicted Error at Different Column Efficiency

The prediction of hybrid serial model and first-principles model was also compared at each experiment run. Fig 4.10 is the plot of distillate composition predicted

errors vs. experiment number. The diamonds are the hybrid serial model distillate composition predicted errors vs. experiment number. The circles are the first-principles model distillate composition predicted errors vs. experiment number. Since data from experiment number 44 – 72 reflect some errors, they were not used in the hybrid serial modeling. One can see from the figure that there are some data "missing" from experiment number 44-72. Figure 4.10 tells that statistically hybrid model gave better distillate composition prediction than first-principles model at each experiment run.

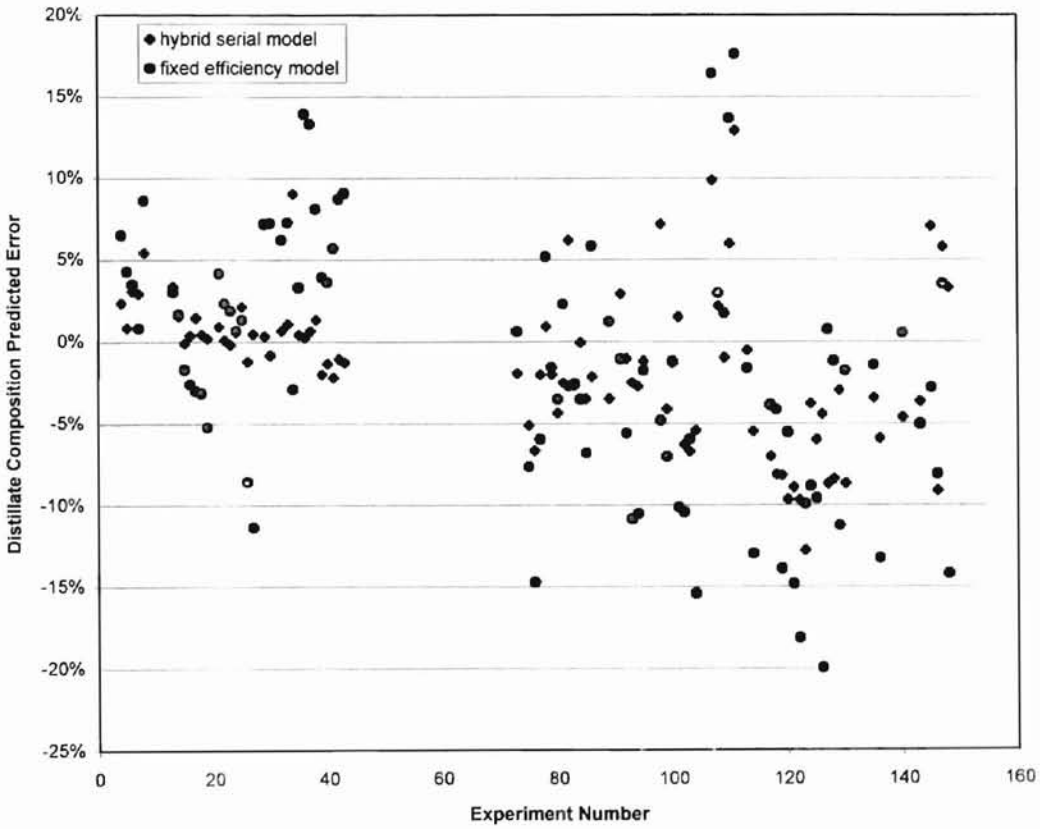

Fig. 4.10 Serial Approach: Distillate Composition Predicted Error vs. Experiment Number

4.3 HYBRID PARALLEL MODELING METHOD

4.3.1 Modeling procedure

The modeling can be described in the following 5 steps.

Step 1: Collect Experiment Data.

148 steady state data points were collected for model evaluation. Which was the same data set collected for hybrid serial modeling. For hybrid parallel modeling, 131 data points from the whole data set were used. The 17 data points that were not used contained some significant experiment errors. Some data points, especially where the column efficiency equals or close to 1.0, contained some not-so-significant experiment errors, were still used for the hybrid parallel modeling. The 131 points used for hybrid parallel modeling could be found in Appendix F.

Step 2: Reconcile Data.

This step was essentially the same as that in hybrid serial modeling, except that the total number of data points was different.

Step 3: Run ChemCAD to Get Distillate and Bottom Product Composition at Fixed Column Efficiency.

ChemCAD inputs were from reconciled data set. The inputs were: feed temperature, feed pressure (14.7 psia), feed methanol flow rate, feed water flow rate (calculated from feed flow rate and feed composition), subcooled delta T (calculated from reflux temperature), reflux flow rate, bottom product flow rate. Other less

important inputs were: distillate flow rate, reflux flow rate, top tray temperature, second top tray temperature. All of the less important inputs were just estimated values for convergence purpose. Over all column efficiency was set to 40%, which was the average efficiency in all runs.

Step 4: Train Neural Network to Predict Residual Error

Till this step, all the process measured variables and residual errors were available. The neural network output was the residual error in first principles model. But neural network inputs should be selected. First, all measured variables were used for training neural network. The procedure of selecting input variables were the same as that for hybrid serial modeling. Based on the selection procedure, the final inputs to neural network were: feed flow rate, feed composition, feed temperature, reflux rate, reboiler temperature and top tray temperature.

Neural network structure is 6-5-1, which happens to be the same structure as hybrid serial modeling. All the other procedures for training neural network, such as data scaling, training set and test set selection, neural network training algorithm selection, output scaling, were essentially the same as that in hybrid serial modeling.

Step 5: Test Hybrid Serial Model.

Various tests were taken to show the performance of the hybrid parallel model. First, the prediction error of the neural network was examined. Secondly, hybrid parallel model predicted distillate composition vs. the true distillate composition was compared to fixed efficiency first-principles model vs. the true distillate composition. Thirdly, the

prediction capability between hybrid parallel model and fixed efficiency first-principles model was compared. Lastly, in each experiment run, the prediction error between hybrid parallel model and fixed efficiency first-principles model was compared.

4.3.2 Experimental Results

In hybrid parallel modeling, the improved model prediction accuracy over first-principles model totally depends on the neural network. As a result, neural network prediction accuracy is so important that must be examined first. The error (error of fixed efficiency model minus error of neural network predicted distillate composition) has a mean of 0.11 (mol% of MeOH) and standard deviation of 2.81 (mol% of MeOH). Fig. 4.11 is the plot of neural network predicted distillate composition residuals vs. the true distillate composition residuals. "True distillate composition residuals" equal to experiment distillate composition minus fixed efficiency first-principles model predicted distillate composition. The fixed efficiency was chosen to be 40%, which was the average column efficiency. Then the true distillate composition residuals were used as the training set to train the neural network. Neural network outputs were the "neural network predicted distillate composition residuals". The closer the diamond point to the diagonal line, the better the neural network prediction is. From the figure, it shows that neural network gives nice prediction results.

The next step is to test hybrid parallel model distillate composition prediction capability vs. the true distillate composition with first-principles model prediction vs. the true distillate composition. As in hybrid serial modeling, first-principles model was run

under fixed column efficiency at 40% (mol% of methanol), which was the average column efficiency of all runs. This test shows whether the hybrid parallel model is better than first-principles model or not.

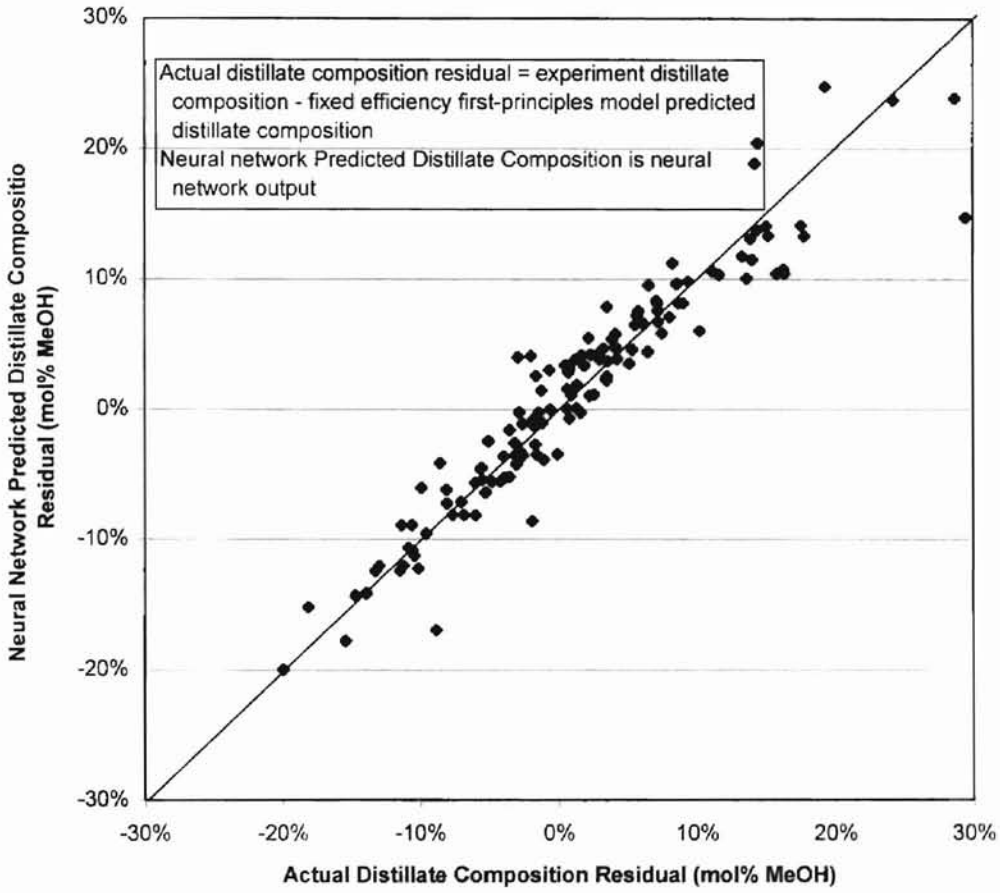

Fig. 4.11 Parallel Approach: Neural Network Predicted Distillate Composition Residual vs. True Distillate Composition Residual

Table 4.3 shows the prediction error of hybrid parallel model and fixed efficiency first-principles model. The mean error of hybrid parallel model is 0.10 mol% MeOH, which is smaller than 1.55 mol% MeOH, mean error of fixed efficiency first principles model. Standard deviation of hybrid parallel model is 2.80 mol% MeOH, which is much smaller than 9.54 mol% MeOH, standard deviation of fixed efficiency first-principles model. Table 4.3 shows that hybrid parallel model provides better model prediction accuracy.

Table 4.3 Comparison of Prediction Error between Hybrid Parallel Model and Fixed Efficiency First-principles Model (unit: mol% MeOH)

	Hybrid Serial Model	**Fixed Efficiency Model**
Mean Error	0.10	1.55
Standard deviation	2.80	9.54

Fig. 4.12 is the model predicted distillate composition vs. actual distillate composition. The circles are the first-principles model predicted distillate composition (at fixed column efficiency) vs. actual distillate composition. The diamonds are the hybrid parallel model predicted distillate composition vs. actual distillate composition. From the plot, one can see that hybrid parallel model does provide better model prediction accuracy.

Hybrid parallel model uses neural network to predict residual errors between the process and first-principles model. Residual errors come from different sources, such as unmodeled parameters, unaccounted process mechanism, inaccurate thermodynamic

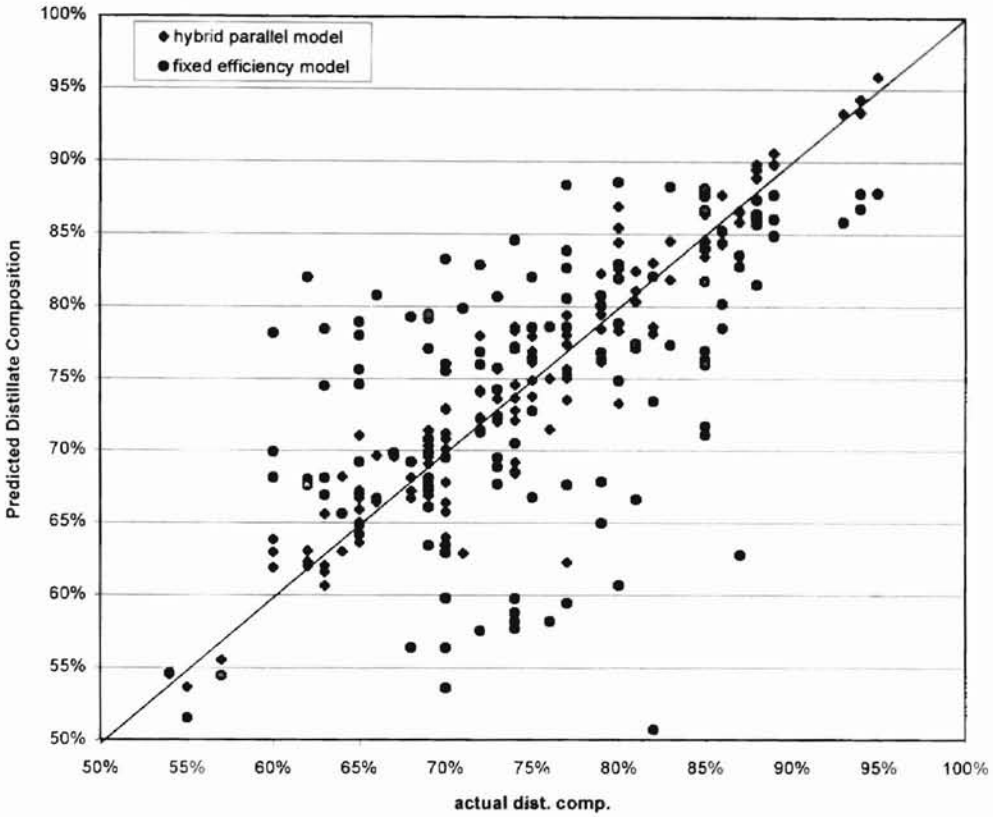

Fig. 4.12 Hybrid Parallel Model Predicted Distillate Composition vs. True Distillate Composition

correlation, etc. In this research, first-principles model residual error mainly came from unmodeled column efficiency. First-principles model assumed the distillation column always works at the condition where column efficiency is fixed. First-principles model should give good distillate composition prediction if the column runs at that efficiency, and it would give bad distillate composition prediction if the true column efficiency deviate from the average column efficiency. Fig. 4.13 shows this conclusion. Fig. 4.13 is the plot of distillate composition predicted errors vs. column efficiency. The diamonds

are the hybrid parallel model distillate composition predicted errors vs. column efficiency. At different column efficiency, it gave statistically the same prediction error. The squares are the fixed efficiency first-principles model distillate composition predicted errors vs. column efficiency. The fixed efficiency first-principles model is the same as that in hybrid serial model section, except that more operating points were added, especially the points where column efficiency equals or close to 1.0, which can be reflected from the cluster of points at efficiency equals to 1.0.

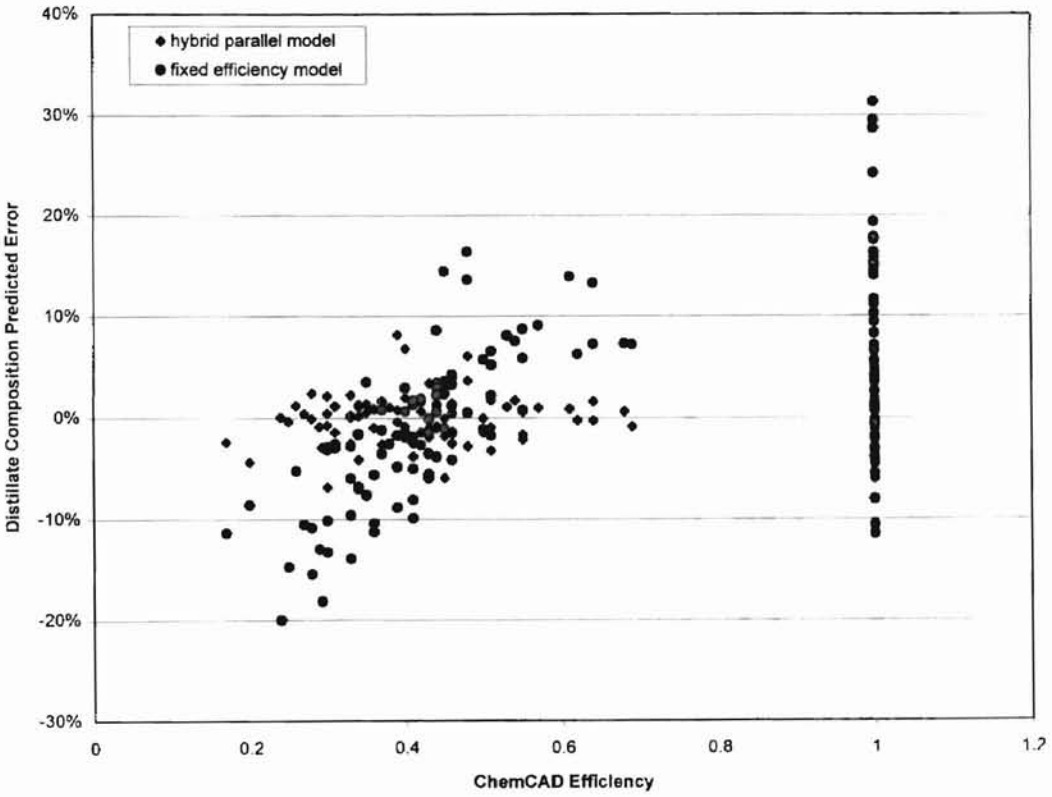

Fig. 4.13 Parallel Approach: Distillate Composition Predicted Error at Different column Efficiency

The prediction of hybrid parallel model and first-principles model is also compared at each experiment run. Fig 4.14 is the plot of distillate composition predicted errors vs. experiment number. The diamonds are the hybrid parallel model distillate composition predicted errors vs. experiment number. The circles are the first-principles model distillate composition predicted errors vs. experiment number. Fig. 4.14 tells that statistically hybrid parallel model gives better distillate composition prediction than first-principles model at each experiment run.

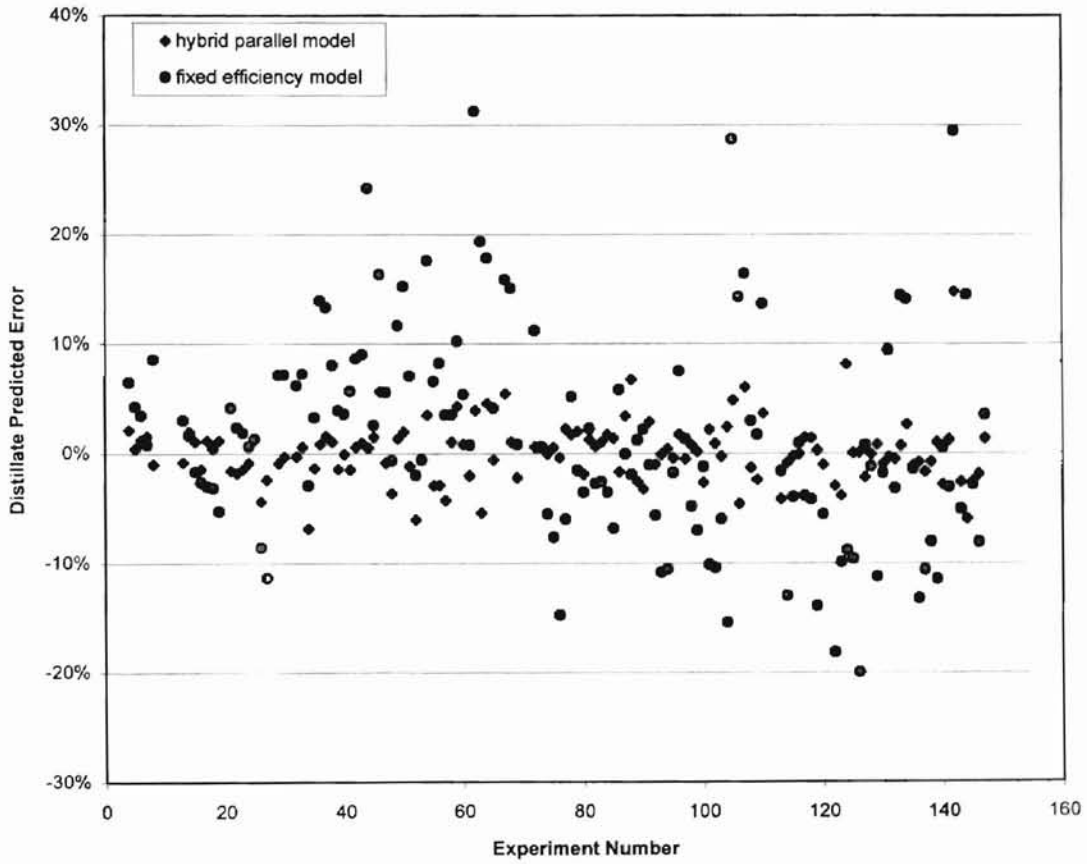

Fig. 4.14 Parallel Approach: Distillate Composition Predicted Error vs. Experiment Number

4.4 Model Evaluation

Mean and Standard Deviation

Two of the criteria of comparing different models are to evaluate mean and standard deviation of residual errors and error. Table 4.4 lists the mean and standard deviation of hybrid serial model and hybrid parallel model. The mean error of hybrid serial model predicted distillate composition is –1.31 mol% of MeOH, significantly larger than that of hybrid parallel model. The standard deviation of hybrid serial model predicted distillate composition is 4.70 mol% of MeOH, larger than that of hybrid parallel model. Both criteria shows that hybrid parallel model is better than hybrid serial model in distillation column modeling.

Table 4.4 Mean Error and Standard Deviation of Hybrid Models (unit: mol% MeOH)

	hybrid serial model	**hybrid parallel model**
Mean Error	-1.31%	0.10%
Standard Deviation	4.70%	2.80%

"Whiteness" of Residual Error

Another important criterion to evaluate the model is to test the whiteness of hybrid model residual error. The data were arranged in experiment sequence since the experiment was carried out in such a way that the adjacent experiment data points were close to each other in the multi-dimensional process variable space.

Fig. 4.15 shows the residual error auto-correlation function in the hybrid serial model. Since auto-correlation function is even symmetric along the y axis, only the right part of the auto-correlation function is shown. The ideal white noise shape should show that auto-correlation function equals to 1.0 at lag k=0, and 0 for all other k value. The 95% significance level is 0.21 ($1.96\sigma/\sqrt{88} = 0.21$, where variance $\sigma = 1.0$), but the auto-correlation function were greater than 0.21 for $k \leq 4$. So, the residual error is not white. The shape is also similar to a damped sine wave, which means that part of the residual noise is predictable, probably by ARMA model. Fig. 4.15 tells that the residual errors in hybrid serial model are not a white noise.

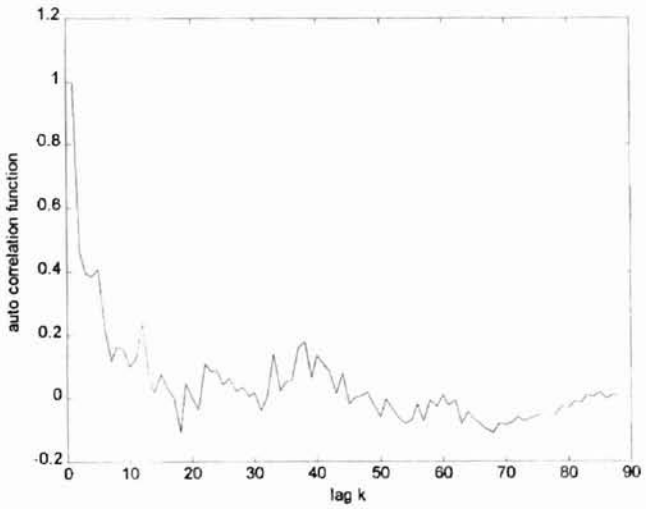

Fig. 4.15 Auto Correlation Function of Residual Error in Hybrid Serial Model

Fig. 4.16 shows the residual error auto-correlation function in hybrid parallel model. Only the right part of the auto-correlation function is shown because of the symmetric characteristic of the function. The ideal white noise shape should show that auto-correlation function equals to 1.0 at lag k=0, and 0 for all other k value. The 95%

significance level is 0.17 ($1.96\sigma / \sqrt{131} = 0.17$, where $\sigma = 1.0$). Fig. 4.16 tells that the residual errors in hybrid serial model are a white noise, which means that the model fit the experiment data well, thus leading to a satisfactory model.

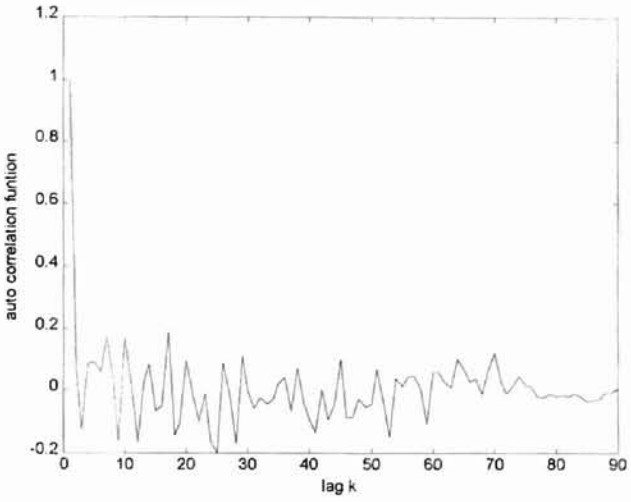

Fig. 4.16 Auto Correlation Function of Residual Error in Hybrid Parallel Model

This result is not surprising. In hybrid serial modeling, all factors that led to model inaccuracy in first-principles model were lumped into one model parameter – column efficiency. Even though neural network may predict the true column efficiency, true column efficiency could not correct all other factors that lead to model inaccuracy. On the other hand, in hybrid parallel modeling, neural network was used to correct the residual errors in first principles model, in which situation that neural network can compensate all factors that led to model inaccuracy.

CHAPTER V

CONCLUSIONS AND RECOMMENDATIONS

5.1 Conclusions

This work outlined a framework of how to incorporate first-principles model, empirical model and historical data into process modeling. There are generally two approaches, i.e., hybrid modeling and gray box modeling. Emphasis was put on the hybrid modeling technique. More specifically, hybrid serial modeling and hybrid parallel modeling. In hybrid modeling technique, the modeling procedure starts from building a rough first-principles model. Neural network (or other forms of empirical correlation) and historical data provide prior information to enhance the accuracy of first-principles model. Generally speaking, the hybrid modeling techniques can be applied to any process, provided that a "rough" first-principles model is available and related process information is available for neural network to "fine-tune" the first-principles model to get a better hybrid model.

Distillation column was used for testing the proposed modeling methods. An experimental distillation column was set up and automated. 148 steady state operating data points were collected as "historical data" for hybrid modeling methods validation. From the data set, 88 points were used for hybrid serial modeling method, 131 data points were used for hybrid parallel modeling method.

Some conclusions can be made as follows:

- Hybrid serial model provided better prediction capability for distillate composition than standalone fixed efficiency first-principles model did. Hybrid serial modeling was to use neural network to predict unmodelled parameters in first principles model. In experimental distillation column modeling application, a feed forward neural network was used to predict the column efficiency from the experiment data collected, which was then provided to first-principles model to predict distillate composition.
- Hybrid parallel model provided better prediction capability for distillate composition than standalone fixed efficiency first-principles model did. Hybrid parallel modeling was to use neural network to predict residual errors in first-principles model. In experimental distillation column modeling application, a feed forward neural network was used to predict the residual errors, which were resulted from the inaccuracy of first-principles model, from the experiment data collected.
- In distillation column modeling, the hybrid parallel model was better than hybrid serial model. First, both mean error and standard deviation of hybrid parallel model were much less than those of hybrid parallel model. Secondly, the prediction errors of the hybrid serial model were "biased", which meant hybrid serial model still had room for improvement under the same process information. On the other hand, the prediction errors of the hybrid parallel model were "white", which was the desired situation.
- Ideally, a first-principles model is preferred in process modeling. Hybrid serial model employs more process mechanism in the model, thus "clearer" than hybrid parallel model. This led to the conclusion that under the same process information, hybrid

serial model was preferred. But in this research, hybrid parallel model is better than serial model. This was partly caused by lump all first-principles model inaccuracy factors into column efficiency. A hybrid serial-parallel model may be able to fix this problem. That is, after the hybrid serial model was built, put another neural network to correct the residual errors from hybrid serial model.

- A better model can be achieved if only few unidentifiable parameters by hybrid serial model. Otherwise, a parallel model is preferred.

5.2 Recommendations

- All the modeling techniques were validated by experimental size distillation column data. It is better that the modeling technique be validated by industrial distillation column data before it is extended to industrial distillation column modeling application. By the time of this writing, no such work was done due to the unavailability of the industrial quality data. .
- One gray box modeling method, gain constrained training, which was still on the simulation stage at the time of this writing, provided promising alternative to hybrid modeling, thus worth of further development. When historical data were sparse in the whole operable region, and process gain information were available at any or most of the points in the operable region, which may came from first-principles model or operator's experience, Gain Constrained Training was better applied. Gain Constrained Training modeling process started from building a neural network structure. Neural network was trained by both sparse historical data and process gain information. Gain Constrained

Training provided an improved neural network for prediction, especially in the regions where the historical data were unavailable.

- Incorporating other prior information in neural network training is worth of further investigation. A priori information incorporated in the neural network can somehow light up the totally "black" box characteristic to "gray". Some of the candidate prior information are derivatives (such as mentioned above in "gain constrained training"), probability distribution of parameters, smoothness, etc.

