NATIONAL PETROCHEMICAL & REFINERS ASSOCIATION
1899 L STREET, N.W., SUITE 1000
WASHINGTON, D.C. 20036

CC-00-148

REFINING AND PETROCHEMICAL PROPERTY PREDICTORS FOR DISTILLATION, FRACTIONATION, AND CRUDE SWITCH

By

Greg Martin
Director, Business Development
Pavilion Technologies, Inc.
Austin, Texas

Gary Barber
Project Director, Information Technology
The Automation Group, Inc.
Houston, Texas

Zak Friedman
Principal Consultant
Petrocontrol
Hoboken, New Jersey

Ed Bullerdiek
Operations Systems Engineer
Marathon Ashland
Robinson, Illinois

Presented at the

NPRA
2000 Computer Conference
November 13-15, 2000
Palmer House Hilton Hotel
Chicago, Illinois

REFINING AND PETROCHEMICAL PROPERTY PREDICTORS FOR DISTILLATION, FRACTIONATION, AND CRUDE SWITCH

Greg Martin
Pavilion Technologies, Inc.
Austin, Texas
gmartin@pav.com

Zak Friedman
Petrocontrol
Hoboken, New Jersey
petrocontrol@earthlink.net

Gary Barber
The Automation Group, Inc.
Houston, Texas
garyb@tagsite.com

Ed Bullerdiek
Marathon Ashland
Robinson, Illinois
eabullerdiek@mapllc.com

KEYWORDS

Property Predictors, Virtual On-line Analyzers (VOAs), Soft Sensors, Refining, Petrochemical, Distillation, Fractionation, Crude Switch

ABSTRACT

This paper discusses the technical feasibility, practical utility, sufficient accuracy, and economic viability of property predictors engineered using datamining software. Model types include empirical models based on neural networks, physical models from engineering equations, and hybrid combinations of both. Simple guidelines are presented to determine where an empirical property predictor will work and where it will not. Several field examples are included, with deployment times ranging from two to four man weeks and installed accuracies approaching that of the lab. ROIs of less than six months are calculated. A rollout program is described where a U.S. refiner is currrently progressing through field installations of property predictors across seven refineries.

INTRODUCTION

Commercial property predictors (aka. “soft sensors”, “virtual analyzers”) based on neural networks were introduced in two 1996 papers [1,2]. A property predictor is a single-output neural network model that is trained on a large set of process and lab data. It is implemented in a field on-line module to replace or supplement an existing analyzer or provide continuous feedback to the operator or a control application.

Crude switch property predictors [3,4,5,6] are quite different, as they are based on high fidelity physical models. The model is called GCC (Generalized Cutpoint Calculation). The technology is also coined by the name “crude switch” because of its ability to provide property calculations through crude switches.

This paper presents the neural network property predictors in the next six sections. The final four sections discuss the crude switch property predictor. The ultimate intent is to combine the two approaches. Use GCC for crude switches. Use the empirical models to model and correct the GCC mismatch against lab data, taking into account secondary factors.

WHEN IS A PROPERTY PREDICTOR LIKELY TO WORK?

In a nutshell, empirical property predictors, whether constructed using neural networks or first principle models, will work on applications where there is a significant temperature profile in the tower. Most distillation columns in refining and petrochemicals are of that category.

The reason for this is the models use temperature information as a primary input to the correlation. Changes in the property being predicted must be reflected in changing measured temperatures. An example of a column that does not lend itself to inference models is a C3 splitter, which has basically the same temperature throughout the entire tower. Overhead C3 or bottoms C3= cannot be inferred from temperature measurements.

The second requirement for a successful property predictor is that the tower operation must exhibit significant changes in the property and or significant changes in the tower variables to achieve a constant property. In other words, there must be information about how the tower operates in the data used to build the model. If the tower runs consistently at the same point and with the same operational settings, then an empirical property predictor is not feasible. This is actually a moot point, however, since such an operation does not call for a property predictor in the first place.

BUILDING A PROPERTY PREDICTOR MODEL

This section uses a field example of a fractionator kerosene 90% point property predictor. This property predictor is currently operational in a refinery in eastern Canada.

Data Collection

Property predictors are modeled from historical process and lab data. The process data may come from a data historian or an information system, it may come from a SCADA package historian, or it may be made up of sets of data that were periodically downloaded from a DCS historian. The lab data are a time-stamped dataset that may come from a lab system or an information system.

