Section 30

Analysis of Plant Performance

Colin S. Howat, Ph.D., P.E., *John E. & Winifred E. Sharp Professors Department of Chemical & Petroleum Engineering, University of Kansas; Member, American Institute of Chemical Engineers; Member, American Society of Engineering Education.*

REFERENCES: The following reference list presents a broad spectrum of the information in the literature regarding plant-performance analysis. The list is not intended to be comprehensive. However, the citations at the ends of these articles lead to essentially all of the relevant literature.

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Nomenclature

Symbol	Definition	SI units	U.S. customary units
$\mathbf{B}$	Matrix of linear constraint coefficients		
$\vec{\mathbf{b}}$	Vector of bias		
b	Bias		
C_p	Heat capacity	kJ/kgmol/K	Btu/lbmole/F
c	Number of components		
$\vec{\mathbf{d}}$	Vector of weighted adjustment in measurements		
d_j	Weighted adjustment to measurement j		
$\vec{f}$	Vector of constraints		
$g\langle\rangle$	Operator on the measurements and equipment boundaries		
H_0	Null hypothesis		
H_a	Alternative hypothesis		
$\mathbf{J}$	Variance-covariance matrix of measurements		
K_{ij}	Equilibrium vaporization ratio for component i on stage j		
k	Specific rate constant		
$\mathbf{Q}$	Variance-covariance matrix of measurement adjustments		
Q	Heat transfer	kJ/hr	Btu/hr
Q_{jj}	Variance of adjustment to measurement j		
$\mathbf{R}$	Variance-covariance matrix of constraint residuals		
R_{ii}	Variance of constraint residual i		
$\vec{\mathbf{r}}$	Constraint equation residuals		
r_j	Single constraint residual		
S	Stream flow	kgmol/hr	lbmole/hr
T	Temperature	K	°F
t	Time		
$\mathbf{X}_1$	Matrix of all measurements		
$\vec{\mathbf{X}}_1^{\mathbf{m}}$	Vector of measurements		
$\hat{\vec{\mathbf{X}}}_1^{\mathbf{m}}$	Vector of adjusted measurements		

Symbol	Definition	SI units	U.S. customary units
$\hat{\vec{\mathbf{X}}}_1^{\mathbf{M}}$	Vector of estimated measurements from the model		
$\delta\vec{\mathbf{X}}_1$	Deviation between adjusted and measured values		
$\mathbf{X}_2$	Matrix of equipment boundaries		
$\vec{\mathbf{X}}_2$	Vector of component flows		
$X_{i,j}$	Component i flow in stream j		
x_{ij}	Entry in the measurement matrix; liquid mole fraction of component i on stage j		
$\hat{x}_i$	Individual adjusted measurement		
x_i	Individual measurement		
$\tilde{x}_i$	True value of individual measurement		
$\bar{x}_i$	Mean value of individual measurement		
y_{ij}	Vapor mole fraction of component i on stage j		
$y^{*}_{i,j}$	Equilibrium vapor mole fraction of component i on stage j		
	Greek Symbols		
$\vec{\beta}$	Vector representation of parameters		
σ_i	Uncertainty in individual measurement		
θ_{ij}	Tray efficiency of component i on stage j		
ρ_j	Stream density	kg/m^3	lbm/ft^3
	Superscripts		
M	Measurement		
$\mathbf{m}$	Measured		
P	Plant		
$\mathbf{T}$	Transpose		
T	Total		
	Subscripts		
i	Matrix, vector position		
j	Matrix, vector position		

GLOSSARY

accuracy Proximity of the measurements to actual values. Data frequently contain bias, a deviation between the measurement and the actual value. The smaller the deviation, the greater the accuracy.

bias Offset between the measurement and the actual value of a measurement.

equipment boundary Limit in equipment operation. This could refer to design limits such as operating pressure and temperature. More often, the concern of the plant-performance analyst is the upper and lower operating limits for the equipment. These boundaries typically describe an operating range beyond which the equipment performance deteriorates markedly.

equipment constraints Limits beyond which the equipment cannot be operated, either due to design or operating boundaries.

fault detection Process of identifying deteriorating unit operating performance. Examples are instrument failure, increased energy consumption, and increased catalyst usage.

gross error Extreme systematic error in a measurement. The bias or systematic error is sufficiently large to distort the reconciliation and model development conclusions. Gross errors are frequently identified during rectification. Validation steps also are used to identify gross errors in measurements.

identification Procedure for developing hypotheses and determining critical measurements. Identification requires an understanding of the intent of the process and intent of the plant-performance analysis to be conducted.

interpretation Procedure for using the plant measurements or adjustments thereof to troubleshoot, detect faults, develop a plant model, or estimate parameters.

measurements Plant information. These provide a window into the operation. They may consist of routinely acquired information such as that recorded by automatic control systems or recorded on shift logs, or they may consist of nonroutine information acquired as part of a plant test.

model Qualitative or quantitative relationship between operating specifications and products. The quantitative model can be relational (e.g., a linear model) or physical (e.g., one comprised of appropriate material and energy balances, equilibrium relations, and rate relations). The parameters of these models (e.g., linear coefficients in the relational model; or tray efficiency, reactor volume efficiency, and heat transfer coefficients in a physical model) can be estimated from plant data.