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APPENDIX A

MATLAB PROGRAM FOR

HYBRID SERIAL MODELING METHOD

```
%HYBRID SERIAL MODEL

%STEP 1: COLLECT EXPERIMENT DATA
%% 148 steady state data points were collected for model evaluation.
%% In each experiment, after the distillation column reached steady
%% state, continue to run for additional 30 minutes, collect data every
%% 30 seconds, Process variables (except liquid level and level related
%% variables, such as distillate rate, bottom rate) were averaged over
%% the 30 minutes period, to reduce measurement noise.


%STEP 2: RECONCILE DATA
%% the characteristics of the experimental distillation
%% column determines that bottom product flow rate and
%% distillate flow rate were measured with least confidence,
%% because those two variables were inferred from distillate tank
%% and bottom tank level.
%% The training data must agree with overall material balance
%% and component material balance as follows:
%%   overall material balance: F=D+B
%%   component material balance: F*xf=D*xd+B*xb
%%     where:      F - feed flow rate (lb/hr)
%%                 D - distillate flow rate (lb/hr)
%%                 B - bottom product flow rate (lb/hr)
%%                 xf - feed composition (mass% of MeOH)
%%                 xd - distillate composition (mass% of MeOH)
%%                 xb - bottom product composition (mass% of MeOH)
%% adjust B and D to comply with the balance equations.
%% this step is done in Microsoft Excel.  The tool "solver"
%% in Excel was used.


%SETP 3: RUN CHEMCAD TO DETERMINE COLUMN EFFICIENCY
%% ChemCAD inputs were from reconciled data set.
%% The inputs were: feed temperature, feed pressure(14.7 psia),
%% feed methanol flow rate, feed water flow rate(calculated from
%% reflux flow rate and feed composition), subcooled delta T
%% (calculated from reflux temperature), reflux mass flow rate, bottom
%% product mass flow rate, and some less important variable estimates,
%% which are only for convergence purpose.
%% Overall tray efficiency was adjusted to make ChemCAD predicted
%% distillate composition match experiment distillate composition,
%% and bottom product composition match experiment bottom product
%% composition.
```

```
%STEP 4: TRAIN NEURAL NETWORK TO PREDICT COLUMN EFFICIENCY
%% load the reconciled data (text format)
%% expSerialData.dat has the following format:
%% column =[1: serialNumber
%%          2: feedRate (lb/hr)
%%          3: feedComp (mol% meOH)
%%          4: feedTemp (C)
%%          5: refluxRate (lb/hr)
%%          6: refluxTemp (C)
%%          7: TReboiler (C)
%%          8: TTray1 (C)
%%          9: TTray2 (C)
%%          10: TTray3 (C)
%%          11: TTray4 (C)
%%          12: TTray5 (C)
%%          13: TTray6 (C)
%%          14: trayEfficiency  ]

%IF YOUR DATA FILE NAME IS NOT CALLED "expSerialData",
%MAKE CHANGES IN THE FOLLOWING TWO LINES.
load expSerialDataall.dat;
data=expSerialDataall;

%% scale all data to [-1 1]
%% each variable scaling was based on the following equation:
%%   (actual-min)/(max-min)=(scaled+1)/2;
%%                where min and max are the minimum measured value
%%                and maximum measured value, respectively.
expDataMax=max(data);
expDataMin=min(data);
[r,c]=size(data);
expDataScale(:,1)=data(:,1);
for i=2:c
   temp=expDataMax(i)-expDataMin(i);
   expDataScale(:,i)=2/(expDataMax(i)-expDataMin(i))...
       *(data(:,i)-expDataMin(i))-ones(r,1);
end

%%neural network training
%%extract neural network inputs from experiment data set matrix.
%% network inputs are:
%% feedRate, feedComp, feedTemp, refluxRate, TReboiler, TTray6
inputs=expDataScale(:,2:13)';
inputs(7:11,:)=[];
inputs(5,:)=[];

%%extract neural network desired output from experiment data set
%% matrix.
%%neural network output: trayEfficiency
outputs=expDataScale(:,14)';

%%divide expData into training set and test set
%%based on the sequence number:
%% training set include:1,2,4,5,7,8...
%% test set include: 3,6,9...
[r,c]=size(inputs);
trainInputs=[];
```

```
testInputs=[];
trainOutput=[];
testOutput=[];
for i=1:c
   if (mod(i,3)==0)
      testInputs=[testInputs,inputs(:,i)];
      testOutput=[testOutput,outputs(:,i)];
   else
      trainInputs=[trainInputs,inputs(:,i)];
      trainOutput=[trainOutput,outputs(:,i)];
   end
end

%%create neural network
numHiddenLayerNode=5;
numOutputLayerNode=1;
net=newff(ones(6,1)*[-1 1],[numHiddenLayerNode,numOutputLayerNode],...
   {'tansig','purelin'},'trainbr');

%%set training parameters and train neural network
net.trainParam.epochs=2000;
net.trainParam.show=20;
net=train(net,trainInputs,trainOutput);

%%get network predicted tray efficiency from training set
trainPredict=sim(net,trainInputs);

%%get network predicted tray efficiency from test set
testPredict=sim(net,testInputs);

%%change scale back to experiment value
trainPredictReal=(trainPredict+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);
testPredictReal=(testPredict+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);
trainOutputReal=(trainOutput+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);
testOutputReal=(testOutput+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);

%% if predicted efficiency is greater than 1.0, set the effciency
%% equals to 1.0. if predicted efficiency is less than -1.0, set the
%% effciency equals to -1.0.
[r,c]=size(trainPredictReal);
for i=1:c
   if trainPredictReal(i)>1.0
      trainPredictReal(i)=1.0;
   end
   if trainPredictReal(i)<-1.0
      trainPredictReal(i)=-1.0;
   end
end

[r,c]=size(testPredictReal);
for i=1:c
   if testPredictReal(i)>1.0
      testPredictReal(i)=1.0;
```

```
    end
    if testPredictReal(i)<-1.0
       testPredictReal(i)=-1.0;
    end
end



%SETP 5: TEST HYBRID SERIAL MODEL
%%plot experiment efficiency vs. predicted efficiency
%%%training set
close;
figure(1);
plot(trainPredictReal,trainOutputReal,'+');
line([0,1],[0,1]);
title('training set');
xlabel('neural network predicted efficiency');
ylabel('true experiment efficiency');

%%%test set
figure(2);
plot(testPredictReal,testOutputReal,'+');
line([0,1],[0,1]);
title('test set');
xlabel('neural network predicted efficiency');
ylabel('true experiment efficiency');

%%sum squared error
errTrainReal=sumsqr(trainOutputReal-trainPredictReal)
errTestReal=sumsqr(testOutputReal-testPredictReal)
```

APPENDIX B

MATLAB SLIDE SHOW FOR

HYBRID SERIAL MODELING METHOD

```
function slide=SSlideShow
% This is a slideshow file for use with playshow.m and makeshow.m
% To see it run, type 'playshow SSlideShow',

if nargout<1,
  playshow SSlideShow
else
  %========== Slide 1 ==========

  slide(1).code={
   'slideData=nnslides(''start'',slideData,''Hybrid Serial Modeling
Method'');',
   'disp(''STEP 1: COLLECT EXPERIMENT DATA'');' };
  slide(1).text={
   'STEP 1: COLLECT EXPERIMENT DATA',
   '148 steady state data points were collected for model evaluation.
When the process reached steady state, the experiment continued to run
for additional 30 minutes in steady state.  Process variables were
measured every 30 seconds during this 30-minutes steady state period.
Process variables (except for liquid level and level related variables,
such as distillate rate, bottom rate) were averaged over this 30
minutes time period to reduce measurement noise.'};

  %========== Slide 2 ==========

  slide(2).code={
   'disp(''STEP 2: RECONCILE DATA'');' };
  slide(2).text={
   'STEP 2: RECONCILE DATA',
   'The characteristic of the experiment distillation column determines
that bottom product flow rate and distillate flow rate were measured
with least confidence.  The training data must agree with overall
material balance and componenet material balance.  i.e.',
   '   F=D+B',
   '   F*xf=D*xd+B*xb',
   '   where F,Dand B are feed, distillate and bottom product flow
rate, respectively.',
   '             xf,xd and xb are feed, distillate and bottom product
composition, respectively.',
   'Adjust D and B to comply with the balance equations.',
   'This step is done in Microsoft Excel.  The "equation sovler"
function in Excel helps in solving balance equations.',
   ''};
```

```
%========== Slide 3 ==========

slide(3).code={
 'disp(''STEP 3: RUN CHEMCAD TO DETERMINE COLUMN EFFICIENCY'');',
 '' };
slide(3).text={
 'STEP 3: RUN CHEMCAD TO DETERMINE COLUMN EFFICIENCY',
 'ChemCAD inputs are from reconciled data set.',
 'The inputs are: feed temperature, feed pressure (14.7 psia), feed
methonal flow rate, feed water flow rate (calculated from feed flow
rate and feed composition), subcooled delta T(calcualted from reflux
temperature), reflux flow rate, bottom product flow rate.  Overall tray
efficiency was adjusted to make ChemCAD predicted distillate
composition match experiment distillate composition.  Double check to
see if the predicted bottom product composition matches experiment
bottom product composition.',
 '',
 'This step is done in ChemCAD.',
 ''};

%========== Slide 4 ==========

slide(4).code={
 'disp(''STEP 4: TRAIN NEURAL NETWORK TO PREDICT COLUMN
EFFICIENCY'');',
 '',
 'load expSerialDataall.dat;',
 'expSerialData=expSerialDataall;',
 '',
 'expDataFirstSet=expSerialData(1,:);',
 'out=evalc(''expDataFirstSet'');',
 'slideData=nnslides(''text'',slideData,out);',
 '' };
slide(4).text={
 'STEP 4: TRAIN NEURAL NETWORK TO PREDICT COLUMN EFFICIENCY',
 'load the reconciled data file.',
 'file "expSerialDatal.dat" has the following format:',
 'column =[   1: serialNumber      2: feedRate (lb/hr)',
 '    3: feedComp (mol% meOH)      4: feedTemp (C)',
 '    5: refluxRate (lb/hr)        6: refluxTemp (C)',
 '    7: TReboiler (C)             8: TTray1 (C)',
 '    9: TTray2 (C)                10: TTray3 (C)',
 '    11: TTray4 (C)               12: TTray5 (C)',
 '    13: TTray6 (C)               14: trayEfficiency  ]',
 '',
 'load expSerialData.dat;',
 '',
 ''};

%========== Slide 5 ==========

slide(5).code={
 'disp(''   scale all data to [-1 1]'');',
 '',
 'expDataMax=max(expSerialData);',
 'expDataMin=min(expSerialData);',
 '[r,c]=size(expSerialData);',
```

```
    'expDataScale(:,1)=expSerialData(:,1);',
    'for i=2:c',
    '   temp=expDataMax(i)-expDataMin(i);',
    '   expDataScale(:,i)=2/(expDataMax(i)-
expDataMin(i))*(expSerialData(:,i)-expDataMin(i))-ones(r,1);',
    'end',
    '',
    'expDataFirstSetAfterScale=expDataScale(1,:);',
    'out=evalc(''expDataFirstSetAfterScale'');',
    'slideData=nnslides(''text'',slideData,out);',
    '',
    '' };
  slide(5).text={
    'STEP 4 (Cont''d):',
    'scale all data to [-1 1]',
    '',
    'for each variable v (corresponding to each column of expSerialData,
except for the first column, which is the experiment serial Number),
perform the following scaling:',
    '(v-vmin)/(vmax-vmin)=(vscale+1)/2',
    'where v-unscaled experiment data, vscale-scaled experiment data,
vmax-maximum value of variable v, vmin-minimum value of variable v;',
    '',
    'expDataMax=max(expSerialData);',
    'expDataMin=min(expSerialData);',
    '[r,c]=size(expSerialData);',
    'expDataScale(:,1)=expSerialData(:,1);',
    'for i=2:c',
    '   temp=expDataMax(i)-expDataMin(i);',
    'expDataScale(:,i)=2/(expDataMax(i)-
expDataMin(i))*(expSerialData(:,i)-expDataMin(i))-ones(r,1);',
    'end',
    ''};

  %========== Slide 6 ==========

  slide(6).code={
    'disp(''   prepare neural network training inputs and output'');',
    '',
    'inputs=expDataScale(:,2:13)'';',
    'inputs(7:11,:)=[];',
    'inputs(5,:)=[];',
    'outputs=expDataScale(:,14)'';',
    '',
    'nn.inputsFirstSet=inputs(:,1);',
    'nn.outputsFirstSet=outputs(1);',
    'out=evalc(''nn'');',
    'slideData=nnslides(''text'',slideData,out);',
    '',
    '' };
  slide(6).text={
    'STEP 4 (Cont''d):',
    'extract neural network training inputs and output from experiment
data sets',
    'neural network inputs:  feedRate, feedComp, feedTemp, refluxRate,
TReboiler, TTray6',
    'neural network output: trayEfficiency',
```

```
 '',
 'inputs=expDataScale(:,2:13)'';',
 'inputs(7:11,:)=[];',
 'inputs(5,:)=[];',
 'outputs=expDataScale(:,14)'';',
 ''};

%========== Slide 7 ==========

slide(7).code={
 'disp(''   divide expData into training set and test set'');',
 '',
 '[r,c]=size(inputs);',
 'trainInputs=[];',
 'testInputs=[];',
 'trainOutput=[];',
 'testOutput=[];',
 'for i=1:c',
 '   if (mod(i,3)==0)',
 '      testInputs=[testInputs,inputs(:,i)];',
 '      testOutput=[testOutput,outputs(:,i)];',
 '   else',
 '      trainInputs=[trainInputs,inputs(:,i)];',
 '      trainOutput=[trainOutput,outputs(:,i)];',
 '   end',
 'end',
 '',
 '',
 'totalPoints.trainingSet=length(trainOutput);',
 'totalPoints.testSet=length(testOutput);',
 'out=evalc(''totalPoints'');',
 'slideData=nnslides(''text'',slideData,out);',
 '' };
slide(7).text={
 'STEP 4 (Cont''d)',
 'divide expData into training set and test set',
 '',
 '[r,c]=size(inputs);',
 'trainInputs=[];',
 'testInputs=[];',
 'trainOutput=[];',
 'testOutput=[];',
 'for i=1:c',
 '   if (mod(i,3)==0)',
 '      testInputs=[testInputs,inputs(:,i)];',
 '      testOutput=[testOutput,outputs(:,i)];',
 '   else',
 '      trainInputs=[trainInputs,inputs(:,i)];',
 '      trainOutput=[trainOutput,outputs(:,i)];',
 '   end',
 'end',
 ''};

%========== Slide 8 ==========

slide(8).code={
 'disp(''   create neural network'');',
```

```
    '',
    'numHiddenLayerNode=5;',
    'numOutputLayerNode=1;',
    'net=newff(ones(6,1)*[-1 1],[numHiddenLayerNode,numOutputLayerNode],
{''tansig'',''purelin''},''trainbr'');',
    '',
    '',
    'nnetNodes.numHiddenLayerNode=numHiddenLayerNode;',
    'nnetNodes.numOutputLayerNode=numOutputLayerNode;',
    'out=evalc(''nnetNodes'');',
    'slideData=nnslides(''text'',slideData,out);' };
  slide(8).text={
    'STEP 4(Cont''d)',
    'create neural network',
    '',
    'numHiddenLayerNode=5;',
    'numOutputLayerNode=1;',
    'net=newff(ones(6,1)*[-1 1],[numHiddenLayerNode,numOutputLayerNode],
{''tansig'',''purelin''},''trainbr'');',
    '',
    ''};

  %========== Slide 9 ==========

  slide(9).code={
    'disp(''   neural network training'');',
    '',
    'slideData=nnslides(''axes'',slideData);',
    'net.trainParam.epochs=2000;',
    'net.trainParam.show=20;',
    'net=train(net,trainInputs,trainOutput);',
    '' };
  slide(9).text={
    'SETP 4: (Cont''d)',
    'neural network training',
    '',
    'net.trainParam.epochs=2000;',
    'net.trainParam.show=20;',
    'net=train(net,trainInputs,trainOutput);',
    ''};

  %========== Slide 10 ==========

  slide(10).code={
    'disp(''   get network predicted tray efficiency from training
set'');',
    '',
    'trainPredict=sim(net,trainInputs);',
    '',
    '',
    'trainPredictScaledFirst10Pts=trainPredict(1:10);',
    'out=evalc(''trainPredictScaledFirst10Pts'');',
    'slideData=nnslides(''text'',slideData,out);',
    '',
    '' };
  slide(10).text={
    'STEP 4(Cont''d)',
```

```
 'get network predicted column efficiency from training set.',
 '',
 'trainPredict=sim(net,trainInputs);',
 ''};

%========== Slide 11 ==========

slide(11).code={
 'disp(''   get network predicted tray efficiency from test set'');',
 '',
 'testPredict=sim(net,testInputs);',
 '',
 'testPredictScaledFirst10Pts=testPredict(1:10);',
 'out=evalc(''testPredictScaledFirst10Pts'');',
 'slideData=nnslides(''text'',slideData,out);' };
slide(11).text={
 'STEP 4(Cont''d)',
 'get network predicted column efficiency from test set.',
 '',
 'testPredict=sim(net,testInputs);',
 ''};


%========== Slide 12 ==========

slide(12).code={
 'disp(''   set upper and lower bound for efficiency'');',
 '',
 '',
 '[r,c]=size(trainPredict);',
 'for i=1:c',
 '   if trainPredict(i)>1.0',
 '      trainPredict(i)=1.0;',
 '   end',
 '   if trainPredict(i)<-1.0',
 '      trainPredict(i)=-1.0;',
 '   end',
 'end',
 '',
 '[r,c]=size(testPredict);',
 'for i=1:c',
 '   if testPredict(i)>1.0',
 '      testPredict(i)=1.0;',
 '   end',
 '   if testPredict(i)<-1.0',
 '      testPredict(i)=-1.0;',
 '   end',
 'end' };
slide(12).text={
 'STEP 4(Cont''d)',
 'set upper and lower bound for efficiency.  If predicted efficicency
is greater than 1.0, set the efficiency equals to 1.0; If predicted
efficiency is less than -1.0, set the efficiency equals to -1.0.',
 '',
 '[r,c]=size(trainPredict);',
 'for i=1:c',
 '   if trainPredict(i)>1.0',
```

```
    '      trainPredict(i)=1.0;',
    '   end',
    '   if trainPredict(i)<-1.0',
    '      trainPredict(i)=-1.0;',
    '   end',
    'end',
    '',
    '[r,c]=size(testPredict);',
    'for i=1:c',
    '   if testPredict(i)>1.0',
    '      testPredict(i)=1.0;',
    '   end',
    '   if testPredict(i)<-1.0',
    '      testPredict(i)=-1.0;',
    '   end',
    'end',
    ''};


  %========== Slide 13 ==========

  slide(13).code={
    'disp(''   change training set scale back to experiment value'');',
    '',
    'trainPredictReal=(trainPredict+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    'trainOutputReal=(trainOutput+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    '',

'trainPredictReal_trainExperiment_First10Pts=[trainPredictReal(1:10);tr
ainOutputReal(1:10)];',
    'out=evalc(''trainPredictReal_trainExperiment_First10Pts'');',
    'slideData=nnslides(''text'',slideData,out);',
    '' };
  slide(13).text={
    'STEP 4(cont''d):',
    'change training set scale back to experiment value',
    '',
    'trainPredictReal=(trainPredict+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    '',
    'trainOutputReal=(trainOutput+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    ''};

  %========== Slide 14 ==========

  slide(14).code={
    ' disp(''   change test set scale back to experiment value'');',
    '',
    'testPredictReal=(testPredict+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    'testOutputReal=(testOutput+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    '',
    '',
```

```
    '
testPredictReal_testExperiment_First10Pts=[testPredictReal(1:10);testOu
tputReal(1:10)];',
    'out=evalc(''testPredictReal_testExperiment_First10Pts'');',
    'slideData=nnslides(''text'',slideData,out);',
    '',
    '',
    '',
    '',
    '' };
  slide(14).text={
    'STEP 4(cont''d):',
    'change test set scale back to experiment value',
    '',
    'testPredictReal=(testPredict+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    'testOutputReal=(testOutput+1)*(expDataMax(14)-
expDataMin(14))/2+expDataMin(14);',
    ''};

  %========== Slide 15 ==========

  slide(15).code={
    'disp(''STEP 5: TEST HYBRID SERIAL MODEL'');',
    'disp(''   plot experiment efficiency vs. predicted efficiency from
training set'');',
    '',
    'figure(2);',
    'plot(trainPredictReal,trainOutputReal,''+'');',
    'line([0,1],[0,1]);',
    'title(''training set'');',
    'xlabel(''neural network predicted efficiency'');',
    'ylabel(''true experiment efficiency'');' };
  slide(15).text={
    'STEP 5: TEST HYBRID SERIAL MODEL',
    'plot experiment efficiency vs. predicted efficiency from training
set',
    '',
    'figure(2);',
    'plot(trainPredictReal,trainOutputReal,''+'');',
    'line([0,1],[0,1]);',
    'title(''training set'');',
    'xlabel(''neural network predicted efficiency'');',
    'ylabel(''true experiment efficiency'');',
    ''};

  %========== Slide 16 ==========

  slide(16).code={
    'disp(''plot experiment efficiency vs. predicted efficiency from
test set'');',
    '',
    'figure(3);',
    'plot(testPredictReal,testOutputReal,''+'');',
    'line([0,1],[0,1]);',
    'title(''test set'');',
    'xlabel(''neural network predicted efficiency'');',
```

```
    'ylabel(''true experiment efficiency'');',
    '',
    '' };
  slide(16).text={
    'STEP 5 (Cont''d)',
    'plot experiment efficiency vs. predicted efficiency test set',
    '',
    'figure(3);',
    'plot(testPredictReal,testOutputReal,''+'');',
    'line([0,1],[0,1]);',
    'title(''test set'');',
    'xlabel(''neural network predicted efficiency'');',
    'ylabel(''true experiment efficiency'');',
    ''};


  %========== Slide 17 ==========

  slide(17).code={
    'disp(''sum squared error'');',
    '',
    'errTrainReal=sumsqr(trainOutputReal-trainPredictReal);',
    'errTestReal=sumsqr(testOutputReal-testPredictReal);',
    '',
    'err.TrainReal=errTrainReal;',
    'err.TestReal=errTestReal;',
    'out=evalc(''err'');',
    'slideData=nnslides(''text'',slideData,out);',
    '' };
  slide(17).text={
    'STEP 5 (Cont''d)',
    'sum squared error',
    '',
    'errTrainReal=sumsqr(trainOutputReal-trainPredictReal)',
    'errTestReal=sumsqr(testOutputReal-testPredictReal)',
    ''};
end
```

APPENDIX C

MATLAB PROGRAM FOR

HYBRID PARALLEL MODELING METHOD

```
%HYBRID PARALLEL MODEL


%STEP 1: COLLECT EXPERIMENT DATA
%% 148 steady state data points were collected for model evaluation.
%% In each experiment, after the distillation column reached steady
%% state, continue to run for additional 30 minutes, collect data every
%% 30 seconds, Process variables (except liquid level and level related
%% variables, such as distillate rate, bottom rate) were averaged over
%% the 30 minutes period, to reduce measurement noise.


%STEP 2: RECONCILE DATA
%% the characteristics of the experimental distillation
%% column determines that bottom product flow rate and
%% distillate flow rate were measured with least confidence,
%% because those two variables were inferred from distillate tank
%% and bottom tank level.
%% The training data must agree with overall material balance
%% and component material balance as follows:
%%   overall material balance: F=D+B
%%   component material balance: F*xf=D*xd+B*xb
%%     where:     F - feed flow rate (lb/hr)
%%                D - distillate flow rate (lb/hr)
%%                B - bottom product flow rate (lb/hr)
%%                xf - feed composition (mass% of MeOH)
%%                xd - distillate composition (mass% of MeOH)
%%                xb - bottom product composition (mass% of MeOH)
%% adjust B and D to comply with the balance equations.
%% this step is done in Microsoft Excel.  The tool "solver"
%% in Excel was used.


%STEP 3: RUN CHEMCAD TO GET DISTILLATE AND BOTTOM PRODUCT
%        COMPOSITION AT FIXED COLUMN EFFICIENCY
%%ChemCAD inputs are from reconciled data set.
%%The inputs are: feed temperature, feed pressure(14.7 psia),
%% feed methanol flow rate, feed water flow rate(calculated from
%% reflux flow rate and feed composition), subcooled delta T
%% (calculated from reflux temperature), reflux flow rate, bottom
%% product mass flow rate, and some other less important variables
%% estimates, which are only for convergence purpose.
%%Overall tray efficiency was set to 40%, which was the average
%%efficiency in all runs.
```

```
%STEP 4: TRAIN NEURAL NETWORK TO PREDICT  RESIDUAL ERROR
%        OF DISTILLATE COMPOSITION
%% load the reconciled data
%% expParallelData.dat has the following format:
%% column =[1: serialNumber
%%          2: feedRate (lb/hr)
%%          3: feedComp (mol% meOH)
%%          4: feedTemp (C)
%%          5: refluxRate (lb/hr)
%%          6: refluxTemp (C)
%%          7: TReboiler (C)
%%          8: TTray1 (C)
%%          9: TTray2 (C)
%%          10: TTray3 (C)
%%          11: TTray4 (C)
%%          12: TTray5 (C)
%%          13: TTray6 (C)
%%          14: trayEfficiency (%)
%%          15: residual error (%) ]

%IF YOUR DATA FILE NAME IS NOT CALLED "expParallelData",
%MAKE CHANGES IN THE FOLLOWING TWO LINES.
load expParallelDataall.dat;
data=expParallelDataall;

%%scale all data to [-1,1]
%% each variable scaling was based on the following equation:
%%   (actual-min)/(max-min)=(scaled+1)/2;
%%    where min and max are the minimum measured value
%%    and maximum measured value, respectively.
expDataMax=max(data);
expDataMin=min(data);
[r,c]=size(data);
expDataScale(:,1)=data(:,1);
for i=2:c
   temp=expDataMax(i)-expDataMin(i);
   expDataScale(:,i)=2/(expDataMax(i)-expDataMin(i))...
      *(data(:,i)-expDataMin(i))-ones(r,1);
end

%%neural network training
%%extract neural network inputs from experiment data set matrix.
%%  neural network inputs are:
%%  feedRate, feedComp, feedTemp, refluxRate, TReboiler, TTray6
inputs=expDataScale(:,2:13)';
inputs(7:11,:)=[];
inputs(5,:)=[];

%%extract neural network desired output from experiment data set
%% matrix.
%%neural network output: residualError
outputs=expDataScale(:,15)';

%%divide expData into training set and test set
%%based on the sequence number:
%% training set include:1,2,4,5,7,8...
%% test set include: 3,6,9...
```

```
[r,c]=size(inputs);
trainInputs=[];
testInputs=[];
trainOutput=[];
testOutput=[];
for i=1:c
   if (mod(i,3)==0)
      testInputs=[testInputs,inputs(:,i)];
      testOutput=[testOutput,outputs(:,i)];
   else
      trainInputs=[trainInputs,inputs(:,i)];
      trainOutput=[trainOutput,outputs(:,i)];
   end
end

%%Create neural network
numHiddenLayerNode=5;
numOutputLayerNode=1;
net=newff(ones(6,1)*[-1 1],[numHiddenLayerNode,numOutputLayerNode],...
   {'tansig','purelin'},'trainbr');

%%set training parameters and train neural network
net.trainParam.epochs=2000;
net.trainParam.show=20;
net=train(net,trainInputs,trainOutput);

%%get network predicted residual error from training set
%%if predicted residual error is greater than 1.0, set the
%%residual error equals to 1.0.  If the predicted residual
%%error is less than -1.0, set the residual error equals to -1.0
trainPredict=sim(net,trainInputs);
[r,c]=size(trainPredict);
for i=1:c
   if trainPredict(i)>1.0
      trainPredict(i)=1.0;
   end
   if trainPredict(i)<-1.0
      trainPredict(i)=-1.0;
   end
end

%%get network predicted residual error from test set
%%if predicted residual error is greater than 1.0, set the
%%residual error equals to 1.0.  If the predicted residual
%%error is less than -1.0, set the residual error equals to -1.0
testPredict=sim(net,testInputs);
[r,c]=size(testPredict);
for i=1:c
   if testPredict(i)>1.0
      testPredict(i)=1.0;
   end
   if testPredict(i)<-1.0
      testPredict(i)=-1.0;
   end
end

%%change scale back to experiment value
```

```
trainPredictReal=(trainPredict+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);
testPredictReal=(testPredict+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);
trainOutputReal=(trainOutput+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);
testOutputReal=(testOutput+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);

%SETP 5: TEST HYBRID SERIAL MODEL
%%plot experiment efficiency vs. predicted efficiency
%%%training set
close;
figure(1);
plot(trainPredictReal,trainOutputReal,'+');
line([-30,30],[-30,30]);
title('training set');
xlabel('neural network predicted residual error');
ylabel('true experiment residual error');

%%%test set
figure(2);
plot(testPredictReal,testOutputReal,'+');
line([-30,30],[-30,30]);
title('test set');
xlabel('neural network predicted residual error');
ylabel('true experiment residual error');

%%sum squared error
errTrainReal=sumsqr(trainOutputReal-trainPredictReal)
errTestReal=sumsqr(testOutputReal-testPredictReal)
```