Data collection amounts to gathering the field and lab data for a period of representative process operation wherein the process moved over the range for which the property predictor will be valid. It is imperative that the data include periods of steady-state behavior, since the property predictor model is a quasi-steady-state* model.

Typically data collection is an iterative exercise, where a first dataset is modeled and then more data are collected to improve the accuracy or range of the property predictor that results.

Data normally arrive in a disorganized flat file format similar to that shown in Figure 1.

Format

The format step transforms the flat file of data into a spreadsheet format for editing.

Formatting does not change the data file in any way, it merely reorganizes it so that it can be edited in an efficient and user-friendly way.

The formatted data are shown in Figure 2.

Preprocess

Preprocess is the data editing step. The engineer examines the data file, removes bad data (such as process upset or shutdown data), filters the data, interpolates through periods of missing data, and introduces transforms (e.g., takes the log of a composition). During this step it is preferable to view the data graphically as shown in Figure 3.

Model

The modeling step trains the neural network on the preprocessed data. During training the engineer usually monitors the training error and the test error to watch for convergence. Training windows for the kerosene 90% point model are shown in Figure 4.

For modeling the data are divided into three sets: the training set, the test set, and the validation set. The validation set is saved away and not used for training or testing. The training set is the set over which the backpropagation algorithm is exercised. The test set is used periodically to determine the accuracy of the model on data that it was not trained on. When train error and test error are minimized the neural network parameters are saved and become the "model". The model is then verified by executing it over the verification set and noting how well the soft sensor output matches the analysis measurement

Analyze

The main purpose of this step is to check the model, to see if the inputs that were determined to be important during training make engineering sense. The sensitivities of the model inputs are examined graphically or in table form as shown in Figure 5.

*The term "quasi-steady-state" is used to indicate a steady-state model with dynamically synchronized inputs (i.e., delays on the inputs).

During the analyze step inputs that do not contribute to the model can be removed and the model step repeated. By this procedure complex models having dozens of inputs can be pared down to simpler, more meaningful models with only a few inputs.

MARATHON ASHLAND ADVANCED CONTROL PROGRAM

The use of property predictor models for quality control is an integral part of Marathon Ashland Petroleum's (MAP) advanced process control strategy. Starting in 1994 MAP has installed over 50 property predictors and expects to install more than 200 in our seven-refinery system. Figure 6 lists some of the property predictors that have been installed.

Why Neural Networks?

From a user's perspective the technology is irrelevant. MAP's goal is to use a technology that is accurate, low cost, has good analysis speed, and is easy to deploy and maintain. For most refinery applications neural networks meet this need. An additional benefit is the model development process improves process understanding.

It is MAP's experience that the accuracy of a property predictor is usually limited by the accuracy of the refinery control lab. Typically the standard deviation of error of the property predictor will be less than 1.5 times the standard deviation of error of the lab test method, and will frequently approach the standard deviation of error of the lab. For example, if the standard deviation of error of a 90% point distillation lab method is 5°F, the standard deviation of error of the property predictor should fall between 5°F and 7.5°F. If an appropriate model bias update routine is used average error will be zero.

The time required for an experienced engineer to develop and install a property predictor model will range between a few days for a straight forward model (most models) to two to four weeks for an unusual or difficult application. The time to update a model can be under a day depending on the extent of the changes. If the models are done in volume the expected installed cost should be under $30,000/model.

The dynamic response of a property predictor is very similar to the dominant process inputs to the model, which in a refinery model are typically temperatures. MAP typically executes the models on 30 to 60 second cycles, although there is no reason cycle time couldn't be pushed under 5 seconds. Property predictors are superior to process analyzers in closed loop control because of their fast update speeds and good dynamic response (read "no deadtime").

MAP has used property predictors as indicators, as inputs to single loop (PID) controllers, and as inputs to multivariable controllers from Aspen (DMC) and Honeywell (RMPCT). When a neural network model is used with a linear controller you should make sure the model response in reasonably linear over the range of interest.

Keys to Success:

Excellent process knowledge is the single most important requirement to develop a successful property predictor. Empirical modeling tools such as neural networks will find relationships between variables that may or may not have engineering merit. The engineer must determine whether the relationship is real and whether it should be included in a final model. For example MAP has found that stream rundown temperatures are almost always related to product endpoint; this is not an input we would include in an online model. In general, the most successful models have the fewest number of inputs consistent with good accuracy.

Obviously lots of good quality process and lab data is required. MAP has had data historians installed in all the refineries for several years. The data used to train a model should cover all normal process operations; it is recommend that a minimum of one year of data be used to train a model. If sufficient data is not available initially a model is built with what is available and later updated when new data becomes available.

A bias update routine is recommended to correct for unmeasured disturbances and meter drift.

Finally, property predictors and process analyzers should be monitored for accuracy. Standard statistical process control tools will work very well.

CRUDE SWITCH PROPERTY PREDICTOR

The crude switch technology was developed by Y. Zak Friedman of Petrocontrol [3] as a unique approach to multi-draw fractionator inferential properties. Fundamentally, the thermal capacitance of the fractionation system is significantly less than its material capacitance. Thus, during a disturbance, such as a crude switch, the tower may be out of material balance for hours depending upon the magnitude of the disturbance. But the energy balance reacts more quickly – in minutes – and can be used to detect the upset, calculate the shift in the overall TBP curve, and calculate the resulting changes in product qualities. The technology works as follows:

Naphtha cutpoint calculation

The column top temperature is indicative of overhead product EFV (Equilibrium Flash Vaporization) endpoint (dew point). GCC applies standard API methods to first correct the top temperature measurement for partial pressure and then convert from EFV to cutpoint TBP.

Flash zone vapor flow calculation from heat balance

Flash zone vapor flow is calculated, not measured. This is one of the important advantages of this method because during upsets the column often operates off mass balance, and the only precise way to measure vapor flow is by heat balance. Moreover, timing of the heat balance calculation is nearly perfect in the sense that it is in phase with crude volatility, i.e., as lighter crude enters the column with higher vapor load, the cooling load immediately increases.

Flash zone cutpoint calculation

The flash zone temperature is indicative of flash zone vapor EFV endpoint. GCC applies standard API methods to first correct the flash zone temperature measurement for partial pressure and then convert from EFV to cutpoint TBP. The conversion technique is the same as the one for naphtha cutpoint calculation.

Crude TBP slope calculation

The model initially assumes a linear boiling curve between naphtha and flash zone cutpoints. Nonlinearities are then estimated from the column temperature profile. The correction of TBP curve nonlinearities is beneficial for cokers and visbreakers, but usually not on crude fractionators, as most crude oils do have a straight line boiling curve.

Sidestream distillation qualities

With the TBP curve reconstructed, front and back cutpoints of all side-streams become known. All distillation qualities are calculated as a function of front and back cuts, and to a lesser extent of internal reflux.

Internal reflux calculation

For cooling load distribution (pumparound) effects the model performs heat balances to compute liquid and vapor flows on critical trays. Constraints such as flooding or weeping are inferred from that data.

CRUDE SWITCH EXAMPLE

An example trend of key variables during a crude switch is shown in Figures 7 and 8. Figure 7 shows minute by minute prediction of crude TBP slope, as well as throughput and sidestream flows (parameter FLIQ is a sum of the sidestream flows). The slope has changed from 5.5 to 5.0 ºC/%, indicating a significant switch from heavy to light crude, and throughput was reduced by 15% to permit this operation. Figure 8 shows how well the product qualities were kept during the switch. Initially all cutpoints dipped, because of physical limits of how quickly the furnace coil outlet temperature and other controllers can move. The bulk of crude switch is over in 40 minutes, and steady state is reached in two hours. Note that the steady state property changes are due to new processing orders associated with the new crude.

NEURAL NETWORK CONTRIBUTION TO THE TECHNOLOGY

The neural network system is used during the learning phase to parameterize the crude switch property predictor thermodynamic equations to fit the column application using plant data and engineering judgement. The nonlinear TBP curve corrections from the neural network fit all column temperature measurements and become an integral part of the learning phase. The two technologies are thus combined to produce the property predictor model that will be implemented on-line. This off-line exercise is illustrated in the top portion of Figure 9.

The on-line executable reads plant data as inputs and calculates the properties, as illustrated in the bottom portion of Figure 9. Typical properties are 90% point, flash point, etc. When a density analyzer is available on one of the sidestreams the model can also predict cold properties: pour, cloud and freeze points.

The ultimate use of physical - neural predictors is to provide continuous feedback, in the form of control variables, to a Model Predictive Control (MPC) application that controls the product properties. The heat balance approach renders the inferential control variables dynamically accurate during an upset, making MPC dynamics simple and easy to tune. Upon a disturbance, the MPC controller reaches its correct manipulated variable positions in minutes, smoothly and quickly countering any process upset.