APPENDIX D

MATLAB SLIDE SHOW FOR

HYBRID PARALLEL MODELING METHOD

```
function slide=PSlideShow
% This is a slideshow file for use with playshow.m and makeshow.m
% To see it run, type 'playshow PSlideShow',

if nargout<1,
  playshow PSlideShow
else
  %========== Slide 1 ==========

  slide(1).code={
   'slideData=nnslides(''start'',slideData,''Hybrid Parallel Modeling
Method'');',
   'disp(''STEP 1: COLLECT EXPERIMENT DATA'');' };
  slide(1).text={
   'STEP 1: COLLECT EXPERIMENT DATA',
   '148 steady state data points were collected for model evaluation.
When the process reached steady state, the experiment continued to run
for additional 30 minutes in steady state.  Process variables were
measured every 30 seconds during this 30-minute steady state period.
Process variables (except for liquid level and level related variables,
such as distillate rate, bottom rate) were averaged over this 30
minutes time period to reduce measurement noise.'};

  %========== Slide 2 ==========

  slide(2).code={
   'disp(''STEP 2: RECONCILE DATA'');' };
  slide(2).text={
   'STEP 2: RECONCILE DATA',
   'The characteristic of the experiment distillation column determines
that bottom product flow rate and distillate flow rate were measured
with least confidence.  The training data must agree with overall
material balance and component material balance.  i.e.',
   '   F=D+B',
   '   F*xf=D*xd+B*xb',
   '   where F,Dand B are feed, distillate and bottom product flow
rate, respectively.',
   '             xf,xd and xb are feed, distillate and bottom product
composition, respectively.',
   'Adjust D and B to comply with the balance equations.',
   'This step is done in Microsoft Excel.  The "equation sovler"
function in Excel helps in solving balance equations.',
   ''};
```

```
%========== Slide 3 ==========

slide(3).code={
 'disp(''STEP 3: RUN CHEMCAD TO GET DISTILLATE AND BOTTOM PRODUCT
COMPOSITION AT FIXED COLUMN EFFICIENCY'');',
 '' };
slide(3).text={
 'STEP 3: RUN CHEMCAD TO GET DISTILLATE AND BOTTOM PRODUCT
COMPOSITION AT FIXED COLUMN EFFICIENCY',
 'ChemCAD inputs are from reconciled data set.',
 'The inputs are: feed temperature, feed pressure (14.7 psia), feed
methonal flow rate, feed water flow rate (calculated from feed flow
rate and feed composition), subcooled delta T(calcualted from reflux
temperature), reflux flow rate, bottom product flow rate.  Overall
column efficiency was set to 40%, which was the average efficiency in
all runs.',
 '',
 'This step is done in ChemCAD.',
 ''};

%========== Slide 4 ==========

slide(4).code={
 'disp(''STEP 4: TRAIN NEURAL NETWORK TO PREDICT RESIDUAL ERROR OF
DISTILLATE COMPOSITION'');',
 '',
 'load expParallelDataall.dat;',
 'expParallelData=expParallelDataall;',
 '',
 'expDataFirstSet=expParallelData(1,:);',
 'out=evalc(''expDataFirstSet'');',
 'slideData=nnslides(''text'',slideData,out);',
 '' ;;
slide(4).text={
 'STEP 4: TRAIN NEURAL NETWORK TO PREDICT RESIDUAL ERROR OF
DISTILLATE COMPOSITION',
 'load the reconciled data file.',
 'file "expParallelData.dat" has the following format:',
 'column =[   1: serialNumber      2: feedRate (lb/hr)',
 '    3: feedComp (mol% meOH)      4: feedTemp (C)',
 '    5: refluxRate (lb/hr)        6: refluxTemp (C)',
 '    7: TReboiler (C)             8: TTray1 (C)',
 '    9: TTray2 (C)                10: TTray3 (C)',
 '    11: TTray4 (C)               12: TTray5 (C)',
 '    13: TTray6 (C)               14: Efficiency',
 '    15:residualError(%)  ]',
 '',
 'load expParallelData.dat;',
 '',
 ''};

%========== Slide 5 ==========

slide(5).code={
 'disp(''   scale all data to [-1 1]'');',
 '',
 'expDataMax=max(expParallelData);',
```

```
    'expDataMin=min(expParallelData);',
    '[r,c]=size(expParallelData);',
    'expDataScale(:,1)=expParallelData(:,1);',
    'for i=2:c',
    '    temp=expDataMax(i)-expDataMin(i);',
    '    expDataScale(:,i)=2/(expDataMax(i)-
expDataMin(i))*(expParallelData(:,i)-expDataMin(i))-ones(r,1);',
    'end',
    '',
    'expDataFirstSetAfterScale=expDataScale(1,:);',
    'out=evalc(''expDataFirstSetAfterScale'');',
    'slideData=nnslides(''text'',slideData,out);',
    '',
    '' };
  slide(5).text={
    'STEP 4 (Cont''d):',
    'scale all data to [-1 1]',
    '',
    'for each variable v (corresponding to each column of
expParallelData, except for the first column, which is the experiment
serial Number), perform the following scaling:',
    '(v-vmin)/(vmax-vmin)=(vscale+1)/2',
    'where v-unscaled experiment data, vscale-scaled experiment data,
vmax-maximum value of variable v, vmin-minimum value of variable v;',
    '',
    'expDataMax=max(expParallelData);',
    'expDataMin=min(expParallelData);',
    '[r,c]=size(expParallelData);',
    'expDataScale(:,1)=expParallelData(:,1);',
    'for i=2:c',
    '    temp=expDataMax(i)-expDataMin(i);',
    'expDataScale(:,i)=2/(expDataMax(i)-
expDataMin(i))*(expParallelData(:,i)-expDataMin(i))-ones(r,1);',
    'end',
    ''};

  %========== Slide 6 ==========

  slide(6).code={
    'disp(''   prepare neural network training inputs and output'');',
    '',
    'inputs=expDataScale(:,2:13)'';',
    'inputs(7:11,:)=[];',
    'inputs(5,:)=[];',
    'outputs=expDataScale(:,15)'';',
    '',
    'nn.inputsFirstSet=inputs(:,1);',
    'nn.outputsFirstSet=outputs(1);',
    'out=evalc(''nn'');',
    'slideData=nnslides(''text'',slideData,out);',
    '',
    '' };
  slide(6).text={
    'STEP 4 (Cont''d):',
    'extract neural network training inputs and output from experiment
data sets',
```

```
   'neural network inputs:  feedRate, feedComp, feedTemp, refluxRate,
TReboiler, TTray6',
   'neural network output: residualError',
   '',
   'inputs=expDataScale(:,2:13)'';',
   'inputs(7:11,:)=[];',
   'inputs(5,:)=[];',
   'outputs=expDataScale(:,15)'';',
   ''};

  %========== Slide 7 ==========

  slide(7).code={
   'disp(''   divide expData into training set and test set'');',
   '',
   '[r,c]=size(inputs);',
   'trainInputs=[];',
   'testInputs=[];',
   'trainOutput=[];',
   'testOutput=[];',
   'for i=1:c',
   '   if (mod(i,3)==0)',
   '      testInputs=[testInputs,inputs(:,i)];',
   '      testOutput=[testOutput,outputs(:,i)];',
   '   else',
   '      trainInputs=[trainInputs,inputs(:,i)];',
   '      trainOutput=[trainOutput,outputs(:,i)];',
   '   end',
   'end',
   '',
   '',
   'totalPoints.trainingSet=length(trainOutput);',
   'totalPoints.testSet=length(testOutput);',
   'out=evalc(''totalPoints'');',
   'slideData=nnslides(''text'',slideData,out);',
   '' };
  slide(7).text={
   'STEP 4 (Cont''d)',
   'divide expData into training set and test set based on the sequence
number:',
   'training set include: 1,2,4,5,7,8...',
   'test set include: 3,6,9...',
   '',
   '[r,c]=size(inputs);',
   'trainInputs=[];',
   'testInputs=[];',
   'trainOutput=[];',
   'testOutput=[];',
   'for i=1:c',
   '   if (mod(i,3)==0)',
   '      testInputs=[testInputs,inputs(:,i)];',
   '      testOutput=[testOutput,outputs(:,i)];',
   '   else',
   '      trainInputs=[trainInputs,inputs(:,i)];',
   '      trainOutput=[trainOutput,outputs(:,i)];',
   '   end',
   'end',
```

```
    ''};

  %========== Slide 8 ==========

  slide(8).code={
   'disp(''   create neural network'');',
   '',
   'numHiddenLayerNode=5;',
   'numOutputLayerNode=1;',
   'net=newff(ones(6,1)*[-1 1],[numHiddenLayerNode,numOutputLayerNode],
{''tansig'',''purelin''},''trainbr'');',
   '',
   '',
   'nnetNodes.numHiddenLayerNode=numHiddenLayerNode;',
   'nnetNodes.numOutputLayerNode=numOutputLayerNode;',
   'out=evalc(''nnetNodes'');',
   'slideData=nnslides(''text'',slideData,out);' };
  slide(8).text={
   'STEP 4(Cont''d)',
   'create neural network',
   '',
   'numHiddenLayerNode=5;',
   'numOutputLayerNode=1;',
   'net=newff(ones(6,1)*[-1 1],[numHiddenLayerNode,numOutputLayerNode],
{''tansig'',''purelin''},''trainbr'');',
   '',
   ''};

  %========== Slide 9 ==========

  slide(9).code={
   'disp(''   neural network training'');',
   '',
   'slideData=nnslides(''axes'',slideData);',
   'net.trainParam.epochs=2000;',
   'net.trainParam.show=20;',
   'net=train(net,trainInputs,trainOutput);',
   '' };
  slide(9).text={
   'SETP 4: (Cont''d)',
   'set training parameters and train neural network',
   '',
   'net.trainParam.epochs=2000;',
   'net.trainParam.show=20;',
   'net=train(net,trainInputs,trainOutput);',
   ''};

  %========== Slide 10 ==========

  slide(10).code={
   'disp(''   get network predicted residual error from training
set'');',
   '',
   'trainPredict=sim(net,trainInputs);',
   '',
   '',
   'trainPredictScaledFirst10Pts=trainPredict(1:10);',
```

```
  'out=evalc(''trainPredictScaledFirst10Pts'');',
  'slideData=nnslides(''text'',slideData,out);',
  '',
  '' };
 slide(10).text={
  'STEP 4(Cont''d)',
  'get network predicted residual error from training set.',
  '',
  'trainPredict=sim(net,trainInputs);',
  ''};

 %========== Slide 11 ==========

 slide(11).code={
  'disp(''   get network predicted residual error from test set'');',
  '',
  'testPredict=sim(net,testInputs);',
  '',
  'testPredictScaledFirst10Pts=testPredict(1:10);',
  'out=evalc(''testPredictScaledFirst10Pts'');',
  'slideData=nnslides(''text'',slideData,out);' };
 slide(11).text={
  'STEP 4(Cont''d)',
  'get network predicted residual error from test set.',
  '',
  'testPredict=sim(net,testInputs);',
  ''};

 %========== Slide 12 ==========

 slide(12).code={
  'disp(''   set upper and lower bound for residual error'');',
  '',
  '',
  '[r,c]=size(trainPredict);',
  'for i=1:c',
  '   if trainPredict(i)>1.0',
  '      trainPredict(i)=1.0;',
  '   end',
  '   if trainPredict(i)<-1.0',
  '      trainPredict(i)=-1.0;',
  '   end',
  'end',
  '',
  '[r,c]=size(testPredict);',
  'for i=1:c',
  '   if testPredict(i)>1.0',
  '      testPredict(i)=1.0;',
  '   end',
  '   if testPredict(i)<-1.0',
  '      testPredict(i)=-1.0;',
  '   end',
  'end' };
 slide(12).text={
  'STEP 4(Cont''d)',
  'set upper and lower bound for residual error (scaled).  If
predicted residual error is greater than 1.0, set the residual error
```

```
equals to 1.0; If predicted residual error is less than -1.0, set the
residual error equals to -1.0.',
   '',
   '[r,c]=size(trainPredict);',
   'for i=1:c',
   '   if trainPredict(i)>1.0',
   '      trainPredict(i)=1.0;',
   '   end',
   '   if trainPredict(i)<-1.0',
   '      trainPredict(i)=-1.0;',
   '   end',
   'end',
   '',
   '[r,c]=size(testPredict);',
   'for i=1:c',
   '   if testPredict(i)>1.0',
   '      testPredict(i)=1.0;',
   '   end',
   '   if testPredict(i)<-1.0',
   '      testPredict(i)=-1.0;',
   '   end',
   'end',
   ''};

  %========== Slide 13 ==========

  slide(13).code={
   'disp(''   change training set scale back to experiment value'');',
   '',
   'trainPredictReal=(trainPredict+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   'trainOutputReal=(trainOutput+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   '',

'trainPredictReal_trainExperiment_First10Pts=[trainPredictReal(1:10);tr
ainOutputReal(1:10)];',
   'out=evalc(''trainPredictReal_trainExperiment_First10Pts'');',
   'slideData=nnslides(''text'',slideData,out);',
   '' };
  slide(13).text={
   'STEP 4(cont''d):',
   'change training set scale back to experiment value',
   '',
   'trainPredictReal=(trainPredict+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   '',
   'trainOutputReal=(trainOutput+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   ''};

  %========== Slide 14 ==========

  slide(14).code={
   ' disp(''   change test set scale back to experiment value'');',
   '',
```

```
   'testPredictReal=(testPredict+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   'testOutputReal=(testOutput+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   '',
   '',
   '
testPredictReal_testExperiment_First10Pts=[testPredictReal(1:10);testOu
tputReal(1:10)];',
   'out=evalc(''testPredictReal_testExperiment_First10Pts'');',
   'slideData=nnslides(''text'',slideData,out);',
   '',
   '',
   '',
   '',
   '' };
  slide(14).text={
   'STEP 4(cont''d):',
   'change test set scale back to experiment value',
   '',
   'testPredictReal=(testPredict+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   'testOutputReal=(testOutput+1)*(expDataMax(15)-
expDataMin(15))/2+expDataMin(15);',
   ''};

  %========== Slide 15 ==========

  slide(15).code={
   'disp(''STEP 5: TEST HYBRID PARALLEL MODEL'');',
   'disp(''   plot experiment residual error vs. predicted residual
error from training set'');',
   '',
   'figure(2);',
   'plot(trainPredictReal,trainOutputReal,''+'');',
   'line([-30,30],[-30,30]);',
   'title(''training set'');',
   'xlabel(''neural network predicted residual error'');',
   'ylabel(''true experiment residual error'');' };
  slide(15).text={
   'STEP 5: TEST HYBRID PARALLEL MODEL',
   'plot experiment residual error vs. predicted residual error from
training set',
   '',
   'figure(2);',
   'plot(trainPredictReal,trainOutputReal,''+'');',
   'line([-30,30],[-30,30]);',
   'title(''training set'');',
   'xlabel(''neural network predicted residual error'');',
   'ylabel(''true experiment residual error'');',
   ''};

  %========== Slide 16 ==========

  slide(16).code={
   'disp(''plot experiment residual error vs. predicted residual error
from test set'');',
```

```
    '',
    'figure(3);',
    'plot(testPredictReal,testOutputReal,''+'');',
    'line([-30,30],[-30,30]);',
    'title(''test set'');',
    'xlabel(''neural network predicted residual error'');',
    'ylabel(''true experiment residual error'');',
    '',
    '' };
  slide(16).text={
    'STEP 5 (Cont''d)',
    'plot experiment residual error vs. predicted residual error test
set',
    '',
    'figure(3);',
    'plot(testPredictReal,testOutputReal,''+'');',
    'line([-30,30],[-30,30]);',
    'title(''test set'');',
    'xlabel(''neural network predicted residual error'');',
    'ylabel(''true experiment residual error'');',
    ''};

  %========== Slide 17 ==========

  slide(17).code={
    'disp(''sum squared error'');',
    '',
    'errTrainReal=sumsqr(trainOutputReal-trainPredictReal);',
    'errTestReal=sumsqr(testOutputReal-testPredictReal);',
    '',
    'err.TrainReal=errTrainReal;',
    'err.TestReal=errTestReal;',
    'out=evalc(''err'');',
    'slideData=nnslides(''text'',slideData,out);',
    '' };
  slide(17).text={
    'STEP 5 (Cont''d)',
    'sum squared error',
    '',
    'errTrainReal=sumsqr(trainOutputReal-trainPredictReal)',
    'errTestReal=sumsqr(testOutputReal-testPredictReal)',
    ''};
end
```

APPENDIX E

HYBRID SERIAL MODELING DATA SET

The data set is on one large spread sheet. It is divided into 7 pages as follows (the number in each of the box correspond to page number):

98	99	100	101	102	103	104

		Data Used for Hybrid Serial Modeling									
Exp No.	original file name	feed	feed	feed	reflux	reflux	reboiler	tray1	tray2	tray3	tray4
		rate	composition	temperature	rate	temperature	temperature	temperature	temperature	temperature	temperature
		(lb/hr)	(mol%)	(C)	(lb/hr)	(C)	(C)	(C)	(C)	(C)	(C)
4	ex990416_ss1	12.05	40	41.8	11.99	50.0	89.8	82.1	77.6	75.7	71.0
5	ex990416_ss2	11.96	40	41.5	14.00	50.0	89.0	81.5	77.7	75.8	70.8
6	ex990416_ss3	12.02	40	41.1	16.01	50.0	88.5	81.4	77.8	75.9	70.8
7	ex990417_ss1	11.94	39	40.9	20.00	50.0	87.0	77.4	80.9	75.9	70.7
8	ex990417_ss2	11.95	39	50.0	30.00	50.1	97.9	91.8	82.2	77.2	71.2
13	ex990430_ss1	14.95	40	38.9	15.01	49.9	83.7	78.6	76.3	75.2	70.2
14	ex990430_ss2	15.02	34	39.7	18.01	50.0	83.5	78.4	76.1	75.1	70.1
15	ex990430_ss3	14.99	33	39.4	20.99	50.0	83.6	78.5	76.1	75.1	70.2
16	ex990501_ss1	15.05	40	39.0	25.00	50.0	83.2	78.1	75.9	74.9	69.8
17	ex990501_ss2	14.97	39	39.1	28.00	50.1	82.9	78.1	75.9	74.9	69.8
18	ex990511_ss1	15.01	40	39.5	28.00	50.0	82.7	77.7	75.6	74.7	69.6
19	ex990511_ss2	15.00	39	39.5	31.01	50.0	82.8	77.8	75.7	74.7	69.8
21	ex990514_ss1	13.89	40	39.6	10.00	50.0	83.9	78.7	76.4	75.2	70.5
22	ex990514_ss2	13.67	40	39.8	14.00	50.0	84.3	78.9	76.1	74.8	69.7
23	ex990514_ss3	13.63	40	40.0	16.01	50.0	84.2	78.5	75.9	74.6	69.5
24	ex990514_ss4	13.68	40	39.5	20.00	50.0	83.1	78.1	75.3	74.1	69.3
25	ex990515_ss1	17.98	40	38.3	24.01	50.0	82.2	77.4	75.1	74.0	68.9
26	ex990515_ss2	17.96	39	37.4	28.02	50.0	81.2	76.8	75.0	74.2	70.1
27	ex990515_ss3	18.01	34	37.5	31.00	50.0	81.6	77.0	75.0	74.2	70.5
29	ex990516_ss2	10.02	35	46.3	10.00	50.0	80.4	75.4	73.8	72.3	67.9
30	ex990516_ss3	10.01	33	45.7	10.00	50.0	83.5	77.8	74.8	73.2	68.7
32	ex990517_ss2	12.05	34	43.0	12.00	50.0	80.4	75.8	72.8	68.3	68.5
33	ex990517_ss3	11.95	35	43.1	10.01	50.0	81.4	77.1	74.7	73.5	69.0
34	ex990519_ss1	17.99	39	36.6	10.00	50.0	85.1	79.6	77.1	76.1	72.9
35	ex990522_ss1	17.94	40	41.2	13.99	50.0	88.4	81.1	76.5	74.4	70.6
36	ex990522_ss2	17.93	34	49.8	16.00	50.0	96.8	91.3	81.1	76.3	70.8
37	ex990522_ss3	17.94	33	49.5	20.00	50.0	97.1	91.8	81.5	76.3	70.7
38	ex990523_ss1	10.03	35	45.9	21.00	50.0	96.0	90.0	80.5	75.7	70.9
39	ex990523_ss2	9.99	34	46.2	25.01	50.0	96.2	90.5	80.7	75.7	70.8
40	ex990523_ss3	9.99	34	46.5	28.00	50.0	96.2	90.4	80.6	75.6	70.7
41	ex990525_ss1	10.04	38	46.7	17.99	50.0	95.5	89.1	79.9	75.4	70.6
42	ex990525_ss2	10.02	38	47.1	15.00	50.0	95.7	89.1	79.9	75.3	70.7
43	ex990529_ss1	10.03	37	46.1	12.01	50.0	95.3	89.0	80.2	75.8	70.9
73	ex990705_ss1	24.00	22	33.9	30.00	50.0	97.3	93.3	86.9	82.0	75.2
75	ex990705_ss3	30.01	21	33.2	59.97	53.8	92.5	85.4	81.3	78.3	72.7
76	ex990706_ss1	29.98	23	31.7	38.01	52.8	90.7	84.1	80.5	78.3	74.5
77	ex990706_ss2	30.02	23	33.9	15.00	50.0	91.4	84.7	81.2	79.1	75.6
78	ex990708_ss1	23.98	23	32.6	10.83	50.0	91.8	86.0	82.0	79.2	73.7
79	ex990708_ss2	24.00	23	31.9	26.43	50.0	92.6	86.0	82.1	78.8	72.9
80	ex990708_ss3	24.02	21	34.5	37.12	49.8	93.7	88.0	82.4	78.4	72.3
81	ex990710_ss1	24.00	23	32.9	23.68	50.9	96.2	91.7	85.3	80.5	74.3
82	ex990710_ss2	23.99	19	32.9	51.71	54.1	96.4	92.7	86.4	80.8	73.9
83	ex990711_ss1	24.00	20	33.9	21.74	50.0	91.7	85.0	81.3	79.1	73.8
84	ex990711_ss2	24.00	20	33.5	33.79	50.0	91.4	85.0	80.9	78.6	72.9
85	ex990711_ss3	24.00	18	34.7	79.72	55.1	90.1	85.0	80.4	78.1	71.5
86	ex990712_ss1	15.02	19	37.4	14.09	50.0	90.1	85.1	79.4	76.5	70.5
89	ex990713_ss1	15.00	20	35.1	19.24	50.0	92.8	87.9	81.5	78.0	72.0
91	ex990714_ss1	14.99	17	35.0	79.31	54.9	95.6	91.1	83.9	79.1	71.4
92	ex990714_ss2	29.98	16	32.0	80.04	54.9	90.9	84.7	81.3	78.6	71.4
93	ex990717_ss1	30.02	20	30.8	59.99	53.9	89.9	84.5	80.9	78.7	72.7
94	ex990717_ss2	30.00	19	34.1	79.96	56.1	88.5	83.0	80.1	78.5	72.6
95	ex990717_ss3	30.00	17	34.8	20.00	50.0	88.0	83.0	80.1	78.2	73.0
98	ex990720_ss2	23.98	18	31.9	80.01	56.2	96.5	92.0	86.1	81.2	73.7
99	ex990720_ss3	30.00	18	34.8	80.02	55.5	91.7	85.7	81.9	79.1	72.4
100	ex990804_ss1	20.99	28	34.8	15.00	50.0	94.4	89.1	82.2	78.3	74.6
101	ex990804_ss2	20.97	28	34.7	44.99	53.6	94.3	88.9	81.6	77.7	73.9
102	ex990804_ss3	21.01	28	34.9	79.97	57.5	95.2	91.0	82.6	78.1	73.6
103	ex990805_ss1	29.96	30	32.2	14.99	50.0	96.1	91.6	83.8	78.8	77.3
104	ex990805_ss2	30.02	28	31.3	80.02	59.5	95.3	90.9	82.8	77.4	75.2
107	ex000114_ss1	24.00	30	35.4	15.75	50.0	99.1	94.5	88.7	81.6	77.5
108	ex000114_ss2	24.01	30	34.8	31.01	50.0	98.7	94.0	88.0	80.6	76.0
109	ex000114_ss3	23.96	29	35.8	28.93	50.0	98.4	94.0	88.0	80.4	75.8
110	ex000114_ss4	24.10	29	34.7	15.87	50.0	98.9	94.4	88.4	80.9	77.1
111	ex000117_ss1	23.97	33	35.9	15.71	50.0	99.3	96.1	88.9	82.4	78.3
113	ex000118_ss1	23.97	30	34.5	15.66	50.0	97.6	93.4	85.2	80.0	77.6
114	ex000118_ss2	23.96	30	33.0	81.90	61.1	96.1	90.6	83.2	78.4	74.8
117	ex000119_ss2	29.94	27	32.1	15.70	50.0	96.6	92.3	84.9	79.6	77.6
118	ex000120_ss1	29.91	26	31.9	15.82	50.0	95.8	91.5	84.2	79.1	76.8
119	ex000120_ss2	29.92	26	32.1	81.71	60.6	95.0	91.2	83.5	77.9	74.7
120	ex000121_ss1	29.94	28	32.3	15.75	50.0	96.4	92.6	84.6	78.7	77.0
121	ex000121_ss2	29.94	28	32.5	81.78	60.7	95.8	92.1	84.0	77.6	75.0
122	ex000126_ss1	29.96	28	30.6	81.80	60.9	95.6	92.2	84.1	77.8	75.3
123	ex000128_ss2	29.95	28	33.1	15.81	50.0	95.5	91.7	83.1	76.8	76.0
124	ex000128_ss3	29.96	28	32.8	81.78	61.3	94.3	90.9	81.6	75.7	74.0
125	ex000131_ss1	29.96	22	31.3	15.92	50.0	92.8	85.9	81.2	77.8	75.7
126	ex000131_ss2	29.95	21	30.0	81.77	61.0	92.0	84.6	79.9	76.9	73.8
127	ex000131_ss3	29.95	20	32.5	16.26	50.0	94.9	90.1	84.3	79.5	74.8
128	ex000201_ss1	29.95	21	32.4	16.01	50.0	95.8	91.3	85.1	80.0	76.1
129	ex000201_ss2	29.95	21	30.6	81.64	59.6	94.6	90.1	83.9	78.6	73.6
130	ex000201_ss3	29.97	20	32.4	16.06	50.0	95.1	90.6	84.5	79.4	75.8
135	ex000203_ss2	23.97	19	27.9	16.40	50.0	92.5	86.1	80.8	77.4	73.6
136	ex000203_ss3	23.91	19	27.4	81.51	58.5	91.0	84.2	79.3	76.4	71.4
140	ex000209_ss1	23.98	28	35.6	16.07	50.0	96.5	93.2	85.1	79.4	76.2
143	ex000210_ss2	23.95	26	34.5	15.88	50.0	96.9	93.5	85.2	79.5	77.5
145	ex000217_ss2	14.98	31	35.0	81.81	60.6	99.1	97.7	93.5	86.6	86.6
146	ex000217_ss3	29.96	29	33.1	15.65	50.0	96.2	92.4	83.8	77.6	76.9
147	ex000218_ss1	29.96	33	33.0	15.14	50.0	99.0	96.1	87.7	81.0	80.1
148	ex000218_ss2	29.95	32	32.2	81.14	61.4	98.5	95.2	87.0	80.1	78.3

	Data Used for Hybrid Serial Modeling				bottom composition	distillate composition	bottom	distillate	bottom
Exp No.	tray5	tray6	efficiency	efficiency	(use efficiency from	(use efficiency from	composition	composition	composition
	temperature	temperature	(actual)	(predicted by	neural network prediction)	neural network prediction)	(set effi=0.4)	(set effi=0.4)	(experiment)
	(C)	(C)	(from ChemCAD)	neural network)	(mol% meOH)	(mol% meOH)	(mol% meOH)	(mol% meOH)	(mol% meOH)
4	70.4	69.3	0.51	0.4836	7.5%	85.7%	7.5%	81.5%	10.0%
5	70.3	69.1	0.46	0.4698	8.4%	86.2%	8.4%	82.7%	11.0%
6	70.2	70.0	0.44	0.4075	9.0%	84.0%	9.0%	83.5%	12.0%
7	70.1	70.0	0.37	0.3603	10.9%	83.1%	10.9%	85.2%	16.0%
8	70.5	69.1	0.44	0.4349	1.1%	76.6%	1.1%	73.4%	3.0%
13	69.7	68.5	0.44	0.3882	16.2%	85.7%	16.2%	86.0%	22.0%
14	69.5	68.3	0.42	0.4019	16.6%	86.5%	16.6%	86.4%	20.0%
15	69.6	68.4	0.34	0.3643	16.4%	85.1%	16.4%	86.7%	20.0%
16	69.3	68.0	0.31	0.3342	17.2%	84.6%	17.2%	87.6%	22.0%
17	69.3	68.0	0.31	0.3054	17.8%	83.6%	17.8%	88.0%	21.0%
18	69.1	67.8	0.30	0.3208	18.2%	84.6%	18.2%	88.1%	23.0%
19	69.3	68.0	0.26	0.2873	18.0%	82.8%	18.0%	88.3%	23.0%
21	70.6	67.9	0.46	0.4918	15.8%	88.1%	15.8%	84.9%	24.0%
22	69.2	68.0	0.45	0.4576	15.1%	87.9%	15.1%	85.7%	17.0%
23	69.0	67.8	0.42	0.4528	15.3%	88.2%	15.3%	86.1%	19.0%
24	68.8	67.6	0.40	0.4015	17.4%	87.4%	17.4%	87.4%	20.0%
25	68.4	67.2	0.41	0.3795	19.2%	86.9%	19.2%	87.7%	23.0%
26	69.5	68.2	0.20	0.2420	21.5%	81.2%	21.5%	88.6%	25.0%
27	69.9	68.6	0.17	0.1803	20.6%	76.6%	20.6%	88.4%	23.0%
29	67.8	66.1	0.69	0.6900	23.5%	94.7%	23.5%	87.8%	26.0%
30	68.8	66.5	0.64	0.6900	16.6%	93.8%	16.6%	85.8%	18.0%
32	68.5	66.4	0.62	0.6124	23.5%	93.4%	23.5%	87.8%	28.0%
33	69.1	66.8	0.68	0.6335	21.1%	93.0%	21.1%	86.8%	23.0%
34	72.3	71.2	0.30	0.1918	13.8%	71.0%	13.8%	82.9%	17.0%
35	70.1	68.9	0.46	0.4610	9.1%	84.6%	9.1%	81.7%	10.0%
36	70.2	68.9	0.61	0.6142	1.8%	84.8%	1.8%	71.1%	2.0%
37	70.1	68.8	0.64	0.5862	1.6%	84.4%	1.6%	71.7%	1.0%
38	70.3	69.0	0.53	0.4944	2.3%	83.7%	2.3%	76.9%	2.0%
39	70.2	68.9	0.46	0.4790	2.2%	83.0%	2.2%	77.1%	2.0%
40	70.1	68.8	0.45	0.4642	2.2%	82.3%	2.2%	77.4%	2.0%
41	70.1	68.8	0.50	0.5186	2.7%	85.2%	2.7%	77.3%	2.0%
42	70.1	68.9	0.55	0.5529	2.5%	86.1%	2.5%	76.3%	2.0%
43	70.3	69.1	0.57	0.5704	2.8%	86.3%	2.8%	75.9%	2.0%
73	73.9	71.4	0.44	0.4287	1.5%	73.9%	1.5%	71.4%	1.0%
75	71.5	69.3	0.35	0.3652	5.0%	78.1%	5.0%	80.7%	3.0%
76	73.6	71.7	0.25	0.2892	6.6%	72.7%	6.6%	80.7%	5.0%
77	74.7	73.0	0.33	0.3367	5.9%	72.0%	5.9%	76.0%	5.0%
78	72.8	71.0	0.51	0.4773	5.6%	79.1%	5.6%	74.8%	5.0%
79	71.9	70.0	0.40	0.4064	4.9%	79.0%	4.9%	78.6%	4.0%
80	71.2	69.0	0.43	0.4118	4.0%	79.4%	4.0%	78.5%	2.0%
81	73.2	71.0	0.44	0.4623	2.2%	77.5%	2.2%	72.7%	2.0%
82	72.6	70.0	0.42	0.3102	2.1%	66.8%	2.1%	75.7%	1.0%
83	72.9	71.0	0.38	0.4015	5.7%	78.7%	5.7%	78.6%	5.0%
84	71.9	70.0	0.37	0.3501	5.9%	77.1%	5.9%	80.5%	5.0%
85	70.4	68.3	0.34	0.3493	7.2%	80.5%	7.2%	83.8%	5.0%
86	69.6	68.0	0.55	0.5678	7.2%	88.1%	7.2%	80.2%	5.0%
89	70.9	69.0	0.46	0.4760	4.7%	83.5%	4.7%	78.5%	3.0%
91	70.2	68.1	0.45	0.3639	2.6%	76.1%	3.0%	80.1%	1.0%
92	70.2	68.0	0.36	0.3347	6.4%	78.1%	6.4%	82.6%	4.0%
93	71.6	69.5	0.28	0.2844	7.4%	74.5%	7.4%	82.8%	6.0%
94	71.5	69.3	0.27	0.2847	9.0%	76.8%	9.0%	84.5%	8.0%
95	72.0	70.2	0.39	0.3894	9.6%	80.2%	9.6%	80.8%	8.0%
98	72.2	69.3	0.39	0.2856	2.0%	64.9%	2.0%	76.8%	1.0%
99	71.2	68.8	0.34	0.3586	5.7%	79.1%	5.7%	82.0%	4.0%
100	73.7	72.1	0.37	0.4006	3.4%	74.3%	3.4%	74.2%	4.0%
101	72.9	71.1	0.30	0.2741	3.5%	67.5%	3.5%	79.1%	3.0%
102	72.5	70.2	0.36	0.3520	2.9%	75.3%	2.9%	79.4%	1.0%
103	76.8	75.2	0.43	0.4095	2.3%	68.7%	2.3%	68.0%	1.0%
104	74.2	71.9	0.28	0.2946	2.8%	68.5%	2.8%	78.4%	1.0%
107	76.6	74.3	0.48	0.4649	0.5%	60.2%	0.5%	53.6%	1.0%
108	74.7	72.2	0.40	0.4075	0.7%	66.8%	0.7%	66.1%	1.0%
109	74.6	72.0	0.41	0.4276	0.9%	70.0%	0.9%	67.3%	1.0%
110	76.1	73.8	0.48	0.4788	0.6%	64.0%	0.6%	56.4%	1.0%
111	77.2	74.7	0.46	0.4480	0.4%	55.1%	0.4%	50.4%	1.0%
113	76.7	75.0	0.34	0.3884	1.3%	64.6%	1.3%	65.6%	2.0%
114	73.5	71.3	0.29	0.3222	2.3%	70.5%	2.3%	78.0%	2.0%
117	76.6	74.6	0.44	0.4400	1.9%	70.0%	1.9%	66.9%	1.0%
118	75.9	74.0	0.46	0.4547	2.5%	73.1%	2.5%	69.2%	1.0%
119	73.3	70.4	0.33	0.3347	3.0%	73.2%	3.0%	78.9%	1.0%
120	76.2	74.5	0.43	0.4543	2.1%	71.7%	2.1%	67.6%	1.0%
121	73.7	71.0	0.32	0.3356	2.5%	71.9%	2.5%	77.8%	1.0%
122	73.9	71.1	0.29	0.3106	2.7%	69.7%	2.6%	78.1%	1.0%
123	75.4	74.2	0.41	0.4398	2.7%	72.6%	2.7%	69.9%	1.0%
124	73.2	71.1	0.39	0.3397	3.5%	74.8%	3.5%	79.8%	1.0%
125	74.9	73.5	0.33	0.3488	4.7%	71.0%	4.7%	74.6%	3.0%
126	72.9	70.8	0.24	0.2274	5.4%	66.5%	5.4%	82.0%	3.0%
127	74.0	71.6	0.55	0.5535	3.1%	80.7%	3.1%	71.3%	1.0%
128	75.2	73.1	0.50	0.5043	2.5%	76.4%	2.5%	69.2%	1.0%
129	72.2	69.4	0.36	0.3082	3.3%	71.0%	3.3%	79.3%	1.0%
130	74.9	72.7	0.51	0.5044	2.9%	77.7%	2.9%	70.8%	1.0%
135	72.5	70.9	0.43	0.4319	5.0%	78.5%	5.0%	76.4%	3.0%
136	70.2	68.1	0.30	0.3029	6.3%	75.9%	6.3%	83.3%	3.0%
140	75.1	72.8	0.48	0.4677	2.0%	74.6%	2.0%	69.5%	1.0%
143	76.5	74.8	0.41	0.3841	1.7%	66.7%	1.7%	68.1%	1.0%
145	80.0	70.5	0.33	0.3210	0.5%	60.0%	0.5%	69.8%	1.0%
146	76.3	75.1	0.41	0.4132	2.2%	69.1%	2.2%	68.1%	1.0%
147	79.4	77.7	0.35	0.3770	0.5%	49.2%	0.5%	51.5%	1.0%
148	77.2	74.6	0.27	0.2605	0.8%	53.8%	0.8%	71.2%	1.0%