In comparison to the heat balance approach, inferences based on flow measurements are slow and often can exhibit an exaggerated inverse response (see Figure 10). To act on the poor inference response behavior, the MPC must be significantly de-tuned, to the point of losing the ability to respond to crude switches or other major disturbances. The physical - neural property predictors permit MPC tuning about five times faster than with flow measured inferences.

The use and fit of the complete column temperature profile, as opposed to only two temperatures, has advantages. First, it permits detection of TBP curves of any general shape. This makes the neural - physical approach easily applicable to any fractionator: crude, coker, FCC, visbreaker or hydrocracker. Second, fitting of many temperatures increases the robustness of the model. The fitting process identifies outlier temperature readings, and disregards them in the inferential formulae. To the extent that draw temperatures exhibit dynamic lags, the neural network easily identifies and accounts for the added dynamic complexity.

The neural – physical inferential technology is implemented as a parameterization of a commercial software package [7]. The significance of this fact is that no custom code needs to be developed or maintained.

CRUDE SWITCH PROPERTY PREDICTOR APPLICATION BENEFITS

Crude units benefit significantly from reduction of the crude switch transition time. With neural - physical predictors supporting MPC crude switches take 1.5 to 2 hours instead of 6 to 8 hours. Dynamic disturbances to the process are reduced from 15-20 °F to 5-10 °F. The limiting factor on this improvement is not model accuracy; it is the response time of column temperature controllers.

These benefits are quite significant for refineries where diverse sources of crude are processed in a single facility. There are also benefits for crude units where multiple feedstocks are held in multiple tanks with unknown mixtures/stratifications, which cause continuous slow changes in crude quality. Under such circumstances it is difficult for the operator to act on lab data and keep product properties at targets without good dynamic inferences.

Cokers mainly benefit from keeping product qualities under control during drum switches. Without good quality control the properties can deviate substantially from targets, causing damage or upsets in downstream equipment. For example, very heavy naphtha may damage reformer catalyst. With physical – neural property feedback for closed-loop control, the product draws are completely synchronized with the drum switch disturbances and the common error of drawing excess light product and emptying the column is virtually eliminated.

FCC’s can be disturbed by changes of feed. For example adding coker gasoil, vacuum resid or changing from sweet to sour feed. Such changes result not only in upsets to the FCC reactor but also in shifts of yields. The physical – neural property feedback acts quickly to allow column conditions to be reset by MPC to keep product properties steady during and after the transients.

Hydrocrackers recycle material heavier than diesel back to the reactor, and thus mistakes in controlling the diesel cut are costly. Recycling diesel to the reactor wastes energy, hydrogen, and consumes reactor capacity. Sometimes diesel range material is intentionally recycled, and then the kerosene cut becomes of major importance. Thus the key to maintaining high unit effectiveness is correct fractionator cutpoint control. When the hydrocracker is on blocked operation, with feed or operating mode changing frequently, accurate inferences assume even more importance.

Last but not least, the object of advanced control is to operate the equipment near constraints. To accomplish operation near constraints, MPC's constantly change process conditions: taking throughput up or down, pressures, compressors, refluxes, etc. Under these "self inflicted" disturbances the fractionator is never at steady-state. However, those up and down steps become counterproductive if product properties cannot be held constant during the perpetual transient. Responsive inferential predictors are mandatory if any form of constraint control is employed on a fractionator.

CAN A REFINER DERIVE THE SAME BENEFIT FROM ON-STREAM PROCESS ANALYZERS?

When an analyzer is available it should be used. When a property predictor is also available and the two trend together it gives the operator a degree of comfort to let the advanced control take aggressive steps when necessary. But an analyzer does not replace the capability of dynamically accurate inferences. All of the conditions stated in the previous section require quick response in minutes, which analyzers simply cannot produce. Responsive inferential calculations provide the only way to accomplish high performance closed-loop control.

In addition to the operator comfort factor, the analyzer data is used as a predictor model input similar to column temperatures. The long dynamic response of the analyzer is not a problem for the neural network system. The analyzer dynamics are identified during the learning phase and are accounted for in the prediction. Analyzers are known to occasionally fail, and upon such failures the predictor model detects the lack of fit, flags the problem for the operator, and continues to provide accurate feedback to the MPC.

REFERENCES

1. Keeler, J. D., and Ferguson, R. B., "Commercial Applications of Soft Sensors: The Virtual On-line Analyzer and the Software CEM", invited paper at the International Forum for Process Analytical Chemistry (IFPAC) Conference, Orlando, Florida, January 22-24, 1996, published in the IFPAC Conference Proceedings, JPAC, 1996.

2. Martin, G., "Soft Sensors", *Advances in Instrumentation and Control*, ISA, 1996, Vol. 51, Part 1, pp. 245-257.

3. Friedman, Y. Zak, "Control of Crude Fractionation Product Qualities during Feedstock Changes by Use of a Simplified Heat Balance, Proceedings of the 1985 Joint Automatic Control Conference, pp. 1084-1089B.

4. Friedman, Y. Zak, "Crude Unit Advanced Control Experience", Hydrocarbon Processing, February, 1994.

5. Hydrocarbon Processing's Advanced Control and Information Systems 97 Handbook, published in Hydrocarbon Processing, September 1997, p. 112.

6. Martin, G., and Z. Friedman, "4th Generation Property Predictors", *Hydrocarbon Engineering* (UK), March, 2000.

7. Pavilion Technologies, Inc., 11100 Metric Blvd., #700, Austin, Texas, (512) 438-1400, www.pavtech.com.

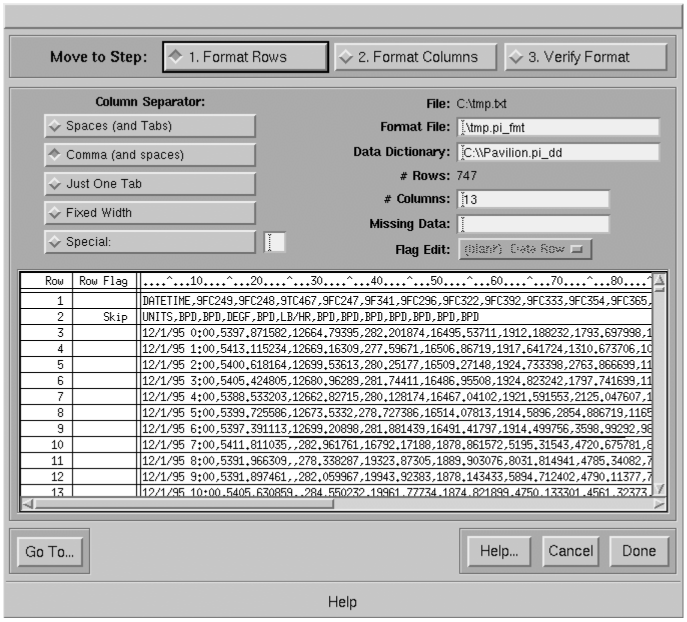

Figure 1. Data in Flat File Format

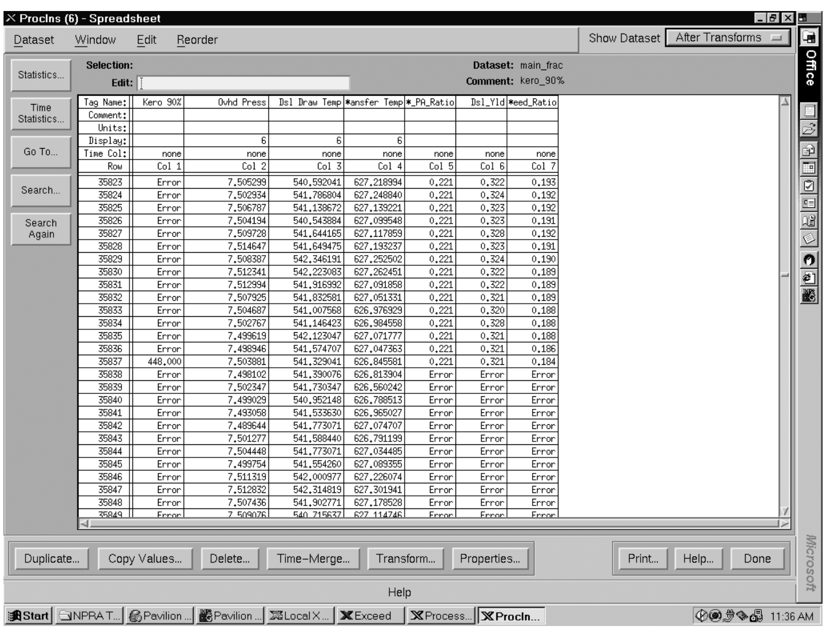

Figure 2. Data Formatted Into Spreadsheet

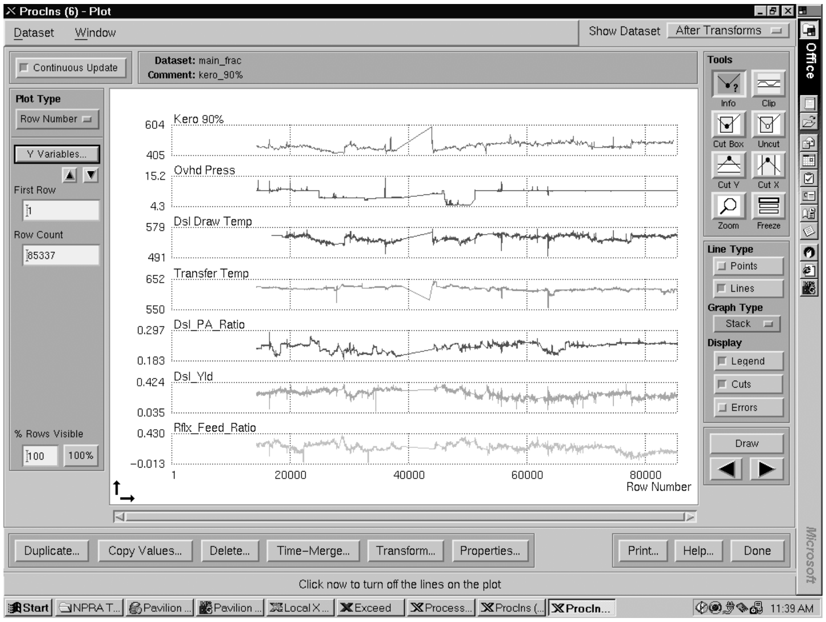

Figure 3. Plotted Data

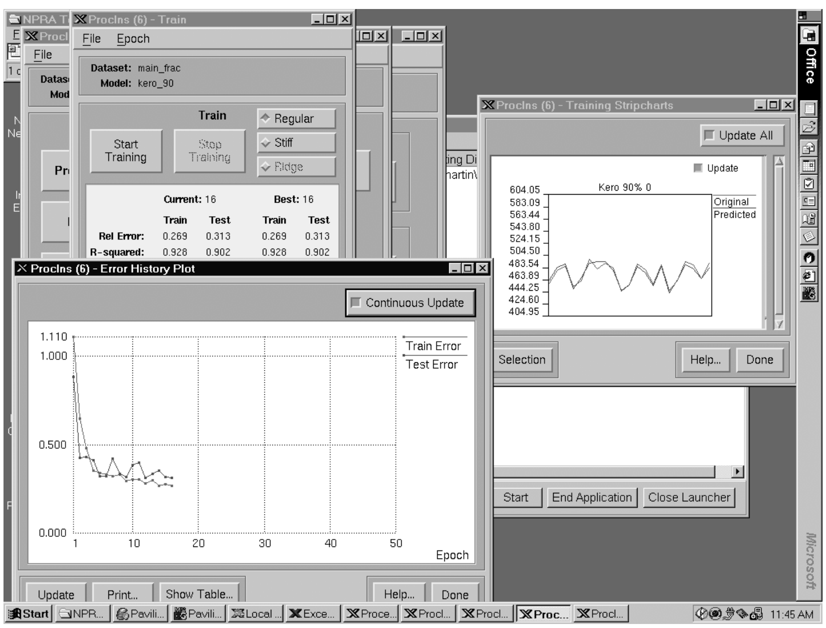

Figure 4. Training Results

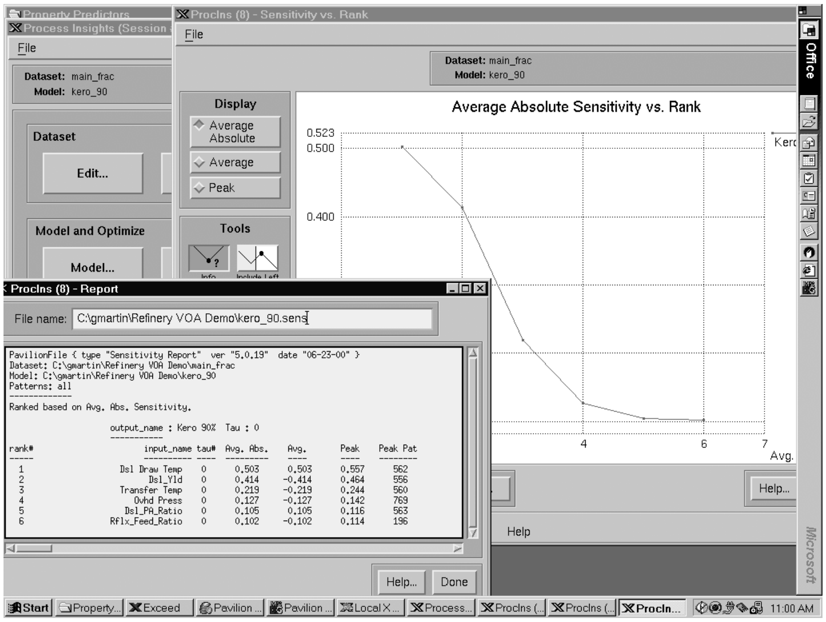

Figure 5. Sensitivities Report and Plot Screen

Unit	**Stream**	**Property**
Crude	**Preflash Gasoline**	**Endpoint**
	Naphtha	**Endpoint**
	Kerosene	**Flash**
		Endpoint
	Distillate	**Flash**
		Endpoint
	AGO	**%@450 F**
	Reduced Crude	**%@500 F**
FCC	**Gasoline**	**Endpoint**
	LCO	**Endpoint**
	Slurry	**Gravity**
Hydrocracker	**Light Naphtha**	**98% Distillation**
	Heavy Unicrackate	**5% Distillation**
		95% Distillation
		Endpoint
	Recycle Oil	**5% Distillation**
Distillate HTU	**Diesel**	**Flash**
Reformers	**Reformate**	**Octane**
Debutanizer	**Bottoms Product**	**RVP**