	distillate	hybrid model	first-principles model	hybrid model	first-principles model	Experiment Data			
Exp No.	composition	error	(with efficiency=0.4)	distillate composition	distillate composition	feed	feed	reflux	bottom
	(experiment)	(actual-model)	(actual-model)	(efficiency from Neural Network)	(fixed efficiency=0.4)	rate	composition	rate	rate
	(mol% meOH)	(mol% meOH)	(mol% meOH)	(mol% MeOH)	(mol% MeOH)	(lb/hr)	(mol% meOH)	(lb/hr)	(lb/hr)
4	88.0%	2.3%	6.5%	85.7%	81.5%	12.05	40%	11.99	8.71
5	87.0%	0.8%	4.3%	86.2%	82.7%	11.96	40%	14.00	8.83
6	87.0%	3.0%	3.5%	84.0%	83.5%	12.02	40%	16.01	9.84
7	86.0%	2.9%	0.8%	83.1%	85.2%	11.94	39%	20.00	8.99
8	82.0%	5.4%	8.6%	76.6%	73.4%	11.95	39%	30.00	3.68
13	89.0%	3.3%	3.0%	85.7%	86.0%	14.95	40%	15.01	12.69
14	88.0%	1.5%	1.6%	86.5%	86.4%	15.02	34%	18.01	12.88
15	85.0%	-0.1%	-1.7%	85.1%	86.7%	14.99	33%	20.99	11.90
16	85.0%	0.4%	-2.6%	84.6%	87.6%	15.05	40%	25.00	13.29
17	85.0%	1.4%	-3.0%	83.6%	88.0%	14.97	39%	28.00	13.27
18	85.0%	0.4%	-3.1%	84.6%	88.1%	15.01	40%	28.00	12.38
19	83.0%	0.2%	-5.3%	82.8%	88.3%	15.00	39%	31.01	12.13
21	89.0%	0.9%	4.1%	88.1%	84.9%	13.69	40%	10.00	9.41
22	88.0%	0.1%	2.3%	87.9%	85.7%	13.67	40%	14.00	11.06
23	88.0%	-0.2%	1.9%	88.2%	86.1%	13.63	40%	16.01	10.98
24	88.0%	0.6%	0.6%	87.4%	87.4%	13.68	40%	20.00	11.76
25	89.0%	2.1%	1.3%	86.9%	87.7%	17.98	40%	24.01	15.24
26	80.0%	-1.2%	-8.6%	81.2%	88.6%	17.96	39%	28.02	14.19
27	77.0%	0.4%	-11.4%	76.6%	88.4%	18.01	34%	31.00	12.76
29	95.0%	0.3%	7.2%	94.7%	87.8%	10.02	35%	10.00	9.41
30	93.0%	-0.8%	7.2%	93.8%	85.8%	10.01	33%	10.00	7.30
32	94.0%	0.6%	6.2%	93.4%	87.8%	12.05	34%	12.00	11.12
33	94.0%	1.0%	7.2%	93.0%	86.8%	11.95	35%	10.01	9.06
34	80.0%	9.0%	-2.9%	71.0%	82.9%	17.99	39%	10.00	13.56
35	85.0%	0.4%	3.3%	84.6%	81.7%	17.94	40%	13.99	8.27
36	85.0%	0.2%	13.9%	84.8%	71.1%	17.93	34%	16.00	3.85
37	85.0%	0.6%	13.3%	84.4%	71.7%	17.94	33%	20.00	4.01
38	85.0%	1.3%	8.1%	83.7%	76.9%	10.03	35%	21.00	4.72
39	81.0%	-2.0%	3.9%	83.0%	77.1%	9.99	34%	25.01	4.91
40	81.0%	-1.3%	3.6%	82.3%	77.4%	9.99	34%	28.00	4.71
41	83.0%	-2.2%	5.7%	85.2%	77.3%	10.04	38%	17.99	4.65
42	85.0%	-1.1%	8.7%	86.1%	76.3%	10.02	36%	15.00	5.02
43	85.0%	-1.3%	9.1%	86.3%	75.9%	10.03	37%	12.01	5.25
73	72.0%	-1.9%	0.6%	73.9%	71.4%	24.00	22%	30.00	16.58
75	73.0%	-5.1%	-7.7%	78.1%	80.7%	30.01	21%	59.97	23.12
76	66.0%	-6.7%	-14.7%	72.7%	80.7%	29.98	23%	36.01	21.95
77	70.0%	-2.0%	-6.0%	72.0%	76.0%	30.02	23%	15.00	22.94
78	80.0%	0.9%	5.2%	79.1%	74.8%	23.98	23%	10.83	19.36
79	77.0%	-2.0%	-1.6%	79.0%	78.6%	24.00	23%	26.43	18.83
80	75.0%	-4.4%	-3.5%	79.4%	78.5%	24.02	21%	37.12	18.67
81	75.0%	-2.5%	2.3%	77.5%	72.7%	24.00	23%	23.68	18.23
82	73.0%	6.2%	-2.7%	66.8%	75.7%	23.99	19%	51.71	17.72
83	76.0%	-2.7%	-2.6%	78.7%	78.6%	24.00	20%	21.74	19.47
84	77.0%	-0.1%	-3.5%	77.1%	80.5%	24.00	20%	33.79	19.88
85	77.0%	-3.5%	-6.8%	80.5%	83.8%	24.00	18%	79.72	21.72
86	86.0%	-2.1%	5.8%	88.1%	80.2%	15.02	19%	14.09	13.16
89	80.0%	-3.5%	1.2%	83.5%	78.8%	15.00	20%	19.24	12.73
91	79.0%	2.9%	-1.1%	76.1%	80.1%	14.99	17%	79.31	13.11
92	77.0%	-1.1%	-5.6%	78.1%	82.6%	29.98	16%	80.04	27.21
93	72.0%	-2.5%	-10.8%	74.5%	82.8%	30.02	20%	59.99	25.56
94	74.0%	-2.8%	-10.5%	76.8%	84.5%	30.00	19%	79.96	26.31
95	79.0%	-1.2%	-1.8%	80.2%	80.8%	30.00	17%	20.00	28.28
98	72.0%	7.1%	-4.8%	64.9%	76.8%	23.98	18%	80.01	19.39
99	75.0%	-4.1%	-7.0%	79.1%	82.0%	30.00	18%	80.02	25.91
100	73.0%	-1.3%	-1.2%	74.3%	74.2%	20.99	28%	15.00	12.61
101	69.0%	1.5%	-10.1%	67.5%	79.1%	20.97	28%	44.99	11.37
102	69.0%	-6.3%	-10.4%	75.3%	79.4%	21.01	28%	79.97	10.80
103	62.0%	-6.7%	-6.0%	68.7%	68.0%	29.96	30%	14.99	11.35
104	63.0%	-5.5%	-15.4%	68.5%	78.4%	30.02	28%	80.02	11.93
107	70.0%	9.8%	16.4%	60.2%	53.6%	24.00	30%	15.75	12.22
108	69.0%	2.2%	2.9%	66.8%	66.1%	24.01	30%	31.01	11.94
109	69.0%	-1.0%	1.7%	70.0%	67.3%	23.98	29%	28.93	11.52
110	70.0%	6.0%	13.6%	64.0%	56.4%	24.10	29%	15.87	11.88
111	68.0%	12.9%	17.6%	55.1%	50.4%	23.97	33%	15.71	11.05
113	64.0%	-0.6%	-1.6%	64.6%	65.6%	23.97	30%	15.66	11.82
114	65.0%	-5.5%	-13.0%	70.5%	78.0%	23.96	30%	81.90	12.03
117	63.0%	-7.0%	-3.9%	70.0%	66.9%	29.94	27%	15.70	14.51
118	85.0%	-8.1%	-4.2%	73.1%	69.2%	29.91	26%	15.82	15.22
119	65.0%	-8.2%	-13.9%	73.2%	78.9%	29.92	26%	81.71	12.82
120	62.0%	-9.7%	-5.6%	71.7%	67.6%	29.94	28%	15.75	11.73
121	63.0%	-8.9%	-14.8%	71.9%	77.8%	29.94	28%	81.78	10.20
122	60.0%	-9.7%	-18.1%	69.7%	78.1%	29.96	28%	81.80	11.11
123	60.0%	-12.8%	-9.9%	72.8%	69.9%	29.95	28%	15.81	8.74
124	71.0%	-3.8%	-8.8%	74.8%	79.8%	29.96	28%	81.78	7.70
125	65.0%	-6.0%	-9.6%	71.0%	74.6%	29.96	22%	15.92	19.05
126	62.0%	-4.5%	-20.0%	66.5%	82.0%	29.95	21%	81.77	17.74
127	72.0%	-8.7%	0.7%	80.7%	71.3%	29.95	20%	16.26	20.59
128	68.0%	-8.4%	-1.2%	76.4%	69.2%	29.95	21%	16.01	19.83
129	68.0%	-3.0%	-11.3%	71.0%	79.3%	29.95	21%	81.64	18.99
130	69.0%	-8.7%	-1.8%	77.7%	70.8%	29.97	20%	16.08	19.56
135	75.0%	-3.5%	-1.4%	78.5%	76.4%	23.97	19%	16.40	17.38
136	70.0%	-5.9%	-13.3%	75.9%	83.3%	23.91	19%	81.51	18.43
140	70.0%	-4.6%	0.5%	74.6%	69.5%	23.98	28%	16.07	9.63
143	63.0%	-3.7%	-5.1%	66.7%	68.1%	23.95	26%	15.68	10.67
145	67.0%	7.0%	-2.8%	60.0%	69.8%	14.96	31%	81.81	6.11
146	60.0%	-9.1%	-8.1%	69.1%	68.1%	29.96	29%	15.65	8.26
147	55.0%	5.8%	3.5%	49.2%	51.5%	29.96	33%	15.14	7.79
148	57.0%	3.2%	-14.2%	53.8%	71.2%	29.95	32%	81.14	6.75

	Experiment Data											
Exp No.	distillate	reboiler	feed	reflux	feed tray	bottom	distillate	reboiler	distillate	tray 1	tray 2	tray 3
	rate	duty	temperature	temperature	Number	composition	composition	temperature	temperature	temperature	temperature	temperature
	(lb/hr)	(% of full power)	(C)	(C)		(mol% meOH)	(mol% meOH)	(C)	(C)	(C)	(C)	(C)
4	2.61	60%	41.8	50.0	3	10%	88%	89.8	29.7	82.1	77.8	75.7
5	2.47	60%	41.5	50.0	3	11%	87%	89.0	29.9	81.5	77.7	75.8
6	1.85	60%	41.1	50.0	3	12%	87%	88.5	30.1	81.4	77.8	75.9
7	2.09	60%	40.9	50.0	3	16%	86%	87.0	31.2	77.4	80.9	75.9
8	2.09	60%	50.0	50.1	3	3%	82%	97.9	33.3	91.8	82.2	77.2
13	1.84	60%	38.9	49.9	3	22%	89%	83.7	30.3	78.6	76.3	75.2
14	1.91	60%	39.7	50.0	3	20%	88%	83.5	31.2	78.4	76.1	75.1
15	2.38	60%	39.4	50.0	3	20%	85%	83.6	32.0	78.5	76.1	75.1
16	1.30	60%	39.0	50.0	3	22%	85%	83.2	32.8	78.1	75.9	74.9
17	1.63	60%	39.1	50.1	3	21%	85%	82.9	33.5	78.1	75.9	74.9
18	1.88	60%	39.5	50.0	3	23%	85%	82.7	33.2	77.7	75.6	74.7
19	2.34	60%	39.5	50.0	3	23%	83%	82.6	33.3	77.8	75.7	74.7
21	3.37	60%	39.8	50.0	3	24%	89%	83.9	30.2	78.7	76.4	75.2
22	2.18	60%	39.8	50.0	3	17%	88%	84.3	30.5	78.9	76.1	74.8
23	2.19	60%	40.0	50.0	3	19%	88%	84.2	30.8	78.5	75.9	74.8
24	2.42	60%	39.5	50.0	3	20%	88%	83.1	31.9	78.1	75.3	74.1
25	1.12	60%	38.3	50.0	3	23%	89%	82.2	32.5	77.4	75.1	74.0
26	2.95	60%	37.4	50.0	3	25%	80%	81.2	33.7	76.8	75.0	74.2
27	3.98	60%	37.5	50.0	3	23%	77%	81.6	34.0	77.0	75.0	74.2
29	0.30	50%	46.3	50.0	3	26%	95%	80.4	28.7	75.4	73.8	72.3
30	1.93	55%	45.7	50.0	3	18%	93%	83.5	29.4	77.8	74.8	73.2
32	0.27	55%	43.0	50.0	3	26%	94%	80.4	29.2	75.6	72.8	68.3
33	1.80	55%	43.1	50.0	3	23%	94%	81.4	29.1	77.1	74.7	73.5
34	4.04	60%	36.6	50.0	3	17%	80%	85.1	30.4	79.6	77.1	76.1
35	4.36	60%	41.2	50.0	3	10%	85%	88.4	31.4	81.1	78.5	74.4
36	3.24	60%	49.8	50.0	3	2%	85%	96.8	31.7	91.3	81.1	76.3
37	3.19	60%	49.5	50.0	3	1%	85%	97.1	32.6	91.8	81.5	76.3
38	4.16	60%	45.9	50.0	3	2%	85%	96.0	33.3	90.0	80.5	75.7
39	4.26	60%	46.2	50.0	3	2%	81%	96.2	33.8	90.5	80.7	75.7
40	4.24	60%	46.5	50.0	3	2%	81%	96.2	34.1	90.4	80.6	75.6
41	4.11	60%	46.7	50.0	3	2%	83%	95.5	32.3	89.1	79.9	75.4
42	5.07	60%	47.1	50.0	3	2%	85%	95.7	31.6	89.1	79.9	75.3
43	3.72	60%	46.1	50.0	3	2%	85%	95.3	30.8	89.0	80.2	75.8
73	7.88	80%	33.9	50.0	3	1%	72%	97.3	35.1	93.3	86.9	82.0
75	8.28	80%	33.2	53.8	3	3%	73%	92.5	36.7	85.4	81.3	78.3
76	9.66	70%	31.7	52.8	3	5%	66%	90.7	35.9	84.1	80.5	78.3
77	8.80	70%	33.9	50.0	3	5%	70%	91.4	33.8	84.7	81.2	79.1
78	6.04	70%	32.6	50.0	3	5%	80%	91.8	32.0	88.0	82.0	79.2
79	6.68	71%	31.9	50.0	3	4%	77%	92.6	34.3	88.0	82.1	78.6
80	7.19	76%	34.5	49.6	3	2%	75%	93.7	34.5	88.0	82.4	78.4
81	7.16	97%	32.9	50.9	3	2%	75%	96.2	34.2	91.7	85.3	80.5
82	7.80	95%	32.9	54.1	3	1%	73%	96.4	37.5	92.7	86.4	80.8
83	6.05	69%	33.9	50.0	3	5%	76%	91.7	33.6	85.0	81.3	79.1
84	6.25	69%	33.5	50.0	3	5%	77%	91.4	35.1	85.0	80.9	78.6
85	4.83	69%	34.7	55.1	3	5%	77%	90.1	38.7	85.0	80.4	78.1
86	2.37	64%	37.4	50.0	3	5%	86%	90.1	34.9	85.1	79.4	76.5
89	2.28	68%	35.1	50.0	3	3%	80%	92.8	34.8	87.9	81.5	78.0
91	3.70	66%	35.0	54.9	3	1%	79%	95.6	37.2	91.1	83.9	79.1
92	5.39	100%	32.0	54.9	3	4%	77%	90.9	36.8	84.7	81.3	78.6
93	6.88	99%	30.6	53.9	3	6%	72%	89.9	36.4	84.5	80.9	78.7
94	5.94	70%	34.1	58.1	3	8%	74%	88.5	37.1	83.0	80.1	78.5
95	3.26	70%	34.8	50.0	3	8%	79%	88.0	34.7	83.0	80.1	78.2
98	6.96	100%	31.9	56.2	3	1%	72%	96.5	37.3	92.0	86.1	81.2
99	7.23	100%	34.8	55.5	3	4%	75%	91.7	37.5	85.7	81.9	79.1
100	8.64	67%	34.8	50.0	3	4%	73%	94.4	33.3	89.1	82.2	78.3
101	10.20	67%	34.7	53.6	3	3%	69%	94.3	36.1	88.9	81.6	77.7
102	10.60	69%	34.9	57.5	3	1%	69%	95.2	37.5	91.0	82.6	78.1
103	17.96	100%	32.2	50.0	3	1%	62%	96.1	35.7	91.6	83.8	78.8
104	17.52	100%	31.3	59.5	3	1%	63%	95.3	38.0	90.9	82.8	77.4
107	11.08	100%	35.4	50.0	3	1%	70%	99.1	41.5	94.5	88.7	81.6
108	11.33	100%	34.8	50.0	3	1%	69%	98.7	44.0	94.0	88.0	80.6
109	11.67	90%	35.8	50.0	3	1%	69%	98.4	44.1	94.0	88.0	80.4
110	11.46	90%	34.7	50.0	3	1%	70%	98.9	41.2	94.4	88.4	80.9
111	11.44	80%	35.9	50.0	3	1%	68%	99.3	41.5	96.1	88.9	82.4
113	11.64	60%	34.5	50.0	3	2%	64%	97.6	42.1	93.4	85.2	80.9
114	11.03	60%	33.0	61.1	3	2%	65%	96.1	48.3	90.8	83.2	78.4
117	14.89	90%	32.1	50.0	3	1%	63%	96.6	43.5	92.3	84.9	79.6
118	14.72	80%	31.9	50.0	3	1%	65%	95.8	43.0	91.5	84.2	79.1
119	16.08	80%	32.1	60.6	3	1%	65%	95.0	49.0	91.2	83.5	77.9
120	17.59	70%	32.3	50.0	3	1%	62%	96.4	43.9	92.6	84.6	78.7
121	18.37	70%	32.5	60.7	3	1%	63%	95.8	48.9	92.1	84.0	77.6
122	18.24	90%	30.8	60.9	3	1%	60%	95.6	49.2	92.2	84.1	77.8
123	20.62	60%	33.1	50.0	3	1%	60%	95.5	44.8	91.7	83.1	76.6
124	20.14	60%	32.8	61.3	3	1%	71%	94.3	49.3	90.9	81.6	75.7
125	11.14	60%	31.3	50.0	3	3%	65%	92.8	42.0	85.9	81.2	77.6
126	12.57	60%	30.0	61.0	3	3%	62%	92.0	48.9	84.6	79.9	76.9
127	9.79	80%	32.5	50.0	3	1%	72%	94.9	39.7	90.1	84.3	79.5
128	10.64	90%	32.4	50.0	3	1%	68%	95.8	40.4	91.3	85.1	80.0
129	11.20	90%	30.6	59.6	3	1%	68%	94.6	48.1	90.1	83.9	78.6
130	10.94	100%	32.4	50.0	3	1%	69%	95.1	40.7	90.6	84.5	79.4
135	6.71	60%	27.9	50.0	3	3%	75%	92.5	38.9	86.1	80.8	77.4
136	6.37	60%	27.4	58.5	3	3%	70%	91.0	47.4	84.2	79.3	76.4
140	12.58	80%	35.6	50.0	3	1%	70%	96.5	41.7	93.2	85.1	79.4
143	12.94	60%	34.5	50.0	3	1%	63%	96.9	42.2	93.5	85.2	79.5
145	8.05	70%	35.0	60.6	3	1%	67%	99.1	48.0	97.7	93.5	86.6
146	20.52	60%	33.1	50.0	3	1%	60%	96.2	45.6	92.4	83.8	77.6
147	20.95	70%	33.0	50.0	3	1%	55%	99.0	45.8	96.1	87.7	81.0
148	21.60	70%	32.2	61.4	3	1%	57%	98.5	49.6	95.2	87.0	80.1

				Data Reconcilliation						CHEMCAD INPUTS			
Exp No.	tray 4	tray 5	tray 6	alpha	beta	overall	MeOH	reconciled	reconciled	MeOH	water	feed	reflux
	temperature	temperature	temperature			material	material	bottom rate	distillate rate	flow rate	flow rate	temperature	rate
	(C)	(C)	(C)			balance	balance	(lb/hr)	(lb/hr)	(lb/hr)	(lb/hr)	(C)	(lb/hr)
4	71.0	70.4	69.3	-2.81	3.34	0.00	0.00	6.10	5.95	6.5356	5.5144	41.8	11.99
5	70.8	70.3	69.1	-2.71	3.37	0.00	0.00	6.12	5.84	6.4888	5.4732	41.5	14.00
6	70.8	70.2	70.0	-3.56	3.89	0.00	0.00	6.28	5.74	6.5193	5.5007	41.1	16.01
7	70.7	70.1	70.0	-2.07	2.93	0.00	0.00	6.92	5.02	6.3517	5.5883	40.9	20.00
8	71.2	70.5	69.1	1.43	4.75	0.00	0.00	5.11	6.84	6.3570	5.5930	50.0	30.00
13	70.2	69.7	68.5	-2.92	3.34	0.00	0.00	9.77	5.18	8.1085	6.8415	38.9	15.01
14	70.1	69.5	68.3	-1.98	2.21	0.00	0.00	10.90	4.12	7.1800	7.8400	39.7	18.01
15	70.2	69.6	68.4	-0.87	1.58	0.00	0.00	11.03	3.98	6.9980	7.9920	39.4	20.99
16	69.8	69.3	68.0	-3.69	4.15	0.00	0.00	9.60	5.45	8.1627	6.8873	39.0	25.00
17	69.8	69.3	68.0	-3.67	3.74	0.00	0.00	9.60	5.37	7.9636	7.0064	39.1	28.00
18	69.6	69.1	67.8	-2.58	3.33	0.00	0.00	9.60	5.21	8.1410	6.8890	39.5	28.00
19	69.8	69.3	68.0	-2.18	2.71	0.00	0.00	9.95	5.05	7.9795	7.0205	39.5	31.01
21	70.5	70.6	67.9	-0.07	0.98	0.00	0.00	9.34	4.35	7.4251	6.2649	39.6	10.00
22	69.7	69.2	68.0	-3.08	3.51	0.00	0.00	7.98	5.69	7.4142	6.2558	39.8	14.00
23	69.5	69.0	67.8	-2.68	3.14	0.00	0.00	8.30	5.33	7.3925	6.2375	40.0	16.01
24	69.3	68.8	67.6	-3.25	2.75	0.00	0.00	8.51	5.17	7.4197	6.2603	39.5	20.00
25	68.9	68.4	67.2	-3.24	4.86	0.00	0.00	12.00	5.98	9.7519	8.2281	38.3	24.01
26	70.1	69.5	68.2	-1.92	2.74	0.00	0.00	12.27	5.69	9.5542	8.4058	37.4	28.02
27	70.5	69.9	68.6	0.61	0.66	0.00	0.00	13.37	4.64	8.6093	9.4007	37.5	31.00
29	67.9	67.8	66.1	-1.18	1.49	0.00	0.00	8.23	1.79	4.9006	5.1194	46.3	10.00
30	68.7	68.8	66.5	-0.04	0.82	0.00	0.00	7.26	2.75	4.6731	5.3369	45.7	10.00
32	68.5	68.5	66.4	-0.57	1.23	0.00	0.00	10.55	1.50	5.7603	6.2897	43.0	12.00
33	69.0	69.1	66.8	0.14	0.95	0.00	0.00	9.20	2.75	5.8445	6.1055	43.1	10.01
34	72.9	72.3	71.2	-3.39	3.78	0.00	0.00	10.17	7.82	9.5701	8.4199	38.6	10.00
35	70.6	70.1	68.9	0.58	4.73	0.00	0.00	8.85	9.09	9.7302	8.2098	41.2	13.99
36	70.8	70.2	68.9	5.00	5.84	0.00	0.00	8.85	9.08	8.5711	9.3589	49.8	16.00
37	70.7	70.1	68.8	4.90	5.84	0.00	0.00	8.91	9.03	8.3752	9.5648	49.5	20.00
38	70.9	70.3	69.0	0.10	1.05	0.00	0.00	4.82	5.21	4.9055	5.1245	45.9	21.00
39	70.8	70.2	68.9	-0.14	0.96	0.00	0.00	4.77	5.22	4.7755	5.2145	46.2	25.01
40	70.7	70.1	68.8	0.06	0.98	0.00	0.00	4.77	5.22	4.7755	5.2145	46.5	28.00
41	70.6	70.1	68.8	-0.28	1.56	0.00	0.00	4.37	5.67	5.2353	4.8047	46.7	17.99
42	70.7	70.1	68.9	-0.57	0.50	0.00	0.00	4.45	5.57	5.2248	4.7952	47.1	15.00
43	70.9	70.3	69.1	-0.68	1.74	0.00	0.00	4.57	5.46	5.1232	4.9068	46.1	12.01
73	75.2	73.9	71.4	-2.04	1.58	0.00	0.00	14.54	9.46	8.0152	15.9848	33.9	30.00
75	72.7	71.5	69.3	-3.51	2.12	0.00	0.00	19.61	10.40	9.6307	20.3793	33.2	59.97
76	74.5	73.6	71.7	-3.33	1.70	0.00	0.00	18.62	11.36	10.3983	19.5817	31.7	36.01
77	75.6	74.7	73.0	-3.81	2.09	0.00	0.00	19.13	10.89	10.4122	19.6078	33.9	15.00
78	73.7	72.8	71.0	-3.30	1.88	0.00	0.00	16.06	7.92	8.3173	15.6627	32.6	19.83
79	72.9	71.9	70.0	-3.30	1.79	0.00	0.00	15.53	8.47	8.3242	15.6758	31.9	26.43
80	72.3	71.2	69.0	-3.16	1.32	0.00	0.00	15.51	8.51	7.7084	16.3116	34.5	37.12
81	74.3	73.2	71.0	-3.50	2.11	0.00	0.00	14.73	9.27	8.3242	15.6758	32.9	23.68
82	73.9	72.6	70.0	-1.92	0.39	0.00	0.00	15.80	8.19	7.0600	16.9300	32.9	51.71
83	73.8	72.9	71.0	-2.45	0.93	0.00	0.00	17.02	6.98	7.3846	16.6154	33.9	21.74
84	72.9	71.9	70.0	-2.80	0.67	0.00	0.00	17.08	6.92	7.3846	16.6154	33.5	33.79
85	71.5	70.4	68.3	-3.80	1.25	0.00	0.00	17.92	6.08	6.7368	17.2632	34.7	79.72
86	70.5	69.6	68.0	-1.91	1.40	0.00	0.00	11.25	3.77	4.4202	10.5998	37.4	14.09
89	72.0	70.9	69.0	-2.38	2.37	0.00	0.00	10.35	4.65	4.6154	10.3846	35.1	19.24
91	71.4	70.2	68.1	-2.50	0.66	0.00	0.00	10.61	4.38	4.0013	10.9887	35.0	79.31
92	71.4	70.2	68.0	-4.24	1.62	0.00	0.00	22.97	7.01	7.5839	22.3961	32.0	80.04
93	72.7	71.6	69.5	-4.14	1.72	0.00	0.00	21.42	8.60	9.2369	20.7631	30.8	59.99
94	72.6	71.5	69.3	-3.17	0.92	0.00	0.00	23.14	6.86	8.8287	21.1713	34.1	79.96
95	73.0	72.0	70.2	-3.70	2.16	0.00	0.00	24.58	5.42	8.0079	21.9921	34.8	20.00
98	73.7	72.2	69.3	-3.27	0.90	0.00	0.00	16.12	7.88	6.7312	17.2488	31.9	80.01
99	72.4	71.2	68.8	-4.13	0.99	0.00	0.00	21.78	8.22	8.4211	21.5789	34.8	80.02
100	74.6	73.7	72.1	-1.02	0.78	0.00	0.00	11.59	9.40	8.5799	12.4101	34.8	15.00
101	73.9	72.9	71.1	-0.42	-0.18	0.00	0.00	10.95	10.02	8.5717	12.3983	34.7	44.99
102	73.6	72.5	70.2	-0.32	-0.07	0.00	0.00	10.48	10.53	8.5880	12.4220	34.9	79.97
103	77.3	76.8	75.2	1.49	-0.84	0.00	0.00	12.84	17.12	12.9557	17.0043	32.2	14.99
104	75.2	74.2	71.9	2.09	-1.52	0.00	0.00	14.02	16.00	12.2709	17.7491	31.3	60.02
107	77.5	76.6	74.3	-0.85	1.55	0.00	0.00	11.37	12.63	10.3784	13.6216	35.4	15.75
108	76.0	74.7	72.2	-0.69	1.43	0.00	0.00	11.25	12.76	10.3827	13.6273	34.8	31.01
109	75.8	74.6	72.0	0.07	0.70	0.00	0.00	11.59	12.37	10.0793	13.8807	35.8	28.93
110	77.1	76.1	73.8	-0.10	0.86	0.00	0.00	11.76	12.32	10.1382	13.9618	34.7	15.67
111	76.3	77.2	74.7	-1.01	2.49	0.00	0.00	10.04	13.93	11.1902	12.7798	35.9	15.71
113	77.6	76.7	75.0	-1.00	1.51	0.00	0.00	10.82	13.15	10.3654	13.6046	34.5	15.66
114	74.8	73.5	71.3	-1.07	1.97	0.00	0.00	10.96	13.00	10.3611	13.5989	33.0	61.90
117	77.6	76.6	74.8	-0.03	0.57	0.00	0.00	14.48	15.46	11.8770	18.0630	32.1	15.70
118	76.8	75.9	74.0	0.06	-0.09	0.00	0.00	15.28	14.63	11.4996	18.4104	31.9	15.82
119	74.7	73.3	70.4	2.46	-1.44	0.00	0.00	15.28	14.64	11.5034	18.4166	32.1	61.71
120	77.0	76.2	74.5	2.08	-1.48	0.00	0.00	13.81	16.13	12.2382	17.7018	32.3	15.75
121	75.0	73.7	71.0	3.79	-2.42	0.00	0.00	13.99	15.95	12.2382	17.7018	32.5	61.78
122	75.3	73.9	71.1	2.34	-1.73	0.00	0.00	13.45	16.51	12.2464	17.7136	30.6	61.80
123	76.0	75.4	74.2	4.70	-4.11	0.00	0.00	13.44	16.51	12.2423	17.7077	33.1	15.81
124	74.0	73.2	71.1	7.53	-5.41	0.00	0.00	15.23	14.73	12.2464	17.7136	32.8	61.78
125	75.7	74.9	73.5	-0.89	0.66	0.00	0.00	18.16	11.80	10.0056	19.9544	31.3	15.92
126	73.8	72.9	70.8	0.57	-0.93	0.00	0.00	18.31	11.64	9.6115	20.3385	30.0	61.77
127	74.8	74.0	71.6	-1.46	1.03	0.00	0.00	19.13	10.82	9.2154	20.7346	32.5	16.26
128	76.1	75.2	73.1	-1.63	1.11	0.00	0.00	18.20	11.75	9.6115	20.3385	32.4	16.01
129	73.6	72.2	69.4	-0.79	0.55	0.00	0.00	18.20	11.75	9.6115	20.3385	30.6	61.64
130	75.8	74.9	72.7	-0.73	0.20	0.00	0.00	18.83	11.14	9.2215	20.7485	32.4	16.08
135	73.6	72.5	70.9	-0.76	0.64	0.00	0.00	16.62	7.35	7.0541	16.9159	27.9	16.40
136	71.4	70.2	68.1	-2.20	1.31	0.00	0.00	16.23	7.68	7.0364	16.8736	27.4	61.51
140	76.2	75.1	72.8	2.45	-0.68	0.00	0.00	12.08	11.90	9.8029	14.1780	35.6	16.07
143	77.5	76.5	74.8	1.31	-0.97	0.00	0.00	11.98	11.97	9.2081	14.7419	34.5	15.68
145	86.6	80.0	70.5	0.52	0.28	0.00	0.00	6.63	8.33	6.6429	6.3171	35.0	61.61
146	76.9	76.3	75.1	4.68	-3.50	0.00	0.00	12.94	17.02	12.6033	17.3567	33.1	15.65
147	80.1	79.4	77.7	2.00	-0.78	0.00	0.00	9.79	20.17	13.9866	15.9734	33.0	15.14
148	78.3	77.2	74.6	4.04	-2.44	0.00	0.00	10.79	19.16	13.6427	16.3073	32.2	61.14

	CHEMCAD INPUTS			CHEMCAD OUTPUTS										
Exp No.	bottom	reflux T	Sub Cooled	feed	feed	reflux	bottom	distillate	reboiler	feed	reflux	feed	bottom	distillate
	rate	temperature	temperature	rate	composition	rate	rate	rate	duty	temperature	temperature	tray	composition	composition
	(lb/hr)	(C)	(C)	(lb/hr)	(mol% meOH)	(lb/hr)	(lb/hr)	(lb/hr)	(MMBtu/hr)	(C)	(C)		(mol% meOH)	(mol% meOH)
4	6.10	50.0	16.0	12.05	40%	11.99	6.10	5.95	0.010064	41.8	50.4	3	10.1%	87.9%
5	6.12	50.0	16.0	11.96	40%	14.00	6.12	5.84	0.011133	41.5	50.5	3	11.0%	86.9%
6	6.28	50.0	17.0	12.02	40%	16.01	6.28	5.74	0.012180	41.1	49.5	3	12.0%	86.9%
7	6.92	50.0	17.0	11.94	39%	20.00	6.92	5.02	0.014022	40.9	49.7	3	16.0%	85.9%
8	5.11	50.1	17.0	11.95	39%	30.00	5.11	6.84	0.020765	50.0	50.3	3	3.0%	82.0%
13	9.77	49.9	16.0	14.95	40%	15.01	9.77	5.18	0.011370	38.9	50.2	3	22.0%	89.0%
14	10.90	50.0	16.0	15.02	34%	16.01	10.90	4.12	0.012527	39.7	50.3	3	20.0%	88.1%
15	11.03	50.0	17.0	14.99	33%	20.99	11.03	3.96	0.014306	39.4	49.8	3	20.0%	85.2%
16	9.60	50.0	17.0	15.05	40%	25.00	9.60	5.45	0.017200	39.0	49.8	3	21.9%	85.1%
17	9.60	50.1	17.0	14.97	39%	28.00	9.60	5.37	0.018803	39.1	49.8	3	21.0%	85.0%
18	9.80	50.0	17.0	15.01	40%	28.00	9.80	5.21	0.018677	39.5	49.8	3	23.0%	85.2%
19	9.95	50.0	17.0	15.00	39%	31.01	9.95	5.05	0.020471	39.5	50.1	3	22.9%	83.2%
21	9.34	50.0	16.0	13.69	40%	10.00	9.34	4.35	0.008215	39.6	50.2	3	24.0%	89.1%
22	7.98	50.0	16.0	13.67	40%	14.00	7.98	5.69	0.011079	39.8	50.3	3	16.9%	88.1%
23	8.30	50.0	16.0	13.63	40%	16.01	8.30	5.33	0.011956	40.0	50.3	3	19.0%	88.0%
24	8.51	50.0	16.0	13.68	40%	20.00	8.51	5.17	0.013994	39.5	50.3	3	20.0%	88.1%
25	12.00	50.0	16.0	17.98	40%	24.01	12.00	5.98	0.016705	38.3	50.2	3	23.0%	89.0%
26	12.27	50.0	16.0	17.96	39%	26.02	12.27	5.69	0.019786	37.4	49.6	3	25.0%	80.1%
27	13.37	50.0	16.0	18.01	34%	31.00	13.37	4.64	0.021341	37.5	50.1	3	23.0%	77.1%
29	8.23	50.0	15.0	10.02	35%	10.00	8.23	1.79	0.006414	46.3	50.3	3	26.0%	94.9%
30	7.26	50.0	16.0	10.01	33%	10.00	7.26	2.75	0.007007	45.7	49.6	3	18.0%	93.1%
32	10.55	50.0	15.0	12.05	34%	12.00	10.55	1.50	0.007480	43.0	50.4	3	26.0%	94.1%
33	9.20	50.0	15.0	11.95	35%	10.01	9.20	2.75	0.007079	43.1	50.4	3	23.0%	94.0%
34	10.17	50.0	16.0	17.99	39%	10.00	10.17	7.82	0.010899	36.6	49.7	3	17.0%	80.0%
35	8.85	50.0	17.0	17.94	40%	13.99	8.85	9.09	0.013309	41.2	49.8	3	10.0%	85.0%
36	8.85	50.0	17.0	17.93	34%	16.00	8.85	9.08	0.014345	49.8	49.8	3	2.0%	85.0%
37	8.91	50.0	17.0	17.94	33%	20.00	8.91	9.03	0.016527	49.5	49.8	3	1.0%	85.0%
38	4.82	50.0	17.0	10.03	35%	21.00	4.82	5.21	0.014668	45.9	49.8	3	2.0%	85.0%
39	4.77	50.0	17.0	9.99	34%	25.01	4.77	5.22	0.017261	46.2	50.5	3	1.9%	81.1%
40	4.77	50.0	17.0	9.99	34%	28.00	4.77	5.22	0.018939	46.5	50.5	3	2.0%	80.9%
41	4.37	50.0	17.0	10.04	38%	17.99	4.37	5.67	0.013413	46.7	50.2	3	2.0%	82.9%
42	4.45	50.0	17.0	10.02	38%	15.00	4.45	5.57	0.011563	47.1	49.8	3	2.0%	85.0%
43	4.57	50.0	17.0	10.03	37%	12.01	4.57	5.46	0.009917	46.1	49.9	3	2.0%	84.9%
73	14.54	50.0	19.0	24.00	22%	30.00	14.54	9.46	0.025246	33.9	50.0	3	1.0%	72.0%
75	19.61	53.8	15.0	30.01	21%	59.97	19.61	10.40	0.043371	33.2	53.8	3	2.9%	73.3%
76	18.62	52.8	17.0	29.98	23%	38.01	18.62	11.36	0.031321	31.7	53.0	3	4.9%	66.2%
77	19.13	50.0	19.0	30.02	23%	15.00	19.13	10.89	0.017746	33.9	50.4	3	5.0%	69.8%
78	16.06	50.0	18.0	23.98	23%	19.83	16.06	7.92	0.012378	32.8	49.7	3	5.0%	79.9%
79	15.53	50.0	18.0	24.00	23%	28.43	15.53	8.47	0.021812	31.9	50.1	3	3.9%	77.2%
80	15.51	49.6	19.0	24.02	21%	28.43	15.53	8.49	0.022135	34.5	49.5	3	2.0%	75.2%
81	14.73	50.9	18.0	24.00	23%	23.68	14.73	9.27	0.020952	32.9	50.5	3	2.0%	75.2%
82	15.80	54.1	15.0	23.99	19%	51.71	15.80	8.19	0.036991	32.9	53.8	3	1.0%	73.1%
83	17.02	50.0	18.0	24.00	20%	21.74	17.02	6.98	0.018388	33.9	50.3	3	4.9%	76.3%
84	17.08	50.0	18.0	24.00	20%	33.79	17.08	6.92	0.025139	33.5	50.1	3	4.9%	77.3%
85	17.92	55.1	13.0	24.00	18%	79.72	17.92	6.08	0.050402	34.7	55.1	3	5.0%	77.2%
86	11.25	50.0	17.0	15.02	19%	14.09	11.25	3.77	0.010781	37.4	49.7	3	5.0%	86.0%
89	10.35	50.0	18.0	15.00	20%	19.24	10.35	4.65	0.014585	35.1	49.6	3	3.0%	80.2%
91	10.61	54.9	13.0	14.99	17%	79.31	10.61	4.38	0.048086	35.0	54.8	3	1.1%	78.8%
92	22.97	54.9	13.0	29.98	16%	80.04	22.97	7.01	0.051943	32.0	55.2	3	4.0%	76.9%
93	21.42	53.9	15.0	30.02	20%	59.99	21.42	8.60	0.042708	30.8	54.0	3	6.0%	72.2%
94	23.14	56.1	12.0	30.00	19%	79.96	23.14	6.86	0.052207	34.1	56.6	3	8.0%	74.4%
95	24.58	50.0	18.0	30.00	17%	20.00	24.58	5.42	0.016784	34.8	49.8	3	8.0%	78.9%
98	16.12	56.2	13.0	23.98	18%	80.01	16.12	7.86	0.053659	31.9	56.0	3	1.0%	71.9%
99	21.78	55.5	13.0	30.00	16%	80.02	21.78	8.22	0.053002	34.0	55.5	3	4.0%	75.2%
100	11.59	50.0	19.0	20.99	28%	15.00	11.59	9.40	0.015733	34.8	49.6	3	4.0%	73.1%
101	10.95	53.6	16.0	20.97	28%	44.99	10.95	10.02	0.034415	34.7	53.5	3	3.0%	69.0%
102	10.48	57.5	12.0	21.01	28%	79.97	10.48	10.53	0.055327	34.9	57.5	3	1.0%	69.0%
103	12.84	50.0	21.0	29.96	30%	14.99	17.12	12.84	0.022381	32.2	49.8	3	1.0%	62.0%
104	14.02	59.5	11.0	30.02	28%	80.02	14.02	16.00	0.062047	31.3	59.8	3	1.6%	61.9%
107	11.37	50.0	19.0	24.00	30%	15.75	11.37	12.63	0.018581	35.4	50.4	3	1.0%	70.0%
108	11.25	50.0	20.0	24.01	30%	31.01	11.25	12.76	0.028034	34.8	49.5	3	1.0%	69.0%
109	11.59	50.0	20.0	23.96	29%	28.93	11.59	12.37	0.026517	35.8	49.5	3	1.0%	69.1%
110	11.78	50.0	19.0	24.10	29%	15.87	11.78	12.32	0.018529	34.7	50.4	3	1.0%	70.0%
111	10.04	50.0	20.0	23.97	33%	15.71	10.04	13.93	0.019459	35.9	49.7	3	1.0%	68.0%
113	10.82	50.0	20.0	23.97	30%	15.66	10.82	13.15	0.019522	34.5	50.4	3	2.0%	64.0%
114	10.96	61.1	9.0	23.96	30%	81.90	10.96	13.00	0.059234	33.0	61.2	3	1.9%	65.2%
117	14.48	50.0	21.0	29.94	27%	15.70	14.48	15.46	0.021784	32.1	49.6	3	1.0%	63.0%
118	15.28	50.0	20.0	29.91	26%	15.82	15.28	14.63	0.021133	31.9	50.2	3	1.0%	65.0%
119	15.28	60.6	10.0	29.92	26%	81.71	15.28	14.64	0.061021	32.1	60.3	3	1.0%	64.9%
120	13.81	50.0	21.0	29.94	28%	15.75	13.81	16.13	0.022309	32.3	49.8	3	1.0%	62.1%
121	13.99	60.7	10.0	29.94	28%	81.76	13.99	15.95	0.062485	32.5	60.6	3	0.9%	63.1%
122	13.45	60.9	10.0	29.96	28%	81.80	13.45	16.51	0.064200	30.6	61.2	3	1.0%	60.0%
123	13.44	50.0	21.0	29.95	28%	15.81	13.44	16.51	0.022611	33.1	50.2	3	0.9%	60.1%
124	15.23	61.3	8.0	29.96	28%	81.78	15.23	14.73	0.058446	32.8	61.2	3	1.0%	71.1%
125	18.16	50.0	20.0	29.96	22%	15.92	18.16	11.80	0.019573	31.3	50.2	3	3.0%	65.1%
126	18.31	61.0	10.0	29.95	21%	81.77	18.31	11.64	0.060533	30.0	60.6	3	3.0%	62.1%
127	19.13	50.0	19.0	29.95	20%	16.26	19.13	10.82	0.018547	32.5	50.2	3	1.0%	72.1%
128	18.20	50.0	20.0	29.95	21%	16.01	18.20	11.75	0.019345	32.4	49.7	3	1.0%	68.1%
129	18.20	59.6	10.0	29.95	21%	81.64	18.20	11.75	0.058346	30.6	59.7	3	1.0%	68.0%
130	18.83	50.0	20.0	29.97	20%	16.08	18.83	11.14	0.018968	32.4	49.5	3	1.0%	69.0%
135	16.62	50.0	18.0	23.97	19%	16.40	16.62	7.35	0.015954	27.9	50.5	3	3.0%	74.9%
136	16.23	58.5	11.0	23.91	19%	81.51	16.23	7.68	0.054861	27.4	58.4	3	3.0%	69.9%
140	12.08	50.0	19.0	23.98	28%	18.07	12.08	11.90	0.018389	35.6	50.4	3	1.0%	70.0%
143	11.98	50.0	21.0	23.95	26%	15.68	11.98	11.97	0.019085	34.5	49.6	3	1.0%	63.1%
145	6.63	60.6	9.0	14.96	31%	81.81	6.63	8.33	0.055038	35.0	60.9	3	1.1%	66.9%
146	12.94	50.0	21.0	29.96	29%	15.65	12.94	17.02	0.022995	33.1	50.2	3	0.9%	60.0%
147	9.79	50.0	22.0	29.96	33%	15.14	9.79	20.17	0.025275	33.0	50.1	3	1.0%	55.0%
148	10.79	61.4	10.0	29.95	32%	81.14	10.79	19.16	0.066528	32.2	61.7	3	1.0%	57.0%

	CHEMCAD OUTPUTS												
Exp No.	reboiler	distillate	tray 1	tray 2	tray 3	tray 4	tray 5	tray 6	tray				
	temperature	temperature	temperature	temperature	temperature	temperature	temperature	temperature	efficiency				
	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)					
4	87.6	50.4	77.8	75.4	74.0	70.8	68.9	67.5	0.51				
5	87.0	50.5	77.1	75.0	73.7	70.5	68.8	67.5	0.46				
6	86.2	49.5	76.5	74.6	73.3	70.2	68.7	67.5	0.44				
7	83.8	49.7	74.9	73.5	72.6	69.8	68.4	67.5	0.37				
8	95.0	50.3	83.8	78.7	75.5	72.4	70.2	68.5	0.44				
13	81.0	50.2	74.3	73.3	72.7	69.2	68.0	67.0	0.44				
14	81.9	50.3	74.8	73.9	73.2	69.3	68.0	67.1	0.42				
15	81.9	49.8	74.6	73.7	73.1	69.5	68.4	67.5	0.34				
16	81.0	49.8	73.5	72.6	72.0	69.2	68.2	67.5	0.31				
17	81.4	49.8	73.6	72.7	72.0	69.2	68.2	67.5	0.31				
18	80.6	49.8	73.2	72.4	71.7	69.0	68.1	67.4	0.30				
19	80.6	50.1	73.0	72.3	71.7	69.2	68.4	67.7	0.26				
21	80.2	50.2	74.4	73.6	73.1	69.5	68.1	67.0	0.46				
22	83.3	50.3	75.3	74.0	73.1	69.8	68.3	67.2	0.45				
23	82.3	50.3	74.6	73.5	72.7	69.4	68.1	67.1	0.42				
24	81.9	50.3	74.1	73.0	72.2	69.1	68.0	67.1	0.40				
25	80.6	50.2	73.7	72.8	72.1	68.9	67.7	66.9	0.41				
26	79.9	49.6	73.0	72.5	72.1	69.4	68.8	68.2	0.20				
27	80.8	50.1	73.5	73.0	72.7	69.8	69.2	68.6	0.17				
29	79.5	50.3	74.2	73.2	72.7	68.4	66.8	65.9	0.69				
30	82.8	49.6	75.6	74.4	73.6	69.2	67.5	66.3	0.64				
32	78.8	50.4	74.0	73.2	72.6	68.3	66.9	66.0	0.62				
33	80.6	50.4	75.0	73.9	73.3	68.9	67.2	66.1	0.68				
34	83.3	49.7	75.9	75.1	74.5	71.6	70.1	68.8	0.30				
35	87.7	49.6	78.0	76.0	74.6	71.7	69.7	68.1	0.46				
36	96.5	49.8	88.2	82.0	78.0	74.4	71.1	68.6	0.61				
37	96.1	49.8	92.2	84.9	79.3	75.1	71.3	68.7	0.64				
38	96.6	49.8	87.3	80.7	76.5	72.6	70.0	68.1	0.53				
39	96.6	50.5	87.1	81.0	76.9	73.3	70.7	68.6	0.46				
40	96.5	50.5	86.7	80.7	76.7	73.1	70.6	68.6	0.45				
41	96.5	50.2	87.0	80.8	76.7	73.3	70.6	68.6	0.50				
42	96.5	49.8	87.3	80.8	76.7	73.1	70.3	68.3	0.55				
43	96.5	49.8	87.7	81.2	77.2	73.6	70.6	68.4	0.57				
73	98.2	50.0	92.5	87.2	82.5	78.0	74.0	71.1	0.44				
75	95.1	53.8	85.0	81.2	78.5	74.3	71.9	70.2	0.35				
76	92.5	53.0	82.1	80.1	78.5	74.9	73.0	71.4	0.25				
77	92.4	50.4	83.6	81.5	80.0	76.7	73.8	71.4	0.33				
78	92.4	49.7	84.2	81.4	79.6	75.7	72.4	69.7	0.51				
79	93.7	50.1	84.1	80.7	78.5	74.0	71.5	69.6	0.40				
80	96.5	49.5	88.5	83.9	80.6	75.9	72.7	70.3	0.43				
81	96.6	50.5	88.7	84.0	80.6	76.3	72.9	70.4	0.44				
82	98.2	53.8	92.0	86.3	81.5	76.3	72.9	70.8	0.42				
83	92.5	50.3	83.3	80.7	79.0	74.0	71.6	69.7	0.38				
84	92.5	50.1	82.4	79.7	77.8	73.1	71.0	69.4	0.37				
85	92.5	55.1	81.0	78.1	76.0	72.2	70.5	69.1	0.34				
86	92.4	49.7	83.5	80.2	78.3	72.4	69.8	68.0	0.55				
89	95.1	49.6	86.0	81.8	78.9	73.8	71.0	69.1	0.46				
91	98.1	54.8	90.8	83.9	78.6	73.9	71.1	69.2	0.45				
92	93.7	55.2	82.9	79.5	77.1	72.7	70.8	69.3	0.36				
93	91.4	54.0	80.5	78.5	76.9	73.0	71.4	70.1	0.28				
94	89.4	56.6	78.5	76.8	75.5	71.9	70.6	69.5	0.27				
95	89.4	49.8	81.6	80.1	79.0	72.9	70.8	69.1	0.39				
98	98.1	56.0	91.3	85.4	80.6	75.8	72.8	70.6	0.39				
99	93.7	55.5	82.8	79.5	77.2	73.1	71.1	69.6	0.34				
100	93.7	49.8	84.1	81.1	78.9	76.0	73.1	70.7	0.37				
101	95.0	53.5	84.2	80.6	78.0	74.9	72.7	70.9	0.30				
102	98.2	57.5	91.2	85.1	80.3	76.4	73.4	71.2	0.36				
103	98.1	49.8	92.3	87.1	82.5	84.5	79.9	75.0	0.43				
104	97.2	59.8	88.3	83.7	80.2	77.2	74.5	72.5	0.28				
107	98.1	50.4	92.4	86.8	82.0	81.2	76.5	72.5	0.48				
108	98.2	49.5	91.8	86.2	81.5	78.7	74.7	71.8	0.40				
109	98.2	49.5	92.2	86.7	81.9	79.0	74.9	71.8	0.41				
110	98.1	50.4	92.4	86.9	82.2	81.2	76.5	72.5	0.48				
111	98.2	49.7	92.4	86.6	81.7	81.9	77.2	73.0	0.46				
113	96.5	50.4	88.1	84.0	80.9	80.4	76.4	73.1	0.34				
114	96.7	51.2	86.9	82.3	78.9	76.0	73.6	71.7	0.29				
117	98.2	49.6	92.7	87.7	83.2	84.2	79.3	74.5	0.44				
118	98.2	50.2	92.8	87.8	83.3	83.7	78.7	74.0	0.46				
119	98.1	50.3	91.1	85.7	81.2	77.5	74.4	72.1	0.33				
120	98.2	49.8	92.7	87.6	83.1	84.5	79.7	74.8	0.43				
121	98.2	50.6	91.4	86.1	81.5	78.1	74.9	72.4	0.32				
122	98.2	51.2	91.1	86.0	81.8	78.6	75.4	73.0	0.29				
123	98.2	50.2	92.7	87.7	83.2	85.1	80.2	75.2	0.41				
124	98.2	51.2	91.5	85.5	80.5	76.5	73.2	70.9	0.39				
125	95.1	50.2	86.7	83.8	81.6	79.2	75.6	72.6	0.33				
126	95.1	50.8	84.2	81.2	78.9	75.7	73.7	72.1	0.24				
127	98.2	50.0	93.6	88.8	84.4	81.9	78.6	72.2	0.55				
128	98.2	49.7	93.4	88.7	84.4	83.0	77.7	73.2	0.50				
129	98.1	59.7	91.5	86.0	81.4	78.9	73.8	71.4	0.36				
130	98.2	49.5	93.5	88.9	84.6	82.7	77.4	72.9	0.51				
135	95.0	50.5	86.9	83.5	81.1	78.3	73.0	70.4	0.43				
136	95.0	58.4	84.1	80.4	77.8	74.2	72.2	70.6	0.30				
140	98.1	50.4	92.6	87.2	82.5	81.2	76.4	72.4	0.48				
143	98.2	49.6	92.8	87.9	83.5	83.2	78.2	73.9	0.41				
145	98.1	60.9	90.3	84.4	79.8	76.3	73.5	71.5	0.33				
146	98.2	50.2	92.6	87.5	83.0	85.1	80.3	75.3	0.41				
147	98.1	50.1	91.7	86.6	82.2	86.1	81.7	76.6	0.35				
148	98.2	61.7	90.8	85.9	81.8	79.3	76.1	73.7	0.27				

APPENDIX F

HYBRID PARALLEL MODELING DATA SET

The data set is on one large spread sheet. It is divided into 16 pages as follows (the number in each of the box correspond to page number):

106	107	108	109	110	111	112	113
114	115	116	117	118	119	120	121

		Data Used for Hybrid Parallel Modeling									
No.	original file name	feed	feed	feed	reflux	reflux	reboiler	tray1	tray2	tray3	tray4
		rate	composition	temperature	rate	temperature	temperature	temperature	temperature	temperature	temperature
		(lb/hr)	(mol% MeOH)	(C)	(lb/hr)	(C)	(C)	(C)	(C)	(C)	(C)
4	ex990416_ss1	12.05	40	41.8	11.99	50.0	89.8	82.1	77.8	75.7	71.0
5	ex990416_ss2	11.96	40	41.5	14.00	50.0	89.0	81.5	77.7	75.8	70.8
6	ex990416_ss3	12.02	40	41.1	16.01	50.0	88.5	81.4	77.8	75.9	70.8
7	ex990417_ss1	11.94	39	40.9	20.00	50.0	87.0	77.4	80.9	75.9	70.7
8	ex990417_ss2	11.95	39	50.0	30.00	50.1	97.9	91.8	82.2	77.2	71.2
13	ex990430_ss1	14.95	40	38.9	15.01	49.9	83.7	78.6	76.3	75.2	70.2
14	ex990430_ss2	15.02	34	39.7	18.01	50.0	83.5	78.4	76.1	75.1	70.1
15	ex990430_ss3	14.99	33	39.4	20.99	50.0	83.8	78.5	76.1	75.1	70.2
16	ex990501_ss1	15.05	40	39.0	25.00	50.0	83.2	78.1	75.9	74.9	69.8
17	ex990501_ss2	14.97	39	39.1	28.00	50.1	82.9	78.1	75.9	74.9	69.8
18	ex990511_ss1	15.01	40	39.5	28.00	50.0	82.7	77.7	75.6	74.7	69.6
19	ex990511_ss2	15.00	39	39.5	31.01	50.0	82.8	77.8	75.7	74.7	69.8
21	ex990514_ss1	13.89	40	39.6	10.00	50.0	83.9	78.7	76.4	75.2	70.5
22	ex990514_ss2	13.67	40	39.8	14.00	50.0	84.3	78.9	76.1	74.8	69.7
23	ex990514_ss3	13.63	40	40.0	16.01	50.0	84.2	78.5	75.9	74.6	69.5
24	ex990514_ss4	13.68	40	39.5	20.00	50.0	83.1	78.1	75.3	74.1	69.3
25	ex990515_ss1	17.98	40	38.3	24.01	50.0	82.2	77.4	75.1	74.0	68.9
26	ex990515_ss2	17.96	39	37.4	28.02	50.0	81.2	76.8	75.0	74.2	70.1
27	ex990515_ss3	18.01	34	37.5	31.00	50.0	81.6	77.0	75.0	74.2	70.5
29	ex990516_ss2	10.02	35	46.3	10.00	50.0	80.4	75.4	73.8	72.3	67.9
30	ex990516_ss3	10.01	33	45.7	10.00	50.0	83.5	77.8	74.8	73.2	68.7
32	ex990517_ss2	12.05	34	43.0	12.00	50.0	80.4	75.8	72.8	68.3	68.5
33	ex990517_ss3	11.95	35	43.1	10.01	50.0	81.4	77.1	74.7	73.5	69.0
34	ex990519_ss1	17.99	39	38.6	10.00	50.0	85.1	79.6	77.1	76.1	72.9
35	ex990522_ss1	17.94	40	41.2	13.99	50.0	88.4	81.1	76.5	74.4	70.6
36	ex990522_ss2	17.93	34	49.8	16.00	50.0	96.8	91.3	81.1	76.3	70.8
37	ex990522_ss3	17.94	33	49.5	20.00	50.0	97.1	91.8	81.5	76.3	70.7
38	ex990523_ss1	10.03	35	45.9	21.00	50.0	96.0	90.0	80.5	75.7	70.9
39	ex990523_ss2	9.99	34	46.2	25.01	50.0	96.2	90.5	80.7	75.7	70.8
40	ex990523_ss3	9.99	34	46.5	28.00	50.0	96.2	90.4	80.6	75.6	70.7
41	ex990525_ss1	10.04	38	46.7	17.99	50.0	95.5	89.1	79.9	75.4	70.6
42	ex990525_ss2	10.02	38	47.1	15.00	50.0	95.7	89.1	79.9	75.3	70.7
43	ex990529_ss1	10.03	37	48.1	12.01	50.0	95.3	89.0	80.2	75.8	70.9
44	ex990614_ss2	14.97	27	49.7	15.00	50.0	98.8	94.8	85.8	79.2	72.3
45	ex990618_ss1	11.99	19	40.8	12.00	50.0	99.4	99.9	98.2	93.9	92.9
46	ex990618_ss2	11.99	19	41.1	18.00	50.0	99.5	100.2	98.7	94.3	90.5
47	ex990618_ss3	11.98	19	41.6	24.00	50.0	99.3	100.1	98.6	94.3	91.0
48	ex990618_ss4	12.00	18	41.5	29.99	50.0	99.1	99.9	98.4	94.2	91.2
49	ex990619_ss1	14.99	20	38.9	12.00	50.0	99.1	99.3	96.7	90.9	88.9
50	ex990619_ss2	14.98	19	49.1	18.00	50.0	99.3	100.1	99.1	95.5	91.3
51	ex990619_ss3	14.97	19	50.0	24.00	50.0	99.2	100.0	99.0	95.5	91.2
52	ex990619_ss4	15.00	18	50.4	30.01	50.0	98.9	99.7	98.8	95.3	91.4
53	ex990623_ss1	17.99	20	46.1	11.99	50.0	99.0	99.6	98.5	94.8	94.3
54	ex990623_ss2	17.98	19	46.4	18.01	50.0	99.1	99.7	98.4	93.6	88.5
55	ex990623_ss3	18.01	19	48.0	24.00	50.0	99.0	99.6	98.3	94.1	89.7
56	ex990626_ss1	18.01	20	36.5	29.99	50.0	98.8	98.6	95.3	89.2	85.3
57	ex990626_ss2	17.97	23	36.7	36.01	50.0	98.3	98.1	94.2	87.7	83.7
58	ex990626_ss3	18.05	23	36.7	51.00	52.2	98.8	97.7	94.1	87.7	84.3
59	ex990627_ss1	15.00	24	39.6	36.00	50.0	99.6	98.7	95.7	90.6	86.9
60	ex990627_ss2	14.73	20	39.1	45.02	51.0	99.1	97.9	94.5	88.8	85.1
61	ex990627_ss3	15.00	20	38.9	54.01	52.7	98.6	97.8	94.7	89.3	84.5
62	ex990628_ss1	12.01	20	42.7	11.36	50.0	99.5	98.0	93.8	86.8	79.1
63	ex990629_ss1	11.99	20	42.3	12.00	50.0	99.0	98.9	95.8	90.0	84.0
64	ex990629_ss2	11.98	20	42.8	23.99	50.0	99.6	98.8	96.2	90.8	85.5
65	ex990629_ss3	11.99	19	42.1	42.00	50.4	99.0	98.3	95.6	90.2	84.8
67	ex990630_ss2	15.00	19	39.9	29.99	50.0	99.6	98.8	95.9	90.9	86.5
68	ex990703_ss1	18.02	19	50.7	12.00	50.0	99.3	99.8	98.9	96.0	92.6
69	ex990703_ss2	18.11	19	50.3	29.99	50.0	99.1	99.8	99.1	96.2	92.4
72	ex990704_ss2	24.00	21	33.8	15.01	50.0	96.8	91.4	85.0	80.1	74.0
73	ex990705_ss1	24.00	22	33.9	30.00	50.0	97.3	93.3	86.9	82.0	76.2
74	ex990705_ss2	24.00	21	32.8	60.01	54.6	96.8	92.7	86.4	81.2	74.3
75	ex990705_ss3	30.01	21	33.2	59.97	53.8	92.5	85.4	81.3	78.3	72.7
76	ex990706_ss1	29.98	23	31.7	36.01	52.8	90.7	84.1	80.5	78.3	74.5
77	ex990706_ss2	30.02	23	33.9	15.00	50.0	91.4	84.7	81.2	79.1	75.6
78	ex990708_ss1	23.98	23	32.6	10.83	50.0	91.8	88.0	82.0	79.2	73.7
79	ex990708_ss2	24.00	23	31.9	26.43	50.0	92.6	88.0	82.1	78.6	72.9
80	ex990708_ss3	24.02	21	34.5	37.12	49.6	93.7	88.0	82.4	78.4	72.3
81	ex990710_ss1	24.00	23	32.9	23.68	50.9	96.2	91.7	85.3	80.5	74.3
82	ex990710_ss2	23.99	19	32.9	51.71	54.1	96.4	92.7	86.4	80.8	73.9
83	ex990711_ss1	24.00	20	33.9	21.74	50.0	91.7	85.0	81.3	79.1	73.6
84	ex990711_ss2	24.00	20	33.5	33.79	50.0	91.4	85.0	80.9	78.6	72.9
85	ex990711_ss3	24.00	18	34.7	79.72	55.1	90.1	85.0	80.4	78.1	71.5
86	ex990712_ss1	15.02	19	37.4	14.09	50.0	90.1	85.1	79.4	76.5	70.5
87	ex990712_ss2	15.01	19	38.1	37.26	50.1	91.5	86.0	80.0	76.9	70.7
88	ex990712_ss3	15.00	19	38.6	79.77	54.6	93.4	87.9	81.4	78.0	71.3
89	ex990713_ss1	15.00	20	35.1	19.24	50.0	92.8	87.9	81.5	78.0	72.0
90	ex990713_ss2	15.01	19	38.2	23.54	50.0	95.0	90.9	83.4	79.0	72.2
91	ex990714_ss1	14.99	17	35.0	79.31	54.9	95.6	91.1	83.9	79.1	71.4
92	ex990714_ss2	29.98	18	32.0	80.04	54.9	90.9	84.7	81.3	78.6	71.4
93	ex990717_ss1	30.02	20	30.8	59.99	53.9	89.9	84.5	80.9	78.7	72.7
94	ex990717_ss2	30.00	19	34.1	79.96	56.1	88.5	83.0	80.1	78.5	72.6
95	ex990717_ss3	30.00	17	34.8	20.00	50.0	88.0	83.0	80.1	78.2	73.0
96	ex990718_ss1	14.98	18	35.0	14.99	50.0	92.1	85.0	80.4	78.1	71.8
97	ex990720_ss1	15.00	18	35.1	80.01	57.2	99.3	98.6	95.6	90.4	86.1
98	ex990720_ss2	23.98	18	31.9	80.01	56.2	96.5	92.0	86.1	81.2	73.7
99	ex990720_ss3	30.00	18	34.8	80.02	55.5	91.7	85.7	81.9	79.1	72.4
100	ex990804_ss1	20.99	28	34.8	15.00	50.0	94.4	89.1	82.2	78.3	74.6
101	ex990804_ss2	20.97	28	34.7	44.99	53.6	94.3	88.9	81.6	77.7	73.9
102	ex990804_ss3	21.01	28	34.9	79.97	57.5	95.2	91.0	82.6	78.1	73.6
103	ex990805_ss1	29.96	30	32.2	14.99	50.0	96.1	91.6	83.8	78.8	77.3
104	ex990805_ss2	30.02	28	31.3	80.02	59.5	95.3	90.9	82.8	77.4	75.2
105	ex000113_ss1	14.96	33	35.0	15.76	50.0	100.7	99.5	95.3	87.7	86.9
106	ex000113_ss2	14.98	33	35.0	34.75	50.0	100.6	98.9	95.1	86.8	84.9