Figure 6. Property Predictor Installations at Marathon-Ashland

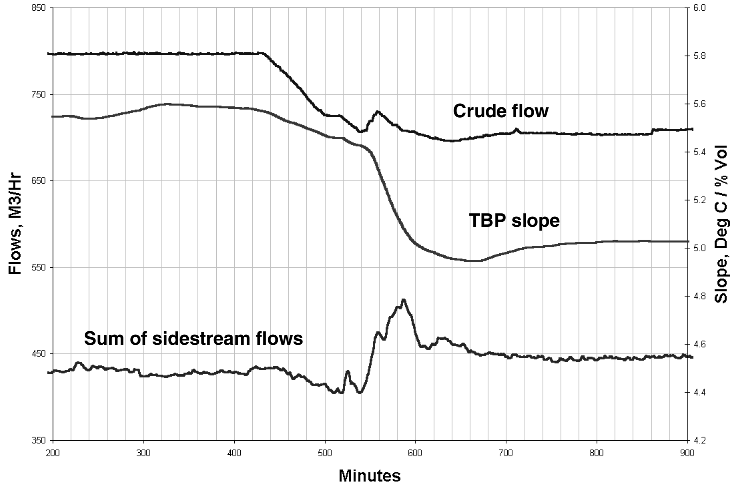

Figure 7. Crude TBP Slope Prediction in a Switch

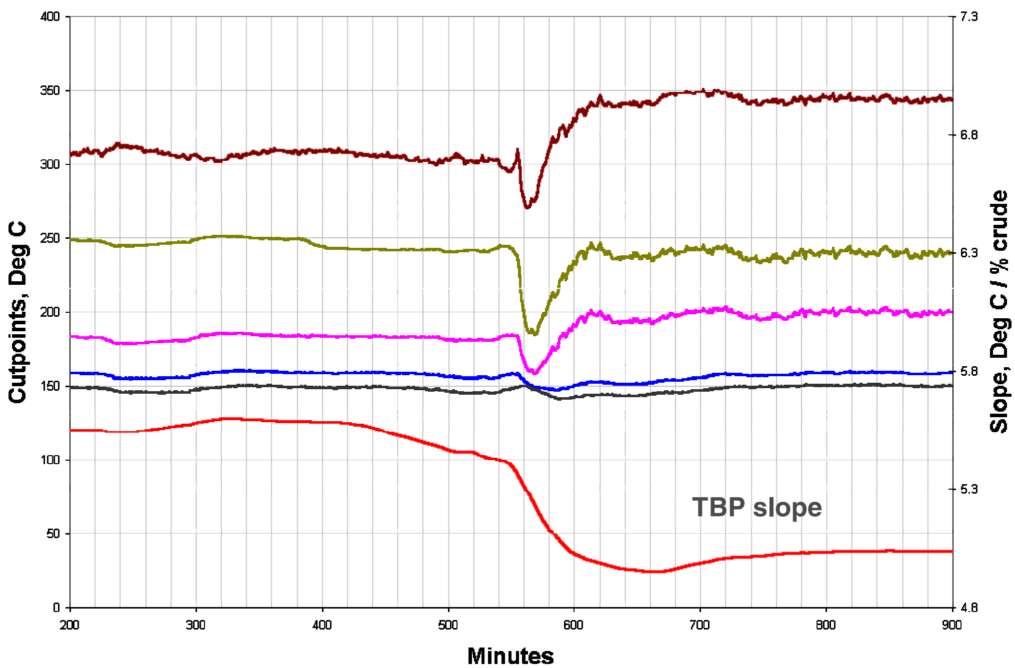

Figure 8. Crude Switch Predictions Used for Closed-Loop Control During a Switch