	Data Used for Hybrid Parallel Modeling			bottom composition	distillate composition	bottom composition
No.	tray5	tray6	efficiency	(with fixed efficiency =0.4)	(with fixed efficiency =0.4)	(experiment)
	temperature	temperature	(actual)			
	(C)	(C)	(from ChemCAD)	(mol% meOH)	(mol% meOH)	(mol% meOH)
4	70.4	69.3	0.51	7.5%	81.5%	10.0%
5	70.3	69.1	0.46	8.4%	82.7%	11.0%
6	70.2	70.0	0.44	9.0%	83.5%	12.0%
7	70.1	70.0	0.37	10.9%	85.2%	16.0%
8	70.5	69.1	0.44	1.1%	73.4%	3.0%
13	69.7	68.5	0.44	16.2%	86.0%	22.0%
14	69.5	68.3	0.42	16.6%	86.4%	20.0%
15	69.6	68.4	0.34	16.4%	86.7%	20.0%
16	69.3	68.0	0.31	17.2%	87.6%	22.0%
17	69.3	68.0	0.31	17.8%	88.0%	21.0%
18	69.1	67.8	0.30	18.2%	88.1%	23.0%
19	69.3	68.0	0.26	18.0%	88.3%	23.0%
21	70.6	67.9	0.46	15.8%	84.9%	24.0%
22	69.2	68.0	0.45	15.1%	85.7%	17.0%
23	69.0	67.8	0.42	15.3%	86.1%	19.0%
24	68.8	67.6	0.40	17.4%	87.4%	20.0%
25	68.4	67.2	0.41	19.2%	87.7%	23.0%
26	69.5	68.2	0.20	21.5%	88.6%	25.0%
27	69.9	68.6	0.17	20.6%	88.4%	23.0%
29	67.8	66.1	0.69	23.5%	87.8%	26.0%
30	68.8	66.5	0.64	16.6%	85.8%	18.0%
32	68.5	66.4	0.62	23.5%	87.8%	28.0%
33	69.1	66.8	0.68	21.1%	86.8%	23.0%
34	72.3	71.2	0.30	13.8%	82.9%	17.0%
35	70.1	68.9	0.46	9.1%	81.7%	10.0%
36	70.2	68.9	0.61	1.8%	71.1%	2.0%
37	70.1	68.6	0.64	1.6%	71.7%	1.0%
38	70.3	69.0	0.53	2.3%	76.9%	2.0%
39	70.2	68.9	0.46	2.2%	77.1%	2.0%
40	70.1	68.8	0.45	2.2%	77.4%	2.0%
41	70.1	68.8	0.50	2.7%	77.3%	2.0%
42	70.1	68.9	0.55	2.5%	76.3%	2.0%
43	70.3	69.1	0.57	2.8%	75.9%	2.0%
44	71.1	69.6	1.00	0.6%	62.8%	0.0%
45	88.8	79.4	1.00	0.3%	54.4%	0.0%
46	84.2	74.4	1.00	0.3%	57.7%	0.0%
47	84.3	74.1	1.00	0.4%	63.4%	0.0%
48	84.2	73.7	1.00	0.5%	66.7%	0.0%
49	83.9	75.4	1.00	0.5%	56.4%	0.0%
50	84.9	74.6	1.00	0.4%	58.8%	0.0%
51	85.1	74.5	1.00	0.4%	62.9%	0.0%
52	85.1	74.2	1.00	0.6%	67.0%	0.0%
53	91.7	82.0	1.00	0.5%	54.6%	0.0%
54	83.4	73.7	1.00	0.5%	59.4%	0.0%
55	84.1	73.7	1.00	0.5%	63.4%	0.0%
56	78.2	70.8	1.00	0.6%	66.7%	0.0%
57	77.1	69.9	1.00	0.9%	70.5%	0.0%
58	77.4	69.6	1.00	0.6%	69.5%	0.0%
59	80.4	71.4	1.00	0.2%	59.8%	0.0%
60	78.5	70.2	1.00	0.5%	67.6%	0.0%
61	77.9	69.6	1.00	0.7%	71.3%	0.0%
62	75.9	70.0	1.00	0.3%	50.7%	0.0%
63	78.7	71.4	1.00	0.5%	60.7%	0.0%
64	79.7	71.5	1.00	0.2%	58.2%	0.0%
65	78.4	70.3	1.00	0.5%	68.9%	0.0%
67	79.4	71.1	1.00	0.2%	58.2%	0.0%
68	86.3	76.4	1.00	0.4%	48.9%	0.0%
69	85.0	74.5	1.00	0.5%	64.2%	0.0%
72	72.7	70.8	1.00	1.8%	67.8%	1.0%
73	73.9	71.4	0.44	1.5%	71.4%	1.0%
74	72.8	70.0	1.00	1.8%	75.5%	0.0%
75	71.5	69.3	0.35	5.0%	80.7%	3.0%
76	73.6	71.7	0.25	6.6%	80.7%	5.0%
77	74.7	73.0	0.33	5.9%	76.0%	5.0%
78	72.8	71.0	0.51	5.6%	74.8%	5.0%
79	71.9	70.0	0.40	4.9%	78.6%	4.0%
80	71.2	69.0	0.43	4.0%	78.5%	2.0%
81	73.2	71.0	0.44	2.2%	72.7%	2.0%
82	72.6	70.0	0.42	2.1%	75.7%	1.0%
83	72.9	71.0	0.38	5.7%	78.6%	5.0%
84	71.9	70.0	0.37	5.9%	80.5%	5.0%
85	70.4	68.3	0.34	7.2%	83.8%	5.0%
86	69.8	68.0	0.55	7.2%	80.2%	5.0%
87	69.7	68.0	0.43	5.9%	82.1%	4.0%
88	70.2	68.3	0.40	4.2%	81.9%	3.0%
89	70.9	69.0	0.46	4.7%	78.8%	3.0%
90	71.0	69.0	0.51	3.0%	76.8%	1.0%
91	70.2	68.1	0.45	3.0%	80.1%	1.0%
92	70.2	68.0	0.36	6.4%	82.6%	4.0%
93	71.6	69.5	0.28	7.4%	82.8%	6.0%
94	71.5	69.3	0.27	9.0%	84.5%	8.0%
95	72.0	70.2	0.39	9.6%	80.8%	8.0%
96	70.9	69.3	0.54	5.3%	78.5%	5.0%
97	79.3	70.5	1.00	0.4%	67.7%	0.0%
98	72.2	69.3	0.39	2.0%	76.8%	1.0%
99	71.2	68.8	0.34	5.7%	82.0%	4.0%
100	73.7	72.1	0.37	3.4%	74.2%	4.0%
101	72.9	71.1	0.30	3.5%	79.1%	3.0%
102	72.5	70.2	0.36	2.9%	79.4%	1.0%
103	76.8	75.2	0.43	2.3%	68.0%	1.0%
104	74.2	71.9	0.28	2.8%	78.4%	1.0%
105	82.9	74.4	1.00	0.2%	45.3%	0%
106	79.1	71.3	1.00	0.2%	59.8%	0%

No.	distillate composition (experiment) (mol% meOH)	error of distillate composition (experiment- fixed efficiency) (mol% meOH)	error of distillate composition (predicted by neural network) (mol% meOH)	distillate composition (hybrid parallel model) (mol% meOH)	residual error (experiment- hybrid parallel model) (mol% meOH)
4	88.0%	6.5%	4.4%	85.9%	2.1%
5	87.0%	4.3%	3.9%	86.6%	0.4%
6	87.0%	3.5%	2.3%	85.8%	1.2%
7	86.0%	0.8%	-0.8%	84.5%	1.5%
8	82.0%	8.6%	9.6%	83.0%	-1.0%
13	89.0%	3.0%	3.8%	89.8%	-0.8%
14	88.0%	1.6%	-0.3%	86.1%	1.9%
15	85.0%	-1.7%	-2.8%	83.9%	1.1%
16	85.0%	-2.6%	-1.1%	86.5%	-1.5%
17	85.0%	-3.0%	-4.1%	83.9%	1.1%
18	85.0%	-3.1%	-3.6%	84.6%	0.4%
19	83.0%	-5.3%	-6.4%	81.8%	1.2%
21	89.0%	4.1%	5.7%	90.6%	-1.6%
22	88.0%	2.3%	4.1%	89.8%	-1.8%
23	88.0%	1.9%	3.3%	89.5%	-1.5%
24	88.0%	0.6%	1.5%	88.9%	-0.9%
25	89.0%	1.3%	0.1%	87.7%	1.3%
26	80.0%	-8.6%	-4.2%	84.4%	-4.4%
27	77.0%	-11.4%	-9.0%	79.4%	-2.4%
29	95.0%	7.2%	8.1%	95.9%	-0.9%
30	93.0%	7.2%	7.5%	93.3%	-0.3%
32	94.0%	6.2%	6.5%	94.3%	-0.3%
33	94.0%	7.2%	6.7%	93.4%	0.6%
34	80.0%	-2.9%	4.0%	86.9%	-6.9%
35	85.0%	3.3%	4.6%	86.4%	-1.4%
36	85.0%	13.9%	13.1%	84.2%	0.8%
37	85.0%	13.3%	11.7%	83.4%	1.6%
38	85.0%	8.1%	7.0%	84.0%	1.0%
39	81.0%	3.9%	5.3%	82.4%	-1.4%
40	81.0%	3.6%	3.7%	81.1%	-0.1%
41	83.0%	5.7%	7.2%	84.5%	-1.5%
42	85.0%	8.7%	8.1%	84.4%	0.6%
43	85.0%	9.1%	8.1%	84.1%	0.9%
44	87.0%	24.2%	23.7%	86.5%	0.5%
45	57.0%	2.6%	1.1%	55.5%	1.5%
46	74.0%	16.3%	10.7%	68.4%	5.6%
47	69.0%	5.6%	6.4%	69.9%	-0.9%
48	66.0%	-0.7%	3.0%	69.6%	-3.6%
49	68.0%	11.6%	10.3%	66.7%	1.3%
50	74.0%	15.2%	13.3%	72.1%	1.9%
51	70.0%	7.1%	8.3%	71.2%	-1.2%
52	65.0%	-2.0%	4.1%	71.0%	-6.0%
53	54.0%	-0.6%	-0.1%	54.5%	-0.5%
54	77.0%	17.6%	14.1%	73.5%	3.5%
55	70.0%	6.6%	9.5%	72.9%	-2.9%
56	75.0%	8.3%	11.2%	77.9%	-2.9%
57	74.0%	3.5%	7.8%	78.3%	-4.3%
58	73.0%	3.5%	2.5%	72.0%	1.0%
59	70.0%	10.2%	6.0%	65.7%	4.3%
60	73.0%	5.4%	4.5%	72.2%	0.8%
61	72.0%	0.7%	2.8%	74.0%	-2.0%
62	82.0%	31.3%	27.4%	78.1%	3.9%
63	80.0%	19.3%	24.8%	85.4%	-5.4%
64	76.0%	17.8%	13.3%	71.5%	4.5%
65	73.0%	4.1%	4.7%	73.6%	-0.6%
67	74.0%	15.8%	10.4%	68.6%	5.4%
68	64.0%	15.1%	14.1%	63.0%	1.0%
69	65.0%	0.8%	3.1%	67.2%	-2.2%
72	79.0%	11.2%	10.6%	78.4%	0.6%
73	72.0%	0.6%	0.0%	71.4%	0.6%
74	70.0%	-5.5%	-5.4%	70.1%	-0.1%
75	73.0%	-7.7%	-8.2%	72.5%	0.5%
76	66.0%	-14.7%	-14.3%	66.4%	-0.4%
77	70.0%	-6.0%	-8.2%	67.8%	2.2%
78	80.0%	5.2%	3.5%	78.3%	1.7%
79	77.0%	-1.6%	-3.5%	75.0%	2.0%
80	75.0%	-3.5%	-1.6%	76.9%	-1.9%
81	75.0%	2.3%	1.0%	73.8%	1.2%
82	73.0%	-2.7%	-3.3%	72.4%	0.6%
83	76.0%	-2.6%	-3.6%	75.0%	1.0%
84	77.0%	-3.5%	-5.2%	75.3%	1.7%
85	77.0%	-6.8%	-8.2%	75.7%	1.3%
86	86.0%	5.8%	7.5%	87.7%	-1.7%
87	82.0%	-0.1%	-3.5%	78.6%	3.4%
88	80.0%	-1.9%	-8.6%	73.3%	6.7%
89	80.0%	1.2%	3.8%	82.6%	-2.6%
90	79.0%	2.2%	5.4%	82.3%	-3.3%
91	79.0%	-1.1%	-3.9%	76.2%	2.8%
92	77.0%	-5.6%	-4.6%	78.0%	-1.0%
93	72.0%	-10.8%	-10.7%	72.1%	-0.1%
94	74.0%	-10.5%	-10.9%	73.6%	0.4%
95	79.0%	-1.8%	-1.3%	79.4%	-0.4%
96	86.0%	7.5%	5.8%	84.3%	1.7%
97	69.0%	1.3%	1.9%	69.5%	-0.5%
98	72.0%	-4.8%	-5.6%	71.3%	0.7%
99	75.0%	-7.0%	-7.2%	74.9%	0.1%
100	73.0%	-1.2%	1.4%	75.7%	-2.7%
101	69.0%	-10.1%	-12.3%	66.9%	2.1%
102	69.0%	-10.4%	-11.3%	68.1%	0.9%
103	62.0%	-6.0%	-5.7%	62.3%	-0.3%
104	63.0%	-15.4%	-17.8%	60.6%	2.4%
105	74.0%	28.7%	23.9%	69.2%	4.8%
106	74.0%	14.2%	18.8%	78.6%	-4.6%

	residual error	EXPERIMENT DATA									
No.	(experiment - fixed	feed	feed	reflux	bottom	distillate	reboiler	feed	reflux	feed	bottom
	efficiency model)	rate	composition	rate	rate	rate	duty	temperature	temperature	tray	composition
	(mol% meOH)	(lb/hr)	(mol% meOH)	(lb/hr)	(lb/hr)	(lb/hr)	(% of full power)	(C)	(C)		(mol% meOH)
4	6.5%	12.05	40%	11.99	8.71	2.61	60%	41.8	50.0	3	10%
5	4.3%	11.96	40%	14.00	8.83	2.47	60%	41.5	50.0	3	11%
6	3.5%	12.02	40%	16.01	9.84	1.85	60%	41.1	50.0	3	12%
7	0.8%	11.94	39%	20.00	8.99	2.09	60%	40.9	50.0	3	16%
8	8.6%	11.95	39%	30.00	3.68	2.09	60%	50.0	50.1	3	3%
13	3.0%	14.95	40%	15.01	12.69	1.84	60%	38.9	49.9	3	22%
14	1.6%	15.02	34%	18.01	12.88	1.91	60%	39.7	50.0	3	20%
15	-1.7%	14.99	33%	20.99	11.90	2.38	60%	39.4	50.0	3	20%
16	-2.6%	15.05	40%	25.00	13.29	1.30	60%	39.0	50.0	3	22%
17	-3.0%	14.97	39%	28.00	13.27	1.63	60%	39.1	50.1	3	21%
18	-3.1%	15.01	40%	28.00	12.38	1.88	60%	39.5	50.0	3	23%
19	-5.3%	15.00	39%	31.01	12.13	2.34	60%	39.5	50.0	3	23%
21	4.1%	13.69	40%	10.00	9.41	3.37	60%	39.6	50.0	3	24%
22	2.3%	13.67	40%	14.00	11.06	2.18	60%	39.8	50.0	3	17%
23	1.9%	13.63	40%	16.01	10.98	2.19	60%	40.0	50.0	3	19%
24	0.6%	13.68	40%	20.00	11.76	2.42	60%	39.5	50.0	3	20%
25	1.3%	17.98	40%	24.01	15.24	1.12	60%	38.3	50.0	3	23%
26	-8.6%	17.96	39%	28.02	14.19	2.95	60%	37.4	50.0	3	25%
27	-11.4%	18.01	34%	31.00	12.76	3.98	60%	37.5	50.0	3	23%
29	7.2%	10.02	35%	10.00	9.41	0.30	50%	46.3	50.0	3	26%
30	7.2%	10.01	33%	10.00	7.30	1.93	55%	45.7	50.0	3	18%
32	6.2%	12.05	34%	12.00	11.12	0.27	55%	43.0	50.0	3	28%
33	7.2%	11.95	35%	10.01	9.06	1.80	55%	43.1	50.0	3	23%
34	-2.9%	17.99	39%	10.00	13.56	4.04	60%	36.6	50.0	3	17%
35	3.3%	17.94	40%	13.99	8.27	4.36	60%	41.2	50.0	3	10%
36	13.9%	17.93	34%	16.00	3.85	3.24	60%	49.8	50.0	3	2%
37	13.3%	17.94	33%	20.00	4.01	3.19	60%	49.5	50.0	3	1%
38	8.1%	10.03	35%	21.00	4.72	4.16	60%	45.9	50.0	3	2%
39	3.9%	9.99	34%	25.01	4.91	4.26	60%	46.2	50.0	3	2%
40	3.6%	9.99	34%	28.00	4.71	4.24	60%	46.5	50.0	3	2%
41	5.7%	10.04	38%	17.99	4.65	4.11	60%	46.7	50.0	3	2%
42	8.7%	10.02	38%	15.00	5.02	5.07	60%	47.1	50.0	3	2%
43	9.1%	10.03	37%	12.01	5.25	3.72	60%	46.1	50.0	3	2%
44	24.2%	14.97	27%	15.00	4.97	2.37	60%	49.7	50.0	3	0%
45	2.6%	11.99	19%	12.00	7.99	4.17	100%	40.8	50.0	3	0%
46	16.3%	11.99	19%	18.00	9.07	3.08	100%	41.1	50.0	3	0%
47	5.6%	11.98	19%	24.00	8.48	3.29	100%	41.6	50.0	3	0%
48	-0.7%	12.00	18%	29.99	8.54	3.53	100%	41.5	50.0	3	0%
49	11.6%	14.99	20%	12.00	10.30	4.82	100%	38.9	50.0	3	0%
50	15.2%	14.98	19%	18.00	4.95	1.77	100%	49.1	50.0	3	0%
51	7.1%	14.97	19%	24.00	4.90	1.80	100%	50.0	50.0	3	0%
52	-2.0%	15.00	18%	30.01	4.60	1.93	100%	50.4	50.0	3	0%
53	-0.6%	17.99	20%	11.99	4.90	3.84	100%	46.1	50.0	3	0%
54	17.6%	17.98	19%	18.01	8.33	2.43	100%	46.4	50.0	3	0%
55	6.6%	18.01	19%	24.00	5.80	2.37	100%	48.0	50.0	3	0%
56	8.3%	18.01	20%	29.99	12.75	5.23	100%	36.5	50.0	3	0%
57	3.5%	17.97	23%	36.01	12.54	5.94	100%	36.7	50.0	3	0%
58	3.5%	18.05	23%	51.00	12.00	8.31	100%	36.7	52.2	3	0%
59	10.2%	15.00	24%	36.00	9.60	4.95	100%	39.6	50.0	3	0%
60	5.4%	14.73	20%	45.02	10.21	4.72	100%	39.1	51.0	3	0%
61	0.7%	15.00	20%	54.01	10.49	4.85	100%	38.9	52.7	3	0%
62	31.3%	12.01	20%	11.36	8.87	3.12	71%	42.7	50.0	3	0%
63	19.3%	11.99	20%	12.00	8.57	3.28	80%	42.3	50.0	3	0%
64	17.8%	11.98	20%	23.99	8.43	3.31	80%	42.6	50.0	3	0%
65	4.1%	11.99	19%	42.00	8.35	3.52	80%	42.1	50.4	3	0%
67	15.8%	15.00	19%	29.99	10.58	4.49	80%	39.9	50.0	3	0%
68	15.1%	18.02	19%	12.00	3.85	1.90	80%	50.7	50.0	3	0%
69	0.8%	18.11	19%	29.99	3.29	1.50	80%	50.3	50.0	3	0%
72	11.2%	24.00	21%	15.01	18.06	6.14	70%	33.8	50.0	3	1%
73	0.6%	24.00	22%	30.00	16.58	7.88	80%	33.9	50.0	3	1%
74	-5.5%	24.00	21%	60.01	16.53	8.25	80%	32.8	54.6	3	0%
75	-7.7%	30.01	21%	59.97	23.12	8.28	80%	33.2	53.8	3	3%
76	-14.7%	29.98	23%	36.01	21.95	9.66	70%	31.7	52.8	3	5%
77	-8.0%	30.02	23%	15.00	22.94	8.80	70%	33.9	50.0	3	5%
78	5.2%	23.98	23%	10.83	19.36	8.04	70%	32.6	50.0	3	5%
79	-1.6%	24.00	23%	26.43	18.83	6.68	71%	31.9	50.0	3	4%
80	-3.5%	24.02	21%	37.12	18.87	7.19	76%	34.5	49.6	3	2%
81	2.3%	24.00	23%	23.88	18.23	7.16	97%	32.9	50.9	3	2%
82	-2.7%	23.99	19%	51.71	17.72	7.80	95%	32.9	54.1	3	1%
83	-2.6%	24.00	20%	21.74	19.47	6.05	69%	33.9	50.9	3	5%
84	-3.5%	24.00	20%	33.79	19.88	6.25	69%	33.5	50.9	3	5%
85	-6.8%	24.00	18%	79.72	21.72	4.83	69%	34.7	55.1	3	5%
86	5.8%	15.02	19%	14.09	13.16	2.37	64%	37.4	50.0	3	5%
87	-0.1%	15.01	19%	37.28	13.23	2.55	64%	38.1	50.1	3	4%
88	-1.9%	15.00	19%	79.77	12.87	3.56	65%	38.6	54.6	3	3%
89	1.2%	15.00	20%	19.24	12.73	2.28	66%	35.1	50.0	3	3%
90	2.2%	15.01	19%	23.54	12.85	2.44	67%	38.2	50.0	3	1%
91	-1.1%	14.99	17%	79.31	13.11	3.70	66%	35.0	54.9	3	1%
92	-5.6%	29.98	18%	80.04	27.21	5.39	100%	32.0	54.9	3	4%
93	-10.8%	30.02	20%	59.99	25.56	6.88	99%	30.8	53.9	3	6%
94	-10.5%	30.00	19%	79.96	26.31	5.94	70%	34.1	56.1	3	8%
95	-1.8%	30.00	17%	20.00	28.28	3.26	70%	34.8	50.0	3	8%
96	7.5%	14.98	18%	14.99	13.33	3.02	64%	35.0	50.0	3	5%
97	1.3%	15.00	18%	80.01	11.53	5.17	100%	35.1	57.2	3	0%
98	-4.8%	23.98	18%	80.01	19.39	6.96	100%	31.9	56.2	3	1%
99	-7.0%	30.00	18%	80.02	25.91	7.23	100%	34.8	55.5	3	4%
100	-1.2%	20.99	28%	15.00	12.61	8.64	67%	34.8	50.0	3	4%
101	-10.1%	20.97	28%	44.99	11.37	10.20	67%	34.7	53.6	3	3%
102	-10.4%	21.01	28%	79.97	10.80	10.60	69%	34.9	57.5	3	1%
103	-6.0%	29.96	30%	14.99	11.35	17.96	100%	32.2	50.0	3	1%
104	-15.4%	30.02	28%	80.02	11.93	17.52	100%	31.3	59.5	3	1%
105	28.7%	14.96	33%	15.76	7.03	6.82	70%	35.0	50.0	3	0%
106	14.2%	14.98	33%	34.75	6.97	6.87	70%	35.0	50.0	3	0%

	EXPERIMENT DATA									DATA RECONCILIATI			
No.	distillate	reboiler	distillate	tray 1	tray 2	tray 3	tray 4	tray 5	tray 6	alpha	beta	overall	MeOH
	composition	temperature	temperature	temperature	temperature	temperature	temperature	temperature	temperature			material	material
	(mol% meOH)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)			balance	balance
4	88%	89.8	29.7	82.1	77.8	75.7	71.0	70.4	69.3	-2.61	3.34	0.00	0.00
5	87%	89.0	29.9	81.5	77.7	75.8	70.8	70.3	69.1	-2.71	3.37	0.00	0.00
6	87%	88.5	30.1	81.4	77.8	75.9	70.8	70.2	70.0	-3.56	3.89	0.00	0.00
7	86%	87.0	31.2	77.4	80.9	75.9	70.7	70.1	70.0	-2.07	2.93	0.00	0.00
8	82%	97.9	33.3	91.8	82.2	77.2	71.2	70.5	69.1	1.43	4.75	0.00	0.00
13	89%	83.7	30.3	78.6	76.3	75.2	70.2	69.7	68.5	-2.92	3.34	0.00	0.00
14	88%	83.5	31.2	78.4	76.1	75.1	70.1	69.5	68.3	-1.98	2.21	0.00	0.00
15	85%	83.6	32.0	78.5	76.1	75.1	70.2	69.6	68.4	-0.87	1.58	0.00	0.00
16	85%	83.2	32.8	78.1	75.9	74.9	69.8	69.3	68.0	-3.69	4.15	0.00	0.00
17	85%	82.9	33.5	78.1	75.9	74.9	69.8	69.3	68.0	-3.67	3.74	0.00	0.00
18	85%	82.7	33.2	77.7	75.6	74.7	69.6	69.1	67.8	-2.58	3.33	0.00	0.00
19	83%	82.8	33.3	77.8	75.7	74.7	69.8	69.3	68.0	-2.16	2.71	0.00	0.00
21	89%	83.9	30.2	78.7	76.4	75.2	70.5	70.6	67.9	-0.07	0.98	0.00	0.00
22	88%	84.3	30.5	78.9	78.1	74.8	69.7	69.2	68.0	-3.08	3.51	0.00	0.00
23	88%	84.2	30.8	78.5	75.9	74.6	69.5	69.0	67.8	-2.68	3.14	0.00	0.00
24	88%	83.1	31.9	78.1	75.3	74.1	69.3	68.8	67.6	-3.25	2.75	0.00	0.00
25	89%	82.2	32.5	77.4	75.1	74.0	68.9	68.4	67.2	-3.24	4.86	0.00	0.00
26	80%	81.2	33.7	76.8	75.0	74.2	70.1	69.5	68.2	-1.92	2.74	0.00	0.00
27	77%	81.6	34.0	77.0	75.0	74.2	70.5	69.9	68.6	0.61	0.66	0.00	0.00
29	95%	80.4	28.7	75.4	73.8	72.3	67.9	67.8	66.1	-1.18	1.49	0.00	0.00
30	93%	83.5	29.4	77.8	74.8	73.2	68.7	68.8	66.5	-0.04	0.82	0.00	0.00
32	94%	80.4	29.2	75.8	72.8	68.3	68.5	68.5	66.4	-0.57	1.23	0.00	0.00
33	94%	81.4	29.1	77.1	74.7	73.5	69.0	69.1	66.8	0.14	0.95	0.00	0.00
34	80%	85.1	30.4	79.6	77.1	76.1	72.9	72.3	71.2	-3.39	3.78	0.00	0.00
35	85%	88.4	31.4	81.1	76.5	74.4	70.6	70.1	68.9	0.58	4.73	0.00	0.00
36	85%	96.8	31.7	91.3	81.1	76.3	70.8	70.2	68.9	5.00	5.84	0.00	0.00
37	85%	97.1	32.6	91.8	81.5	76.3	70.7	70.1	68.6	4.90	5.84	0.00	0.00
38	85%	96.0	33.3	90.0	80.5	75.7	70.9	70.3	69.0	0.10	1.05	0.00	0.00
39	81%	96.2	33.8	90.5	80.7	75.7	70.8	70.2	68.9	-0.14	0.96	0.00	0.00
40	81%	96.2	34.1	90.4	80.6	75.6	70.7	70.1	68.8	0.06	0.98	0.00	0.00
41	83%	95.5	32.3	89.1	79.9	75.4	70.6	70.1	68.8	-0.28	1.56	0.00	0.00
42	85%	95.7	31.6	89.1	79.9	75.3	70.7	70.1	68.9	-0.57	0.50	0.00	0.00
43	85%	95.3	30.8	89.0	80.2	75.8	70.9	70.3	69.1	-0.68	1.74	0.00	0.00
44	87%	98.8	31.1	94.8	85.8	79.2	72.3	71.1	69.6	3.56	4.07	0.00	0.00
45	57%	100.4	32.9	99.9	98.2	93.9	92.9	88.8	79.4	-1.03	0.86	0.00	0.00
46	74%	100.5	32.0	100.2	98.7	94.3	90.5	84.2	74.4	-1.31	1.15	0.00	0.00
47	69%	100.3	33.7	100.1	98.6	94.3	91.0	84.3	74.1	-0.92	1.13	0.00	0.00
48	66%	100.1	35.2	99.9	98.4	94.2	91.2	84.2	73.7	-0.88	0.81	0.00	0.00
49	68%	100.1	32.4	99.3	96.7	90.9	88.9	83.9	75.4	-1.14	1.01	0.00	0.00
50	74%	100.3	32.2	100.1	99.1	95.5	91.3	84.9	74.6	4.75	3.51	0.00	0.00
51	70%	100.2	33.4	100.0	99.0	95.5	91.2	85.1	74.5	4.60	3.67	0.00	0.00
52	65%	99.9	34.6	99.7	98.8	95.3	91.4	85.1	74.2	4.91	3.56	0.00	0.00
53	54%	100.0	33.2	99.6	98.5	94.8	94.3	91.7	82.0	4.90	4.35	0.00	0.00
54	77%	100.1	31.9	99.7	98.4	93.6	88.5	83.4	73.7	5.47	3.75	0.00	0.00
55	70%	100.0	33.1	99.6	98.3	94.1	89.7	84.1	73.7	5.63	4.21	0.00	0.00
56	75%	99.8	34.5	98.8	95.3	89.2	85.3	78.2	70.8	-1.32	1.35	0.00	0.00
57	74%	99.3	35.1	98.1	94.2	87.7	83.7	77.1	69.9	-2.03	1.52	0.00	0.00
58	73%	98.8	36.3	97.7	94.1	87.7	84.3	77.4	69.6	-1.51	1.25	0.00	0.00
59	70%	99.6	35.5	98.7	95.7	90.6	86.9	80.4	71.4	-1.49	1.74	0.00	0.00
60	73%	99.1	36.2	97.9	94.5	88.8	85.1	78.5	70.2	-0.96	0.76	0.00	0.00
61	72%	98.6	36.7	97.8	94.7	89.3	84.5	77.9	69.6	-1.11	0.77	0.00	0.00
62	82%	99.5	31.4	98.0	93.6	86.8	79.1	75.9	70.0	-1.01	1.93	0.00	0.00
63	80%	100.0	31.6	98.9	95.6	90.0	84.0	78.7	71.4	-0.79	0.93	0.00	0.00
64	76%	99.6	33.6	98.8	96.2	90.8	85.5	79.7	71.5	-0.79	1.03	0.00	0.00
65	73%	99.0	35.7	98.3	95.6	90.2	84.8	78.4	70.3	-0.62	0.74	0.00	0.00
67	74%	99.6	35.4	98.8	95.9	90.9	86.5	79.4	71.1	-0.87	0.80	0.00	0.00
68	64%	100.3	32.8	99.8	98.9	96.0	92.6	86.3	76.4	7.19	5.08	0.00	0.00
69	65%	100.1	34.7	99.8	99.1	96.2	92.4	85.0	74.5	7.88	5.44	0.00	0.00
72	79%	98.8	32.7	91.4	85.0	80.1	74.0	72.7	70.8	-2.60	2.40	0.00	0.00
73	72%	97.3	35.1	93.3	86.9	82.0	75.2	73.9	71.4	-2.04	1.58	0.00	0.00
74	70%	96.8	36.7	92.7	86.4	81.2	74.3	72.8	70.0	-2.09	1.31	0.00	0.00
75	73%	92.5	36.7	85.4	81.3	78.3	72.7	71.5	69.3	-3.51	2.12	0.00	0.00
76	66%	90.7	35.9	84.1	80.5	78.3	74.5	73.6	71.7	-3.33	1.70	0.00	0.00
77	70%	91.4	33.8	84.7	81.2	79.1	75.6	74.7	73.0	-3.81	2.09	0.00	0.00
78	80%	91.8	32.0	86.0	82.0	79.2	73.7	72.8	71.0	-3.30	1.88	0.00	0.00
79	77%	92.6	34.3	88.0	82.1	78.6	72.9	71.9	70.0	-3.30	1.79	0.00	0.00
80	75%	93.7	34.5	88.0	82.4	78.4	72.3	71.2	69.0	-3.16	1.32	0.00	0.00
81	75%	96.2	34.2	91.7	85.3	80.5	74.3	73.2	71.0	-3.50	2.11	0.00	0.00
82	73%	96.4	37.5	92.7	86.4	80.8	73.9	72.6	70.0	-1.92	0.39	0.00	0.00
83	76%	91.7	33.6	85.0	81.3	79.1	73.8	72.9	71.0	-2.45	0.93	0.00	0.00
84	77%	91.4	35.1	85.0	80.9	78.6	72.9	71.9	70.0	-2.80	0.67	0.00	0.00
85	77%	90.1	36.7	85.0	80.4	78.1	71.5	70.4	68.3	-3.80	1.25	0.00	0.00
86	86%	90.1	34.9	85.1	79.4	76.5	70.5	69.6	68.0	-1.91	1.40	0.00	0.00
87	82%	91.5	35.0	86.0	80.0	76.9	70.7	69.7	68.0	-2.34	1.57	0.00	0.00
88	80%	93.4	37.3	87.9	81.4	78.0	71.3	70.2	68.3	-2.28	0.83	0.00	0.00
89	80%	92.8	34.8	87.9	81.5	78.0	72.0	70.9	69.0	-2.38	2.37	0.00	0.00
90	79%	95.0	34.8	90.9	83.4	79.0	72.2	71.0	69.0	-2.71	2.43	0.00	0.00
91	79%	95.6	37.2	91.1	83.9	79.1	71.4	70.2	68.1	-2.50	0.68	0.00	0.00
92	77%	90.9	36.8	84.7	81.3	78.6	71.4	70.2	68.0	-4.24	1.62	0.00	0.00
93	72%	89.9	38.4	84.5	80.9	78.7	72.7	71.6	69.5	-4.14	1.72	0.00	0.00
94	74%	88.5	37.1	83.0	80.1	78.5	72.6	71.5	69.3	-3.17	0.92	0.00	0.00
95	79%	88.0	34.7	83.0	80.1	78.2	73.0	72.0	70.2	-3.70	2.16	0.00	0.00
96	86%	92.1	31.9	85.0	80.4	78.1	71.8	70.9	69.3	-1.87	0.50	0.00	0.00
97	69%	99.3	37.7	98.6	95.8	90.4	86.1	79.3	70.5	-1.80	0.10	0.00	0.00
98	72%	96.5	37.3	92.0	86.1	81.2	73.7	72.2	69.3	-3.27	0.99	0.00	0.00
99	75%	91.7	37.5	85.7	81.9	79.1	72.4	71.2	68.8	-4.13	0.99	0.00	0.00
100	73%	94.4	33.3	89.1	82.2	78.3	74.6	73.7	72.1	-1.02	0.76	0.00	0.00
101	69%	94.3	36.1	88.9	81.6	77.7	73.9	72.9	71.1	-0.42	-0.18	0.00	0.00
102	69%	95.2	37.5	91.0	82.6	78.1	73.6	72.5	70.2	-0.32	-0.07	0.00	0.00
103	62%	96.1	35.7	91.6	83.8	78.8	77.3	76.8	75.2	1.49	-0.84	0.00	0.00
104	63%	95.3	38.0	90.9	82.8	77.4	75.2	74.2	71.9	2.09	-1.52	0.00	0.00
105	74%	100.7	39.0	99.5	95.3	87.7	86.9	82.9	74.4	-0.43	1.54	0.00	0.00
106	74%	100.6	43.5	98.9	95.1	86.8	84.9	79.1	71.3	-0.37	1.51	0.00	0.00

	DATA RECONCILIATION		CHEMCAD INPUTS							CHEMCAD OUTPUTS		
No.	reconciled	reconciled	MeOH	water	feed	reflux	bottom	reflux T	sub cooled	feed	feed	reflux
	bottom rate	distillate rate	flow rate	flow rate	temperature	rate	rate	temperature	temperature	rate	composition	rate
	(lb/hr)	(lb/hr)	(lb/hr)	(lb/hr)	(C)	(lb/hr)	(lb/hr)	(C)	(C)	(lb/hr)	(mol% meOH)	(lb/hr)
4	6.10	5.95	6.5356	5.5144	41.8	11.99	6.10	50.0	16	12.05	40%	11.99
5	6.12	5.84	6.4868	5.4732	41.5	14.00	6.12	50.0	16	11.96	40%	14.00
6	6.28	5.74	6.5193	5.5007	41.1	16.01	6.28	50.0	17	12.02	40%	16.01
7	6.92	5.02	6.3517	5.5883	40.9	20.00	6.92	50.0	17	11.94	39%	20.00
8	5.11	6.84	6.3570	5.5930	50.0	30.00	5.11	50.1	17	11.95	39%	30.00
13	9.77	5.18	8.1085	6.8415	38.9	15.01	9.77	49.9	16	14.95	40%	15.01
14	10.90	4.12	7.1800	7.8400	39.7	18.01	10.90	50.0	16	15.02	34%	18.01
15	11.03	3.96	6.9980	7.9920	39.4	20.99	11.03	50.0	17	14.99	33%	20.99
16	9.60	5.45	8.1627	6.8873	39.0	25.00	9.60	50.0	17	15.05	40%	25.00
17	9.60	5.37	7.9636	7.0064	39.1	28.00	9.60	50.1	17	14.97	39%	28.00
18	9.80	5.21	8.1410	6.8690	39.5	28.00	9.80	50.0	17	15.01	40%	28.00
19	9.95	5.05	7.9795	7.0205	39.5	31.01	9.95	50.0	17	15.00	39%	31.01
21	9.34	4.35	7.4251	6.2649	39.6	10.00	9.34	50.0	16	13.69	40%	10.00
22	7.98	5.69	7.4142	6.2558	39.8	14.00	7.98	50.0	16	13.67	40%	14.00
23	8.30	5.33	7.3925	6.2375	40.0	16.01	8.30	50.0	16	13.63	40%	16.01
24	8.51	5.17	7.4197	6.2603	39.5	20.00	8.51	50.0	16	13.68	40%	20.00
25	12.00	5.98	9.7519	8.2281	38.3	24.01	12.00	50.0	16	17.98	40%	24.01
26	12.27	5.69	9.5542	8.4058	37.4	28.02	12.27	50.0	18	17.96	39%	28.02
27	13.37	4.64	8.6093	9.4007	37.5	31.00	13.37	50.0	18	18.01	34%	31.00
29	8.23	1.79	4.9008	5.1194	46.3	10.00	8.23	50.0	15.0	10.02	35%	10.00
30	7.26	2.75	4.6731	5.3369	45.7	10.00	7.26	50.0	16.0	10.01	33%	10.00
32	10.55	1.50	5.7603	6.2897	43.0	12.00	10.55	50.0	15.0	12.05	34%	12.00
33	9.20	2.75	5.8445	6.1055	43.1	10.01	9.20	50.0	15.0	11.95	35%	10.01
34	10.17	7.82	9.5701	8.4199	36.8	10.00	10.17	50.0	18.0	17.99	39%	10.00
35	8.85	9.09	9.7302	8.2098	41.2	13.99	8.85	50.0	17.0	17.94	40%	13.99
36	8.85	9.08	8.5711	9.3589	49.8	16.00	8.85	50.0	17.0	17.93	34%	16.00
37	8.91	9.03	8.3752	9.5648	49.5	20.00	8.91	50.0	17.0	17.94	33%	20.00
38	4.82	5.21	4.9055	5.1245	45.9	21.00	4.82	50.0	17.0	10.03	35%	21.00
39	4.77	5.22	4.7755	5.2145	46.2	25.01	4.77	50.0	17.0	9.99	34%	25.01
40	4.77	5.22	4.7755	5.2145	46.5	28.00	4.77	50.0	17.0	9.99	34%	28.00
41	4.37	5.67	5.2353	4.8047	48.7	17.99	4.37	50.0	17.0	10.04	38%	17.99
42	4.45	5.57	5.2248	4.7952	47.1	15.00	4.45	50.0	17.0	10.02	38%	15.00
43	4.57	5.46	5.1232	4.9068	48.1	12.01	4.57	50.0	17.0	10.03	37%	12.01
44	8.53	6.44	5.9385	9.0315	49.7	15.00	8.53	50.0	17.0	14.97	27%	15.00
45	6.96	5.03	3.5285	8.4615	40.8	12.00	6.96	50.0	22.0	11.99	19%	12.00
46	7.76	4.23	3.5285	8.4615	41.1	18.00	7.76	50.0	19.0	11.99	19%	18.00
47	7.56	4.42	3.5256	8.4544	41.6	24.00	7.56	50.0	20.0	11.98	19%	24.00
48	7.66	4.34	3.3884	8.6316	41.5	29.99	7.66	50.0	20.0	12.00	18%	29.99
49	9.16	5.83	4.6123	10.3777	38.9	12.00	9.16	50.0	20.0	14.99	20%	12.00
50	9.70	5.28	4.4084	10.5716	49.1	18.00	9.70	50.0	19.0	14.98	19%	18.00
51	9.50	5.47	4.4055	10.5645	50.0	24.00	9.50	50.0	19.0	14.97	19%	24.00
52	9.51	5.49	4.2105	10.7895	50.4	30.01	9.51	50.0	20.0	15.00	18%	30.01
53	9.80	8.19	5.5354	12.4646	46.1	11.99	9.80	50.0	22.0	17.99	20%	11.99
54	11.80	6.18	5.2913	12.6887	46.4	18.01	11.80	50.0	18.0	17.98	19%	18.01
55	11.43	6.58	5.3001	12.7099	48.0	24.00	11.43	50.0	19.0	18.01	19%	24.00
56	11.43	6.58	5.5415	12.4685	36.5	29.99	11.43	50.0	19.0	18.01	20%	29.99
57	10.51	7.46	6.2328	11.7372	36.7	36.01	10.51	50.0	19.0	17.97	23%	36.01
58	10.49	7.56	6.2605	11.7895	36.7	51.00	10.49	52.2	17.0	18.05	23%	51.00
59	8.31	6.69	5.3933	9.6067	39.6	36.00	8.31	50.0	19.0	15.00	24%	36.00
60	9.25	5.48	4.5323	10.1977	39.1	45.02	9.25	51.0	18.0	14.73	20%	45.02
61	9.38	5.62	4.6154	10.3846	38.9	54.01	9.38	52.7	18.0	15.00	20%	54.01
62	7.86	4.15	3.6954	8.3146	42.7	11.36	7.86	50.0	17.0	12.01	20%	11.36
63	7.78	4.21	3.6892	8.3008	42.3	12.00	7.78	50.0	18.0	11.99	20%	12.00
64	7.64	4.34	3.6862	8.2938	42.6	23.99	7.64	50.0	18.0	11.98	20%	23.99
65	7.73	4.26	3.5285	8.4615	42.1	42.00	7.73	50.4	18.0	11.99	19%	42.00
67	9.71	5.29	4.4143	10.5857	39.9	29.99	9.71	50.0	19.0	15.00	19%	29.99
68	11.04	6.98	5.3031	12.7169	50.7	12.00	11.04	50.0	20.0	18.02	19%	12.00
69	11.17	6.94	5.3296	12.7804	50.3	29.99	11.17	50.0	20.0	18.11	19%	29.99
72	15.46	8.54	7.7020	16.2980	33.8	15.01	15.46	50.0	18.0	24.00	21%	15.01
73	14.54	9.46	8.0152	15.9848	33.9	30.00	14.54	50.0	19.0	24.00	22%	30.00
74	14.44	9.56	7.7020	16.2980	32.8	60.01	14.44	54.6	15.00	24.00	21%	60.01
75	19.61	10.40	9.6307	20.3793	33.2	59.97	19.61	53.8	15.00	30.01	21%	59.97
76	18.62	11.36	10.3983	19.5817	31.7	36.01	18.62	52.8	17.00	29.98	23%	36.01
77	19.13	10.89	10.4122	19.6078	33.9	15.00	19.13	50.0	19.00	30.02	23%	15.00
78	16.06	7.92	8.3173	15.6627	32.6	10.83	16.06	50.0	18.00	23.98	23%	10.83
79	15.53	8.47	8.3242	15.6758	31.9	26.43	15.53	50.0	18.00	24.00	23%	26.43
80	15.51	8.51	7.7084	16.3116	34.5	37.12	15.51	49.6	19.00	24.02	21%	26.43
81	14.73	9.27	8.3242	15.6758	32.9	23.68	14.73	50.9	18.00	24.00	23%	23.68
82	15.80	8.19	7.0600	16.9300	32.9	51.71	15.80	54.1	15.00	23.99	19%	51.71
83	17.02	6.98	7.3846	16.6154	33.9	21.74	17.02	50.0	18.00	24.00	20%	21.74
84	17.08	6.92	7.3846	16.6154	33.5	33.79	17.08	50.0	18.00	24.00	20%	33.79
85	17.92	6.08	6.7368	17.2632	34.7	79.72	17.92	55.1	13.00	24.00	18%	79.72
86	11.25	3.77	4.4202	10.5998	37.4	14.09	11.25	50.0	17.00	15.02	19%	14.09
87	10.89	4.12	4.4173	10.5927	38.1	37.26	10.89	50.1	17.00	15.01	19%	37.26
88	10.59	4.41	4.4143	10.5857	38.6	79.77	10.59	54.6	13.00	14.99	19%	79.77
89	10.35	4.65	4.6154	10.3846	35.1	19.24	10.35	50.0	18.00	15.00	20%	19.24
90	10.14	4.87	4.4173	10.5927	38.2	23.54	10.14	50.0	18.00	15.01	19%	23.54
91	10.61	4.38	4.0013	10.9887	35.0	79.31	10.61	54.9	13.00	14.99	17%	79.31
92	22.97	7.01	7.5839	22.3961	32.0	80.04	22.97	54.9	13.00	29.98	16%	80.04
93	21.42	8.60	9.2369	20.7831	30.8	59.99	21.42	53.9	15.00	30.02	20%	59.99
94	23.14	6.86	8.8287	21.1713	34.1	79.96	23.14	56.1	12.00	30.00	19%	79.96
95	24.58	5.42	8.0079	21.9921	34.8	20.00	24.58	50.0	18.00	30.00	17%	20.00
96	11.46	3.52	4.2049	10.7751	35.0	14.99	11.46	50.0	17.00	14.98	18%	14.99
97	9.73	5.27	4.2105	10.7895	35.1	80.01	9.73	57.2	12.00	15.00	18%	80.01
98	16.12	7.86	6.7312	17.2488	31.9	80.01	16.12	56.2	13.00	23.98	18%	80.01
99	21.78	8.22	8.4211	21.5789	34.8	80.02	21.78	55.5	13.00	30.00	18%	80.02
100	11.59	9.40	8.5799	12.4101	34.8	15.00	11.59	50.0	19.00	20.99	28%	15.00
101	10.95	10.02	8.5717	12.3983	34.7	44.99	10.95	53.6	16.00	20.97	28%	44.99
102	10.48	10.53	8.5880	12.4220	34.9	79.97	10.48	57.5	12.00	21.01	28%	79.97
103	12.84	17.12	12.9557	17.0043	32.2	14.99	12.84	50.0	21.00	29.96	30%	14.99
104	14.02	16.00	12.2709	17.7491	31.3	80.02	14.02	59.5	11.00	30.02	28%	80.02
105	6.60	8.36	6.9840	7.9760	35.0	15.76	6.60	50.0	19.00	14.96	33%	15.76
106	6.60	8.38	6.9933	7.9867	35.0	34.75	6.60	50.0	19.00	14.98	33%	34.75

	CHEMCAD OUTPUTS											
No.	bottom	distillate	reboiler	feed	reflux	feed	bottom	distillate	reboiler	distillate	tray 1	tray 2
	rate	rate	duty	temperature	temperature	tray	composition	composition	temperature	temperature	temperature	temperature
	(lb/hr)	(lb/hr)	(MMBtu/hr)	(C)	(C)		(mol% meOH)	(mol% meOH)	(C)	(C)	(C)	(C)
4	6.10	5.95	0.010084	41.8	50.4	3	10.1%	87.9%	87.6	50.4	77.8	75.4
5	6.12	5.84	0.011133	41.5	50.5	3	11.0%	86.9%	87.0	50.5	77.1	75.0
6	6.28	5.74	0.012180	41.1	49.5	3	12.0%	86.9%	86.2	49.5	76.5	74.6
7	6.92	5.02	0.014022	40.9	49.7	3	16.0%	85.9%	83.8	49.7	74.9	73.5
8	5.11	6.84	0.020765	50.0	50.3	3	3.0%	82.0%	95.0	50.3	83.8	78.7
13	9.77	5.18	0.011370	38.9	50.2	3	22.0%	89.0%	81.0	50.2	74.3	73.3
14	10.90	4.12	0.012527	39.7	50.3	3	20.0%	88.1%	81.9	50.3	74.8	73.9
15	11.03	3.96	0.014306	39.4	49.8	3	20.0%	85.2%	81.9	49.8	74.6	73.7
16	9.60	5.45	0.017200	39.0	49.8	3	21.9%	85.1%	81.0	49.8	73.5	72.6
17	9.60	5.37	0.018803	39.1	49.8	3	21.0%	85.0%	81.4	49.8	73.6	72.7
18	9.80	5.21	0.018677	39.5	49.8	3	23.0%	85.2%	80.6	49.8	73.2	72.4
19	9.95	5.05	0.020471	39.5	50.1	3	22.9%	83.2%	80.6	50.1	73.0	72.3
21	9.34	4.35	0.008215	39.6	50.2	3	24.0%	89.1%	80.2	50.2	74.4	73.6
22	7.98	5.69	0.011079	39.8	50.3	3	16.9%	88.1%	83.3	50.3	75.3	74.0
23	8.30	5.33	0.011956	40.0	50.3	3	19.0%	88.0%	82.3	50.3	74.6	73.5
24	8.51	5.17	0.013994	39.5	50.3	3	20.0%	88.1%	81.9	50.3	74.1	73.0
25	12.00	5.98	0.016705	38.3	50.2	3	23.0%	89.0%	80.6	50.2	73.7	72.8
26	12.27	5.69	0.019786	37.4	49.6	3	25.0%	80.1%	79.9	49.6	73.0	72.5
27	13.37	4.64	0.021341	37.5	50.1	3	23.0%	77.1%	80.6	50.1	73.5	73.0
28	8.23	1.79	0.006414	46.3	50.3	3	28.0%	94.9%	79.5	50.3	74.2	73.2
30	7.26	2.75	0.007007	45.7	49.6	3	18.0%	93.1%	82.8	49.6	75.8	74.4
32	10.55	1.50	0.007480	43.0	50.4	3	28.0%	94.1%	78.8	50.4	74.0	73.2
33	9.20	2.75	0.007079	43.1	50.4	3	23.0%	94.0%	80.6	50.4	75.0	73.9
34	10.17	7.82	0.010899	36.6	49.7	3	17.0%	80.0%	83.3	49.7	75.9	75.1
35	8.85	9.09	0.013309	41.2	49.8	3	10.0%	85.0%	87.7	49.8	78.0	76.9
36	8.85	9.08	0.014345	49.8	49.8	3	2.0%	85.0%	96.5	49.8	88.2	82.0
37	8.91	9.03	0.016527	49.5	49.8	3	1.0%	85.0%	98.1	49.8	92.2	84.9
38	4.82	5.21	0.014668	45.9	49.8	3	2.0%	85.0%	96.6	49.8	87.3	80.7
39	4.77	5.22	0.017261	46.2	50.5	3	1.9%	81.1%	96.6	50.5	87.1	81.0
40	4.77	5.22	0.018939	46.5	50.5	3	2.0%	80.9%	96.5	50.5	86.7	80.7
41	4.37	5.67	0.013413	46.7	50.2	3	2.0%	82.9%	96.5	50.2	87.0	80.8
42	4.45	5.57	0.011563	47.1	49.8	3	2.0%	85.0%	96.5	49.8	87.3	80.8
43	4.57	5.46	0.009917	46.1	49.9	3	2.0%	84.9%	96.5	49.8	87.7	81.2
44	8.53	6.44	0.012304	49.7	49.6	3	0.1%	86.6%	99.8	49.6	99.1	96.2
45	6.96	5.03	0.012144	40.8	49.8	3	0.0%	56.9%	100.0	49.8	99.8	98.8
46	7.76	4.23	0.013955	41.1	49.7	3	0.0%	73.8%	100.0	49.7	99.8	98.9
47	7.56	4.42	0.018178	41.6	49.6	3	0.0%	68.9%	100.0	49.5	99.9	99.3
48	7.66	4.34	0.022206	41.5	50.0	3	0.0%	66.1%	100.0	50.0	99.9	99.5
49	9.16	5.83	0.012040	38.9	49.7	3	0.0%	67.9%	99.9	49.7	99.5	97.9
50	9.70	5.28	0.014592	49.1	49.7	3	0.0%	73.8%	99.9	49.7	99.7	98.6
51	9.50	5.47	0.018675	50.0	50.4	3	0.0%	69.9%	100.0	50.4	99.8	99.1
52	9.51	5.49	0.023110	50.4	50.3	3	0.0%	64.9%	100.0	50.3	99.9	99.4
53	9.80	6.19	0.014723	46.1	50.4	3	0.0%	53.9%	99.9	50.4	99.6	98.2
54	11.80	6.18	0.015093	46.4	50.2	3	0.0%	76.8%	99.9	50.2	99.6	98.0
55	11.43	6.58	0.019580	48.0	50.4	3	0.0%	69.9%	100.0	50.4	99.8	98.9
56	11.43	6.58	0.022776	36.5	49.5	3	0.0%	74.9%	100.0	49.5	99.8	99.0
57	10.51	7.46	0.026868	36.7	49.7	3	0.0%	74.0%	100.0	49.7	99.9	99.1
58	10.49	7.56	0.035845	36.7	51.8	3	0.0%	73.0%	100.0	51.8	99.9	99.4
59	8.31	6.69	0.026780	39.6	50.3	3	0.0%	70.0%	100.0	50.3	99.9	99.3
60	9.25	5.48	0.030946	39.1	50.9	3	0.0%	72.9%	100.0	50.9	99.9	99.5
61	9.38	5.62	0.036418	38.9	53.0	3	0.0%	72.1%	100.0	53.0	99.9	99.6
62	7.86	4.15	0.009468	42.7	50.4	3	0.1%	81.7%	99.9	50.4	99.4	97.4
63	7.78	4.21	0.009997	42.3	49.7	3	0.1%	79.7%	99.9	49.7	99.5	97.8
64	7.64	4.34	0.017226	42.8	50.3	3	0.0%	76.0%	100.0	50.3	99.9	99.2
65	7.73	4.26	0.028165	42.1	50.8	3	0.0%	73.0%	100.0	50.8	99.9	99.6
67	9.71	5.29	0.021874	39.9	49.7	3	0.0%	73.9%	100.0	49.7	99.9	99.2
68	11.04	6.98	0.012968	50.7	50.5	3	0.1%	63.8%	99.9	50.5	99.4	97.7
69	11.17	6.94	0.024139	50.3	50.2	3	0.0%	65.0%	100.0	50.2	99.9	99.2
72	15.46	8.54	0.015259	33.8	49.8	3	1.0%	79.1%	98.2	49.8	93.5	88.1
73	14.54	9.46	0.025246	33.9	50.0	3	1.0%	72.0%	98.2	50.0	92.5	87.2
74	14.44	9.56	0.043690	32.8	54.4	3	0.0%	69.9%	100.0	54.4	99.9	99.4
75	19.61	10.40	0.043371	33.2	53.8	3	2.9%	73.3%	95.1	53.8	85.0	81.2
76	18.62	11.36	0.031321	31.7	53.0	3	4.9%	66.2%	92.5	53.0	82.1	80.1
77	19.13	10.89	0.017746	33.9	50.4	3	5.0%	69.8%	92.4	50.4	83.6	81.5
78	16.06	7.92	0.012378	32.6	49.7	3	5.0%	79.9%	92.4	49.7	84.2	81.4
79	15.53	8.47	0.021812	31.9	50.1	3	3.9%	77.2%	93.7	50.1	84.1	80.7
80	15.53	8.49	0.022135	34.5	49.5	3	2.0%	75.2%	96.5	49.5	88.5	83.9
81	14.73	9.27	0.020952	32.9	50.5	3	2.0%	75.2%	96.6	50.5	88.7	84.0
82	15.80	8.19	0.036991	32.9	53.8	3	1.0%	73.1%	98.2	53.8	92.0	86.3
83	17.02	6.98	0.018388	33.9	50.3	3	4.9%	76.3%	92.5	50.3	83.3	80.7
84	17.08	6.92	0.025139	33.5	50.1	3	4.9%	77.3%	92.5	50.1	82.4	79.7
85	17.92	6.08	0.050402	34.7	55.1	3	5.0%	77.2%	92.5	55.1	81.0	78.1
86	11.25	3.77	0.010761	37.4	49.7	3	5.0%	86.0%	92.4	49.7	83.5	80.2
87	10.89	4.12	0.023981	38.1	50.3	3	4.0%	82.0%	93.7	50.3	83.0	79.0
88	10.59	4.41	0.047814	38.8	54.6	3	3.0%	80.0%	95.1	54.6	83.8	79.0
89	10.35	4.65	0.014565	35.1	49.6	3	3.0%	80.2%	95.1	49.6	86.0	81.6
90	10.14	4.87	0.017202	38.2	49.8	3	1.0%	79.0%	98.1	49.8	92.4	86.4
91	10.61	4.38	0.048086	35.0	54.8	3	1.1%	78.8%	98.1	54.8	90.8	83.9
92	22.97	7.01	0.051943	32.0	55.2	3	4.0%	76.9%	93.7	55.2	82.9	79.5
93	21.42	8.60	0.042708	30.8	54.0	3	6.0%	72.2%	91.4	54.0	80.5	78.5
94	23.14	6.86	0.052207	34.1	56.6	3	8.0%	74.4%	89.4	56.6	78.5	76.8
95	24.58	5.42	0.016764	34.8	49.8	3	8.0%	78.9%	89.4	49.8	81.6	80.1
96	11.46	3.52	0.011940	35.0	49.7	3	5.0%	85.9%	92.4	49.7	83.5	80.2
97	9.73	5.27	0.052356	35.1	57.5	3	0.0%	69.1%	100.0	57.5	100.0	99.8
98	16.12	7.86	0.053559	31.9	56.0	3	1.0%	71.9%	98.1	56.0	91.3	85.4
99	21.78	8.22	0.053002	34.0	55.5	3	4.0%	75.2%	93.7	55.5	82.8	79.5
100	11.59	9.40	0.015733	34.8	49.8	3	4.0%	73.1%	93.7	49.8	84.1	81.1
101	10.95	10.02	0.034415	34.7	53.5	3	3.0%	69.0%	95.0	53.5	84.2	80.6
102	10.48	10.53	0.055327	34.9	57.5	3	1.0%	69.0%	98.2	57.5	91.2	85.1
103	17.12	12.84	0.022381	32.2	49.8	3	1.0%	62.0%	98.1	49.8	92.3	87.1
104	14.02	16.00	0.062047	31.3	59.6	3	1.6%	61.9%	97.2	59.6	88.3	83.7
105	6.60	8.36	6.600000	35.0	49.7	3	0.0%	74.0%	99.9	49.7	99.6	97.8
106	6.60	8.38	0.026295	35.0	49.7	3	0.0%	73.9%	100.0	49.7	99.9	99.1

	CHEMCAD OUTPUTS				
No.	tray 3 temperature (C)	tray 4 temperature (C)	tray 5 temperature (C)	tray 6 temperature (C)	tray efficiency
4	74.0	70.8	68.9	67.5	0.51
5	73.7	70.5	68.8	67.5	0.46
6	73.3	70.2	68.7	67.5	0.44
7	72.6	69.6	68.4	67.5	0.37
8	75.5	72.4	70.2	68.5	0.44
13	72.7	69.2	68.0	67.0	0.44
14	73.2	69.3	68.0	67.1	0.42
15	73.1	69.5	68.4	67.5	0.34
16	72.0	69.2	68.2	67.5	0.31
17	72.0	69.2	68.2	67.5	0.31
18	71.7	69.0	68.1	67.4	0.30
19	71.7	69.2	68.4	67.7	0.26
21	73.1	69.5	68.1	67.0	0.46
22	73.1	69.8	68.3	67.2	0.45
23	72.7	69.4	68.1	67.1	0.42
24	72.2	69.1	68.0	67.1	0.40
25	72.1	68.9	67.7	66.9	0.41
26	72.1	69.4	68.8	68.2	0.20
27	72.7	69.8	69.2	68.6	0.17
29	72.7	68.4	66.8	65.9	0.69
30	73.6	69.2	67.5	66.3	0.64
32	72.8	68.3	66.9	66.0	0.62
33	73.3	68.9	67.2	66.1	0.68
34	74.5	71.6	70.1	68.8	0.30
35	74.6	71.7	69.7	68.1	0.46
36	78.0	74.4	71.1	68.6	0.61
37	79.3	75.1	71.3	68.7	0.64
38	78.5	72.6	70.0	68.1	0.53
39	76.9	73.3	70.7	68.8	0.46
40	76.7	73.1	70.6	68.8	0.45
41	76.7	73.3	70.6	68.6	0.50
42	76.7	73.1	70.3	68.3	0.55
43	77.2	73.6	70.6	68.4	0.57
44	88.6	83.3	75.5	69.8	1.00
45	94.9	94.4	91.6	82.3	1.00
46	95.3	93.4	86.0	75.2	1.00
47	96.5	95.2	89.0	77.3	1.00
48	97.3	96.2	90.6	78.5	1.00
49	92.8	91.8	87.3	77.6	1.00
50	94.3	92.5	85.5	75.2	1.00
51	95.8	94.4	88.1	76.9	1.00
52	96.8	95.9	90.7	79.0	1.00
53	93.3	93.0	91.1	83.4	1.00
54	93.2	90.8	83.3	74.0	1.00
55	95.1	93.8	87.8	76.9	1.00
56	95.4	93.3	85.4	74.7	1.00
57	95.7	93.7	86.1	75.1	1.00
58	96.8	94.9	87.1	75.6	1.00
59	96.4	95.0	88.4	76.8	1.00
60	97.3	95.4	87.5	75.6	1.00
61	97.6	95.9	88.1	76.0	1.00
62	91.8	88.1	79.7	71.8	1.00
63	92.5	89.4	91.3	72.7	1.00
64	95.9	93.6	85.1	74.3	1.00
65	97.6	95.8	87.6	75.6	1.00
67	96.2	94.3	86.4	75.2	1.00
68	92.5	91.8	88.4	79.5	1.00
69	96.1	95.2	90.2	79.0	1.00
72	83.3	79.3	74.3	70.5	1.00
73	82.5	78.0	74.0	71.1	0.44
74	96.8	95.4	88.7	76.9	1.00
75	78.5	74.3	71.9	70.2	0.35
76	78.5	74.9	73.0	71.4	0.25
77	80.0	76.7	73.8	71.4	0.33
78	79.6	75.7	72.4	69.7	0.51
79	78.5	74.0	71.5	69.6	0.40
80	80.6	75.9	72.7	70.3	0.43
81	80.6	76.3	72.9	70.4	0.44
82	81.5	76.3	72.9	70.6	0.42
83	79.0	74.0	71.6	69.7	0.38
84	77.8	73.1	71.0	69.4	0.37
85	76.0	72.2	70.5	69.1	0.34
86	78.3	72.4	69.8	68.0	0.55
87	76.5	72.0	69.9	68.4	0.43
88	75.8	72.2	70.2	68.7	0.40
89	78.9	73.8	71.0	69.1	0.46
90	81.5	75.8	72.1	69.6	0.51
91	78.6	73.9	71.1	69.2	0.45
92	77.1	72.7	70.8	69.3	0.36
93	76.9	73.0	71.4	70.1	0.28
94	75.5	71.9	70.6	69.5	0.27
95	79.0	72.9	70.8	69.1	0.39
96	78.2	72.3	69.7	67.9	0.54
97	98.5	97.1	90.0	77.2	1.00
98	80.6	75.6	72.8	70.6	0.39
99	77.2	73.1	71.1	69.6	0.34
100	78.9	76.0	73.1	70.7	0.37
101	78.0	74.9	72.7	70.9	0.30
102	80.3	76.4	73.4	71.2	0.36
103	82.5	84.5	79.9	75.0	0.43
104	80.2	77.2	74.5	72.5	0.28
105	91.2	89.6	83.9	75.2	1.00
106	95.1	93.2	85.8	75.2	1.00