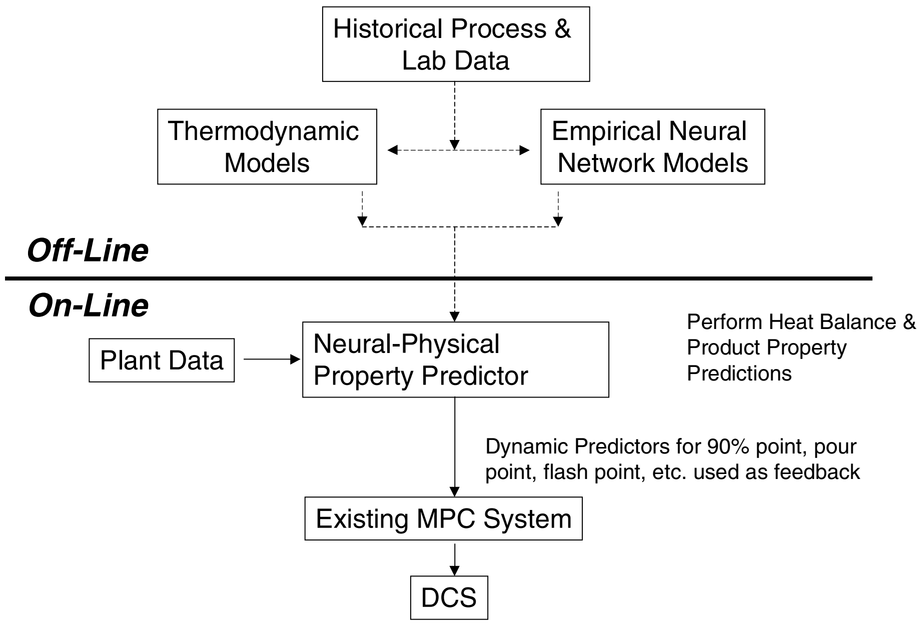

Figure 9. Neural - Physical Crude Switch Property Predictor Architecture

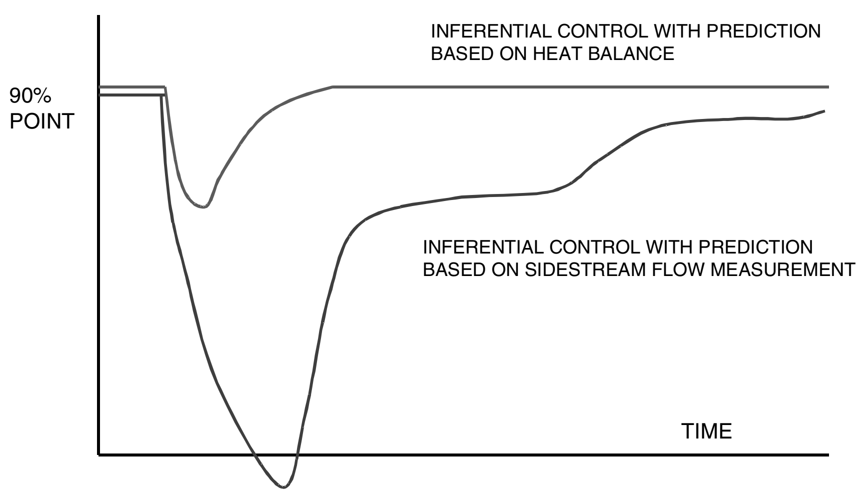

Figure 10. Crude Switch Property Predictor Response vs. Flow Measurement Based Inference