		Data Used for Hybrid Parallel Modeling									
No.	original file name	feed	feed	feed	reflux	reflux	reboiler	tray1	tray2	tray3	tray4
		rate	composition	temperature	rate	temperature	temperature	temperature	temperature	temperature	temperature
		(lb/hr)	(mol% MeOH)	(C)	(lb/hr)	(C)	(C)	(C)	(C)	(C)	(C)
107	ex000114_ss1	24.00	30	35.4	15.75	50.0	99.1	94.5	88.7	81.6	77.5
108	ex000114_ss2	24.01	30	34.8	31.01	50.0	98.7	94.0	88.0	80.6	76.0
109	ex000114_ss3	23.96	29	35.8	28.93	50.0	98.4	94.0	88.0	80.4	75.8
110	ex000114_ss4	24.10	29	34.7	15.87	50.0	98.9	94.4	88.4	80.9	77.1
113	ex000118_ss1	23.97	30	34.5	15.66	50.0	97.6	93.4	85.2	80.0	77.6
114	ex000118_ss2	23.96	30	33.0	81.90	61.1	96.1	90.8	83.2	78.4	74.8
115	ex000118_ss3	15.00	30	34.9	81.58	58.3	97.6	95.0	87.7	81.3	73.3
116	ex000119_ss1	14.97	29	35.0	81.76	59.6	99.3	97.7	93.6	87.1	85.4
117	ex000119_ss2	29.94	27	32.1	15.70	50.0	96.6	92.3	84.9	79.6	77.6
118	ex000120_ss1	29.91	26	31.9	15.82	50.0	95.8	91.5	84.2	79.1	76.8
119	ex000120_ss2	29.92	26	32.1	81.71	60.6	95.0	91.2	83.5	77.9	74.7
120	ex000121_ss1	29.94	28	32.3	15.75	50.0	96.4	92.6	84.6	78.7	77.0
122	ex000128_ss1	29.96	28	30.6	81.80	60.9	95.6	92.2	84.1	77.8	75.3
123	ex000128_ss2	29.95	28	33.1	15.81	50.0	95.5	91.7	83.1	76.8	76.0
124	ex000128_ss3	29.96	28	32.8	81.78	61.3	94.3	90.9	81.6	75.7	74.0
125	ex000131_ss1	29.96	22	31.3	15.92	50.0	92.8	85.9	81.2	77.8	75.7
126	ex000131_ss2	29.95	21	30.0	81.77	61.0	92.0	84.6	79.9	76.9	73.8
127	ex000131_ss3	29.95	20	32.5	16.26	50.0	94.9	90.1	84.3	79.5	74.8
128	ex000201_ss1	29.95	21	32.4	16.01	50.0	95.8	91.3	85.1	80.0	76.1
129	ex000201_ss2	29.95	21	30.6	81.84	59.6	94.6	90.1	83.9	78.6	73.6
130	ex000201_ss3	29.97	20	32.4	16.08	50.0	95.1	90.6	84.5	79.4	75.8
131	ex000202_ss1	23.98	20	34.7	16.31	50.0	97.1	94.8	88.8	83.4	79.7
132	ex000202_ss2	23.97	20	33.9	81.50	57.8	96.4	94.1	87.9	82.1	76.7
133	ex000202_ss3	23.95	20	34.1	16.63	50.0	96.8	94.3	88.0	82.5	78.1
134	ex000203_ss1	14.99	20	29.1	16.26	50.0	98.6	97.2	94.0	88.4	85.6
135	ex000203_ss2	23.97	19	27.9	16.40	50.0	92.5	86.1	80.8	77.4	73.6
136	ex000203_ss3	23.91	19	27.4	81.51	58.5	91.0	84.2	79.3	76.4	71.4
137	ex000204_ss1	23.96	28	34.2	42.90	54.4	96.3	92.8	83.7	76.5	74.6
138	ex000204_ss2	23.96	28	34.1	81.66	59.5	96.8	93.7	85.1	78.1	76.4
139	ex000204_ss3	29.94	28	31.5	42.61	55.2	96.4	93.5	84.4	76.7	75.4
140	ex000209_ss1	23.98	28	35.6	16.07	50.0	96.5	93.2	85.1	79.4	76.2
141	ex000209_ss2	23.98	28	35.2	81.40	57.4	96.6	94.8	89.0	82.1	79.7
142	ex000210_ss1	23.98	26	35.3	16.17	50.0	99.4	97.6	91.8	85.3	83.4
143	ex000210_ss2	23.95	26	34.5	15.68	50.0	96.9	93.5	85.2	79.5	77.5
144	ex000217_ss1	14.98	31	35.0	15.77	50.0	100.3	98.6	94.2	87.5	87.9
145	ex000217_ss2	14.96	31	35.0	81.81	60.6	99.1	97.7	93.5	86.6	86.6
146	ex000217_ss3	29.96	29	33.1	15.65	50.0	96.2	92.4	83.8	77.6	76.9
147	ex000218_ss1	29.96	33	33.0	15.14	50.0	99.0	96.1	87.7	81.0	80.1

	Data Used for Hybrid Parallel Modeling			bottom composition	distillate composition	bottom composition
No.	tray5 temperature (C)	tray6 temperature (C)	efficiency (actual) (from ChemCAD)	(with fixed efficiency =0.4) (mol% meOH)	(with fixed efficiency =0.4) (mol% meOH)	(experiment) (mol% meOH)
107	78.8	74.3	0.48	0.5%	53.6%	1%
108	74.7	72.2	0.40	0.7%	66.1%	1%
109	74.6	72.0	0.41	0.9%	67.3%	1%
110	76.1	73.8	0.48	0.6%	56.4%	1%
113	76.7	75.0	0.34	1.3%	65.6%	2%
114	73.5	71.3	0.29	2.3%	78.0%	2%
115	71.6	68.8	1.00	1.3%	76.0%	0%
116	78.8	69.9	1.00	0.4%	68.1%	0%
117	76.6	74.8	0.44	1.9%	66.9%	1%
118	75.9	74.0	0.46	2.5%	69.2%	1%
119	73.3	70.4	0.33	3.0%	78.9%	1%
120	76.2	74.5	0.43	2.1%	67.6%	1%
122	73.9	71.1	0.29	2.6%	78.1%	1%
123	75.4	74.2	0.41	2.7%	69.9%	1%
124	73.2	71.1	0.39	3.5%	79.8%	1%
125	74.9	73.5	0.33	4.7%	74.6%	3%
126	72.9	70.8	0.24	5.4%	82.0%	3%
127	74.0	71.8	0.55	3.1%	71.3%	1%
128	75.2	73.1	0.50	2.5%	69.2%	1%
129	72.2	69.4	0.36	3.3%	79.3%	1%
130	74.9	72.7	0.51	2.9%	70.8%	1%
131	75.8	71.3	1.00	1.6%	67.6%	0%
132	72.5	67.9	1.00	2.1%	77.2%	0%
133	74.3	69.6	1.00	1.8%	66.6%	0%
134	80.6	71.6	1.00	0.7%	65.0%	0%
135	72.5	70.9	0.43	5.0%	76.4%	3%
136	70.2	68.1	0.30	6.3%	83.3%	3%
137	73.6	71.7	1.00	2.1%	75.6%	0%
138	73.8	69.5	1.00	1.9%	77.1%	0%
139	74.6	72.4	1.00	2.1%	74.5%	0%
140	75.1	72.8	0.48	2.0%	69.5%	1%
141	74.2	67.2	1.00	1.9%	77.0%	0%
142	78.5	72.1	1.00	0.3%	47.5%	0%
143	76.5	74.8	0.41	1.7%	68.1%	1%
144	83.1	74.3	0.45	0.4%	57.5%	1%
145	80.0	70.5	0.33	0.5%	69.8%	1%
146	76.3	75.1	0.41	2.2%	68.1%	1%
147	79.4	77.7	0.35	0.5%	51.5%	1%

No.	distillate composition (experiment) (mol% meOH)	error of distillate composition (experiment- fixed efficiency) (mol% meOH)	error of distillate composition (predicted by neural network) (mol% meOH)	distillate composition (hybrid parallel model) (mol% meOH)	residual error (experiment- hybrid parallel model) (mol% meOH)
107	70.0%	16.4%	10.4%	64.0%	6.0%
108	69.0%	2.9%	4.2%	70.3%	-1.3%
109	69.0%	1.7%	4.1%	71.4%	-2.4%
110	70.0%	13.6%	10.0%	66.4%	3.6%
113	64.0%	-1.6%	2.5%	68.2%	-4.2%
114	65.0%	-13.0%	-12.1%	65.9%	-0.9%
115	72.0%	-4.0%	-3.7%	72.3%	-0.3%
116	69.0%	0.9%	1.0%	69.1%	-0.1%
117	63.0%	-3.9%	-5.3%	61.6%	1.4%
118	65.0%	-4.2%	-5.6%	63.6%	1.4%
119	65.0%	-13.9%	-14.2%	64.8%	0.2%
120	62.0%	-5.6%	-4.5%	63.0%	-1.0%
122	60.0%	-18.1%	-15.2%	63.0%	-3.0%
123	60.0%	-9.9%	-6.1%	63.8%	-3.8%
124	71.0%	-8.8%	-17.0%	62.9%	8.1%
125	65.0%	-9.6%	-9.6%	65.0%	0.0%
126	62.0%	-20.0%	-20.0%	62.0%	0.0%
127	72.0%	0.7%	2.9%	74.2%	-2.2%
128	68.0%	-1.2%	-1.1%	68.1%	-0.1%
129	68.0%	-11.3%	-12.1%	67.2%	0.8%
130	69.0%	-1.8%	-0.8%	70.0%	-1.0%
131	77.0%	9.4%	9.8%	77.4%	-0.4%
132	74.0%	-3.2%	-2.6%	74.6%	-0.6%
133	81.0%	14.4%	13.7%	80.3%	0.7%
134	79.0%	14.0%	11.5%	76.4%	2.6%
135	75.0%	-1.4%	-0.3%	76.1%	-1.1%
136	70.0%	-13.3%	-12.5%	70.8%	-0.8%
137	65.0%	-10.6%	-8.9%	66.7%	-1.7%
138	69.0%	-8.1%	-7.3%	69.8%	-0.8%
139	63.0%	-11.5%	-12.5%	62.0%	1.0%
140	70.0%	0.5%	3.3%	72.8%	-2.8%
141	74.0%	-3.0%	-4.3%	72.8%	1.2%
142	77.0%	29.5%	14.7%	62.3%	14.7%
143	63.0%	-5.1%	-2.5%	65.6%	-2.6%
144	72.0%	14.5%	20.4%	78.0%	-6.0%
145	67.0%	-2.8%	-0.3%	69.5%	-2.5%
146	60.0%	-8.1%	-6.2%	61.9%	-1.9%
147	55.0%	3.5%	2.1%	53.6%	1.4%

	residual error	EXPERIMENT DATA									
No.	(experiment - fixed	feed	feed	reflux	bottom	distillate	reboiler	feed	reflux	feed	bottom
	efficiency model)	rate	composition	rate	rate	rate	duty	temperature	temperature	tray	composition
	(mol% meOH)	(lb/hr)	(mol% meOH)	(lb/hr)	(lb/hr)	(lb/hr)	(% of full power)	(C)	(C)		(mol% meOH)
107	16.4%	24.00	30%	15.75	12.22	11.08	100%	35.4	50.0	3	1%
108	2.9%	24.01	30%	31.01	11.94	11.33	100%	34.8	50.0	3	1%
109	1.7%	23.96	29%	28.93	11.52	11.67	90%	35.8	50.0	3	1%
110	13.6%	24.10	29%	15.67	11.88	11.46	90%	34.7	50.0	3	1%
113	-1.8%	23.97	30%	15.66	11.82	11.64	60%	34.5	50.0	3	2%
114	-13.0%	23.96	30%	81.90	12.03	11.03	60%	33.0	61.1	3	2%
115	-4.0%	15.00	30%	81.58	7.53	6.26	60%	34.9	58.3	3	0%
116	0.9%	14.97	29%	81.78	7.04	6.61	70%	35.0	59.6	3	0%
117	-3.9%	29.94	27%	15.70	14.51	14.89	90%	32.1	50.0	3	1%
118	-4.2%	29.91	26%	15.82	15.22	14.72	80%	31.9	50.0	3	1%
119	-13.9%	29.92	26%	81.71	12.82	16.08	80%	32.1	60.6	3	1%
120	-5.6%	29.94	28%	15.75	11.73	17.59	70%	32.3	50.0	3	1%
122	-18.1%	29.96	28%	81.80	11.11	18.24	90%	30.6	60.9	3	1%
123	-9.9%	29.95	28%	15.81	8.74	20.62	60%	33.1	50.0	3	1%
124	-8.8%	29.96	28%	81.78	7.70	20.14	60%	32.8	61.3	3	1%
125	-9.6%	29.96	22%	15.92	19.05	11.14	60%	31.3	50.0	3	3%
126	-20.0%	29.95	21%	81.77	17.74	12.57	60%	30.0	61.0	3	3%
127	0.7%	29.95	20%	16.26	20.59	9.79	80%	32.5	50.0	3	1%
128	-1.2%	29.95	21%	16.01	19.83	10.64	90%	32.4	50.0	3	1%
129	-11.3%	29.95	21%	81.64	18.99	11.20	90%	30.6	59.6	3	1%
130	-1.8%	29.97	20%	16.08	19.56	10.94	100%	32.4	50.0	3	1%
131	9.4%	23.98	20%	16.31	15.98	8.05	90%	34.7	50.0	3	0%
132	-3.2%	23.97	20%	81.50	15.67	8.45	90%	33.9	57.8	3	0%
133	14.4%	23.95	20%	16.63	16.81	7.55	80%	34.1	50.0	3	0%
134	14.0%	14.99	20%	16.28	9.61	4.95	90%	29.1	50.0	3	0%
135	-1.4%	23.97	19%	16.40	17.38	6.71	80%	27.9	50.0	3	3%
136	-13.3%	23.91	19%	81.51	18.43	6.37	60%	27.4	58.5	3	3%
137	-10.8%	23.96	28%	42.90	4.03	17.33	60%	34.2	54.4	3	0%
138	-8.1%	23.96	28%	81.66	6.06	16.16	80%	34.1	59.5	3	0%
139	-11.5%	29.94	28%	42.61	4.21	23.69	100%	31.5	55.2	3	0%
140	0.5%	23.98	28%	16.07	9.63	12.58	80%	35.6	50.0	3	1%
141	-3.0%	23.98	28%	81.40	7.35	9.25	80%	35.2	57.4	3	0%
142	29.5%	23.98	26%	16.17	9.05	7.93	70%	35.3	50.0	3	0%
143	-5.1%	23.95	26%	15.68	10.67	12.94	60%	34.5	50.0	3	1%
144	14.5%	14.98	31%	15.77	8.87	7.02	70%	35.0	50.0	3	1%
145	-2.8%	14.96	31%	81.81	8.11	8.05	70%	35.0	60.8	3	1%
146	-8.1%	29.96	29%	15.85	8.26	20.52	60%	33.1	50.0	3	1%
147	3.5%	29.96	33%	15.14	7.79	20.95	70%	33.0	50.0	3	1%

	EXPERIMENT DATA									DATA RECONCILIATI			
No.	distillate	reboiler	distillate	tray 1	tray 2	tray 3	tray 4	tray 5	tray 6	alpha	beta	overall	MeOH
	composition	temperature	temperature	temperature	temperature	temperature	temperature	temperature	temperature			material	material
	(mol% meOH)	(C)	(C)	(C)	(C)	(C)	(C)	(C)	(C)			balance	balance
107	70%	99.1	41.5	94.5	88.7	81.6	77.5	76.5	74.3	-0.85	1.55	0.00	0.00
108	69%	98.7	44.0	94.0	88.0	80.6	76.0	74.7	72.2	-0.69	1.43	0.00	0.00
109	69%	98.4	44.1	94.0	88.0	80.4	75.8	74.6	72.0	0.07	0.70	0.00	0.00
110	70%	98.9	41.2	94.4	88.4	80.9	77.1	76.1	73.8	-0.10	0.86	0.00	0.00
113	64%	97.6	42.1	93.4	85.2	80.0	77.6	76.7	75.0	-1.00	1.51	0.00	0.00
114	65%	96.1	48.3	90.8	83.2	78.4	74.8	73.5	71.3	-1.07	1.97	0.00	0.00
115	72%	97.6	47.5	95.0	87.7	81.3	73.3	71.6	68.8	-0.44	1.65	0.00	0.00
116	69%	99.3	47.6	97.7	93.6	87.1	85.4	78.6	69.9	0.04	1.28	0.00	0.00
117	63%	96.6	43.5	92.3	84.9	79.6	77.6	76.6	74.8	-0.03	0.57	0.00	0.00
118	65%	95.8	43.0	91.5	84.2	79.1	76.8	75.9	74.0	0.06	-0.09	0.00	0.00
119	65%	95.0	49.0	91.2	83.5	77.9	74.7	73.3	70.4	2.46	-1.44	0.00	0.00
120	62%	96.4	43.9	92.6	84.6	78.7	77.0	76.2	74.5	2.08	-1.46	0.00	0.00
122	60%	95.6	49.2	92.2	84.1	77.8	75.3	73.9	71.1	2.34	-1.73	0.00	0.00
123	60%	95.5	44.8	91.7	83.1	76.8	76.0	75.4	74.2	4.70	-4.11	0.00	0.00
124	71%	94.3	49.3	90.9	81.6	75.7	74.0	73.2	71.1	7.53	-5.41	0.00	0.00
125	65%	92.8	42.0	85.9	81.2	77.8	75.7	74.9	73.5	-0.89	0.66	0.00	0.00
126	62%	92.0	48.9	84.6	79.9	76.9	73.8	72.9	70.8	0.57	-0.93	0.00	0.00
127	72%	94.9	39.7	90.1	84.3	79.5	74.6	74.0	71.6	-1.46	1.03	0.00	0.00
128	68%	95.8	40.4	91.3	85.1	80.0	76.1	75.2	73.1	-1.63	1.11	0.00	0.00
129	68%	94.6	48.1	90.1	83.9	78.6	73.6	72.2	69.4	-0.79	0.55	0.00	0.00
130	69%	95.1	40.7	90.6	84.5	79.4	75.8	74.9	72.7	-0.73	0.20	0.00	0.00
131	77%	97.1	38.5	94.8	88.8	83.4	79.7	75.8	71.3	-0.62	0.57	0.00	0.00
132	74%	96.4	47.1	94.1	87.9	82.1	76.7	72.5	67.9	-0.53	0.38	0.00	0.00
133	81%	96.8	37.7	94.3	88.0	82.5	78.1	74.3	69.6	-1.20	0.79	0.00	0.00
134	79%	98.6	36.7	97.2	94.0	88.4	85.6	80.6	71.6	0.08	0.35	0.00	0.00
135	75%	92.5	38.9	86.1	80.8	77.4	73.6	72.5	70.9	-0.76	0.64	0.00	0.00
136	70%	91.0	47.4	84.2	79.3	76.4	71.4	70.2	68.1	-2.20	1.31	0.00	0.00
137	65%	96.3	46.9	92.8	83.7	76.5	74.6	73.6	71.7	7.17	-4.57	0.00	0.00
138	69%	96.6	48.0	93.7	85.1	78.1	76.4	73.8	69.5	5.63	-3.89	0.00	0.00
139	63%	96.4	47.4	93.5	84.4	78.7	75.4	74.6	72.4	9.45	-7.41	0.00	0.00
140	70%	96.5	41.7	93.2	85.1	79.4	76.2	75.1	72.8	2.45	-0.68	0.00	0.00
141	74%	96.6	47.1	94.8	89.0	82.1	79.7	74.2	67.2	4.89	2.49	0.00	0.00
142	77%	99.4	38.1	97.6	91.8	85.3	83.4	78.5	72.1	4.16	2.84	0.00	0.00
143	63%	96.9	42.2	93.5	85.2	79.5	77.5	76.5	74.8	1.31	-0.97	0.00	0.00
144	72%	100.3	39.2	98.6	94.2	87.5	87.9	83.1	74.3	0.15	0.94	0.00	0.00
145	67%	99.1	48.0	97.7	93.5	86.6	86.6	80.0	70.5	0.52	0.28	0.00	0.00
146	60%	96.2	45.6	92.4	83.8	77.6	76.9	76.3	75.1	4.68	-3.50	0.00	0.00
147	55%	99.0	45.8	96.1	87.7	81.0	80.1	79.4	77.7	2.00	-0.76	0.00	0.00

	DATA RECONCILIATION		CHEMCAD INPUTS							CHEMCAD OUTPUTS		
No.	reconciled	reconciled	MeOH	water	feed	reflux	bottom	reflux T	sub cooled	feed	feed	reflux
	bottom rate	distillate rate	flow rate	flow rate	temperature	rate	rate	temperature	temperature	rate	composition	rate
	(lb/hr)	(lb/hr)	(lb/hr)	(lb/hr)	(C)	(lb/hr)	(lb/hr)	(C)	(C)	(lb/hr)	(mol% meOH)	(lb/hr)
107	11.37	12.63	10.3784	13.6216	35.4	15.75	11.37	50.0	19.00	24.00	30%	15.75
108	11.25	12.76	10.3627	13.6273	34.8	31.01	11.25	50.0	20.00	24.01	30%	31.01
109	11.59	12.37	10.0793	13.8807	35.8	28.93	11.59	50.0	20.00	23.96	29%	28.93
110	11.78	12.32	10.1382	13.9618	34.7	15.87	11.78	50.0	19.00	24.10	29%	15.87
113	10.82	13.15	10.3654	13.6046	34.5	15.66	10.82	50.0	20.00	23.97	30%	15.66
114	10.96	13.00	10.3811	13.5989	33.0	81.90	10.96	61.1	9.00	23.96	30%	81.90
115	7.09	7.91	6.4865	8.5135	34.9	81.58	7.09	58.3	11.00	15.00	30%	81.58
116	7.08	7.89	6.2974	8.6726	35.0	81.76	7.08	59.6	10.00	14.97	29%	81.76
117	14.48	15.46	11.8770	18.0630	32.1	15.70	14.48	50.0	21.00	29.94	27%	15.70
118	15.28	14.63	11.4996	18.4104	31.9	15.82	15.28	50.0	20.00	29.91	26%	15.82
119	15.28	14.64	11.5034	18.4166	32.1	81.71	15.28	60.6	10.00	29.92	26%	81.71
120	13.81	16.13	12.2382	17.7018	32.3	15.75	13.81	50.0	21.00	29.94	28%	15.75
122	13.45	16.51	12.2464	17.7136	30.8	81.80	13.45	60.9	10.00	29.96	28%	81.80
123	13.44	16.51	12.2423	17.7077	33.1	15.81	13.44	50.0	21.00	29.95	28%	15.81
124	15.23	14.73	12.2464	17.7136	32.8	81.78	15.23	61.3	8.00	29.96	28%	81.78
125	18.18	11.80	10.0056	19.9544	31.3	15.92	18.18	50.0	20.00	29.96	22%	15.92
126	18.31	11.64	9.6115	20.3385	30.0	81.77	18.31	61.0	10.00	29.95	21%	81.77
127	19.13	10.82	9.2154	20.7346	32.5	16.26	19.13	50.0	19.00	29.95	20%	16.26
128	18.20	11.75	9.6115	20.3385	32.4	16.01	18.20	50.0	20.00	29.95	21%	16.01
129	18.20	11.75	9.6115	20.3385	30.8	81.64	18.20	59.6	10.00	29.95	21%	81.64
130	18.83	11.14	9.2215	20.7485	32.4	16.08	18.83	50.0	20.00	29.97	20%	16.08
131	15.36	8.62	7.3785	16.6015	34.7	16.31	15.36	50.0	18.00	23.98	20%	16.31
132	15.14	8.83	7.3754	16.5948	33.9	81.50	15.14	57.8	11.00	23.97	20%	81.50
133	15.61	8.34	7.3692	16.5808	34.1	16.63	15.61	50.0	18.00	23.95	20%	16.63
134	9.69	5.30	4.6123	10.3777	29.1	16.28	9.69	50.0	18.00	14.99	20%	16.28
135	16.62	7.35	7.0541	16.9159	27.9	16.40	16.62	50.0	18.00	23.97	19%	16.40
136	16.23	7.68	7.0364	16.8736	27.4	81.51	16.23	58.5	11.00	23.91	19%	81.51
137	11.20	12.76	9.7939	14.1661	34.2	42.90	11.20	54.4	16.00	23.96	28%	42.90
138	11.69	12.27	9.7939	14.1661	34.1	81.66	11.69	59.5	10.00	23.96	28%	81.66
139	13.66	16.28	12.2382	17.7018	31.5	42.61	13.66	55.2	15.00	29.94	28%	42.61
140	12.08	11.90	9.8020	14.1780	35.6	16.07	12.08	50.0	19.00	23.98	28%	16.07
141	12.24	11.74	9.8020	14.1780	35.2	81.40	12.24	57.4	11.00	23.98	28%	81.40
142	13.21	10.77	9.2197	14.7803	35.3	16.17	13.21	50.0	18.00	23.98	26%	16.17
143	11.98	11.97	9.2081	14.7419	34.5	15.68	11.98	50.0	21.00	23.95	26%	15.68
144	7.02	7.96	6.6518	8.3282	35.0	15.77	7.02	50.0	19.00	14.98	31%	15.77
145	6.63	8.33	6.6429	8.3171	35.0	81.81	6.63	60.6	9.00	14.96	31%	81.81
146	12.94	17.02	12.6033	17.3567	33.1	15.65	12.94	50.0	21.00	29.96	29%	15.65
147	9.79	20.17	13.9866	15.9734	33.0	15.14	9.79	50.0	22.00	29.96	33%	15.14

	CHEMCAD OUTPUTS											
No.	bottom	distillate	reboiler	feed	reflux	feed	bottom	distillate	reboiler	distillate	tray 1	tray 2
	rate	rate	duty	temperature	temperature	tray	composition	composition	temperature	temperature	temperature	temperature
	(lb/hr)	(lb/hr)	(MMBtu/hr)	(C)	(C)		(mol% meOH)	(mol% meOH)	(C)	(C)	(C)	(C)
107	11.37	12.63	0.018581	35.4	50.4	3	1.0%	70.0%	98.1	50.4	92.4	86.8
108	11.25	12.76	0.028034	34.8	49.5	3	1.0%	69.0%	98.2	49.5	91.8	86.2
109	11.59	12.37	0.026517	35.8	49.5	3	1.0%	69.1%	98.2	49.5	92.2	86.7
110	11.78	12.32	0.018529	34.7	50.4	3	1.0%	70.0%	98.1	50.4	92.4	86.9
113	10.82	13.15	0.019522	34.5	50.4	3	2.0%	64.0%	96.5	50.4	88.1	84.0
114	10.96	13.00	0.059234	33.0	61.2	3	1.9%	65.2%	96.7	61.2	86.9	82.3
115	7.09	7.91	0.053495	34.9	58.0	3	0.0%	71.9%	100.0	58.0	100.0	99.7
116	7.08	7.89	0.054563	35.0	59.5	3	0.0%	69.0%	100.0	59.5	100.0	99.7
117	14.48	15.46	0.021784	32.1	49.6	3	1.0%	63.0%	98.2	49.6	92.7	87.7
118	15.28	14.63	0.021133	31.9	50.2	3	1.0%	65.0%	98.2	50.2	92.8	87.8
119	15.28	14.64	0.061021	32.1	60.3	3	1.0%	64.9%	98.1	60.3	91.1	85.7
120	13.81	16.13	0.022309	32.3	49.8	3	1.0%	62.1%	98.2	49.8	92.7	87.6
122	13.45	16.51	0.064200	30.6	61.2	3	1.0%	60.0%	98.2	61.2	91.1	86.0
123	13.44	16.51	0.022811	33.1	50.2	3	0.9%	60.1%	98.2	50.2	92.7	87.7
124	15.23	14.73	0.058446	32.8	61.2	3	1.0%	71.1%	98.2	61.2	91.5	85.5
125	18.16	11.80	0.019573	31.3	50.2	3	3.0%	65.1%	95.1	50.2	86.7	83.8
126	18.31	11.64	0.060533	30.0	60.8	3	3.0%	62.1%	95.1	60.8	84.2	81.2
127	19.13	10.82	0.018547	32.5	50.2	3	1.0%	72.1%	98.2	50.0	93.6	88.8
128	18.20	11.75	0.019345	32.4	49.7	3	1.0%	68.1%	98.2	49.7	93.4	88.7
129	18.20	11.75	0.058346	30.6	59.7	3	1.0%	68.0%	98.1	59.7	91.5	86.0
130	18.83	11.14	0.018968	32.4	49.5	3	1.0%	69.0%	98.2	49.5	93.5	88.9
131	15.36	8.62	0.016341	34.7	50.2	3	0.1%	76.5%	99.8	50.2	99.2	96.8
132	15.14	8.83	0.054238	33.9	57.7	3	0.0%	74.0%	100.0	57.7	99.9	99.6
133	15.61	8.34	0.016026	34.1	49.6	3	0.1%	80.5%	99.8	49.6	99.0	96.4
134	9.69	5.30	0.013621	29.1	49.8	3	0.0%	78.8%	99.9	49.8	99.6	98.1
135	16.62	7.35	0.015954	27.9	50.5	3	3.0%	74.9%	95.0	50.5	86.9	83.5
136	16.23	7.68	0.054861	27.4	58.4	3	3.0%	69.9%	95.0	58.4	84.1	80.4
137	11.20	12.76	0.036247	34.2	54.2	3	0.0%	65.0%	100.0	54.2	99.9	99.1
138	11.69	12.27	0.057627	34.1	59.5	3	0.0%	69.0%	100.0	59.5	99.9	99.5
139	13.66	16.28	0.039227	31.5	55.6	3	0.0%	63.0%	100.0	55.6	99.8	98.9
140	12.08	11.90	0.018389	35.6	50.4	3	1.0%	70.0%	98.1	50.4	92.6	87.2
141	12.24	11.74	0.055568	35.2	57.7	3	0.0%	74.0%	100.0	57.7	99.9	99.5
142	13.21	10.77	0.017251	35.3	50.2	3	0.1%	76.7%	99.8	50.2	99.1	96.3
143	11.98	11.97	0.019085	34.5	49.6	3	1.0%	63.1%	98.2	49.6	92.8	87.9
144	7.02	7.96	0.015014	35.0	50.0	3	1.0%	72.0%	98.2	50.0	92.2	86.3
145	6.63	8.33	0.055038	35.0	60.9	3	1.1%	66.9%	98.1	60.9	90.3	84.4
146	12.94	17.02	0.022995	33.1	50.2	3	0.9%	60.0%	98.2	50.2	92.6	87.5
147	9.79	20.17	0.025275	33.0	50.1	3	1.0%	55.0%	98.1	50.1	91.7	86.6

	CHEMCAD OUTPUTS				
No.	tray 3 temperature (C)	tray 4 temperature (C)	tray 5 temperature (C)	tray 6 temperature (C)	tray efficiency
107	82.0	81.2	76.5	72.5	0.48
108	81.5	78.7	74.7	71.8	0.40
109	81.9	79.0	74.9	71.8	0.41
110	82.2	81.2	76.5	72.5	0.48
113	80.9	80.4	76.4	73.1	0.34
114	78.9	76.0	73.6	71.7	0.29
115	97.8	98.1	88.2	76.0	1.00
116	97.9	98.6	89.7	77.3	1.00
117	83.2	84.2	79.3	74.5	0.44
118	83.3	83.7	78.7	74.0	0.46
119	81.2	77.5	74.4	72.1	0.33
120	83.1	84.5	79.7	74.8	0.43
122	81.8	78.6	75.4	73.0	0.29
123	83.2	85.1	80.2	75.2	0.41
124	80.5	76.5	73.2	70.9	0.39
125	81.6	79.2	75.6	72.6	0.33
126	78.9	75.7	73.7	72.1	0.24
127	84.4	81.9	76.8	72.2	0.55
128	84.4	83.0	77.7	73.2	0.50
129	81.4	76.9	73.8	71.4	0.36
130	84.6	82.7	77.4	72.9	0.51
131	90.7	86.6	82.4	74.1	1.00
132	97.4	95.4	86.9	75.1	1.00
133	90.1	87.0	79.9	72.4	1.00
134	93.1	90.2	82.0	73.0	1.00
135	81.1	76.3	73.0	70.4	0.43
136	77.8	74.2	72.2	70.6	0.30
137	95.3	94.4	89.7	79.0	1.00
138	97.0	95.7	89.2	77.3	1.00
139	94.5	93.8	89.9	79.8	1.00
140	82.5	81.2	76.4	72.4	0.48
141	96.7	94.8	86.6	75.2	1.00
142	89.1	87.2	81.6	74.0	1.00
143	83.5	83.2	78.2	73.9	0.41
144	81.4	78.8	74.6	71.4	0.45
145	79.8	76.3	73.5	71.5	0.33
146	83.0	85.1	80.3	75.3	0.41
147	82.2	86.1	81.7	76.6	0.35

VITA

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