plant A group of processing units. Within this context, it is the entire processing facility, typically too large to be the focus of a single plant-performance analysis. The terminology in plant-performance analysis is inconsistent. Often the study is of a particular unit and rarely of the entire plant. However, the terms *plant test* and *plant data* refer to unit tests and unit data and will be used consistent with *practice.*

parameters Model constants that relate the operating specifications to measures of product quality and quantity. Estimation of these is a frequent goal of plant-performance analysis.

precision Measurement of the random deviations around some mean value. Precision is compromised by sampling methods, instrument calibrations, and laboratory calibrations. Reconciliation methods have been developed to minimize the impact of measurement precision.

process constraints Chemical engineering fundamental relations for the unit. Examples include material balances, energy balances, hydraulic balances and, at times, thermodynamic equilibria. These constraints may be equality constraints such as material balances or inequality constraints such as those found in hydraulic balances (i.e., $P_{out} \leq P_{in}$ for a process vessel). Obvious process constraints may not always apply due to internal or external leaks, vents, and process misunderstanding.

reconciliation Procedure for the adjustment of the measurements to close the process constraints. The purpose of reconciliation is to provide a set of measurements that better represent the actual plant operation.

rectification Procedure for the identification of measurements that contain gross errors. This process is frequently done simultaneously or cyclically with the reconciliation.

systematic error Measure of the bias in the measurements. It is a constant deviation or offset between the measurement and the actual value. This term is frequently used interchangeably with *bias.*

troubleshooting Procedure to identify and solve a problem in operating unit. This is the most frequent interpretation step in plant-performance analysis.

uncertainty A general term used for measurement error. This includes random and systematic errors in measurements.

unit Battery limits of equipment under study. The unit under study may consist of a single piece of equipment, a group (e.g., a distillation tower with auxiliary equipment), an entire process (e.g., reactors and the corresponding separation train), or the entire plant.

unit test Special operating procedure. The unit is operated at prescribed conditions. Special measurements may be made to supplement routine ones. One of the principal goals is to establish nearly constant material and energy balances to provide a firmer foundation for model development.

validation Procedure for screening measurements to determine whether they are consistent with known unit characteristics. Measurements are compared to other measurements, expected operating limits, actual equipment status, and equipment performance characteristics. It is a useful tool to eliminate potentially distorting measurements from further consideration.

INTRODUCTION TO ANALYSIS OF PLANT PERFORMANCE

MOTIVATION

The goal of plant-performance analysis is to develop an accurate understanding of plant operations. This understanding can be used to:

- Identify problems in the current operation.
- Identify deteriorating performance in instruments, energy usage, equipment, or catalysts.
- Identify better operating regions leading to improved product or operating efficiency.
- Identify a better model leading to better designs.

The results of plant-performance analysis ultimately lead to a more efficient, safe, profitable operation.

FOCUS

Section 30 is written for engineers responsible for day-to-day interpretations of plant operation, those responsible for developing unit (plant) tests, and those responsible for analyzing plant data. The content focuses on aspects of troubleshooting, fault detection, parameter estimation, and model discrimination. In order to reach reliable conclusions, methods of identification, validation, reconciliation, rectification and interpretation are included. The emphasis is on guidelines that assist in avoiding many of the pitfalls of plant-performance analysis. While there are numerous mathematical and statistical methods in the technical literature, most of them apply only to restricted plant situations atypical of normal operations or to situations where enormous amounts of measurements are handled on a routine basis. Typical plant measurements are incomplete, their statistical distributions are unknown, the plant fluctuations are too great, and/or the volume of data makes the methods intractable. The numerical methods are useful to provide some insight, and an overview is presented. However, because of the limitations to measurement and numerical methods, the engineering judgment of plant-performance analysts is critical. Analysts must develop an accurate understanding of plant operations in order to draw valid conclusions about current operation, alternative operating regimes, and proposed designs founded upon the current plant configuration.

OVERVIEW

Historical Definition Plant-performance analysis has been defined as the reconciliation, rectification, and interpretation of plant measurements to develop an adequate understanding of plant operation. Measurements taken from the operating plant are the foundation for the analysis. The measurements are reconciled to meet the constraints on the process, such as material balances, energy balances, and phase relations. The measurements are rectified to identify and eliminate those measurements that contain bias (i.e., systematic errors) sufficiently large to distort conclusions. The data are interpreted to troubleshoot, develop plant models, or estimate values for significant operating parameters. Ultimately, the results are used to discriminate among causes for deterioration of performance, operating regions, models, and possible operating decisions. The purpose of plant-performance analysis is to understand plant operations such that relational or physical models of the plant can be developed. The intended results are better profits, better control, safer operation, and better subsequent designs.

Plant-Performance Triangle This view of plant-performance analysis is depicted in Fig. 30-1 as a plant-performance triangle. Figure 30-2 provides a key to the symbols used.

The three vertices are the operating plant, the plant data, and the plant model. The plant produces a product. The data and their uncertainties provide the history of plant operation. The model along with values of the model parameters can be used for troubleshooting, fault detection, design, and/or plant control.

The vertices are connected with lines indicating information flow. Measurements from the plant flow to plant data, where raw measurements are converted to typical engineering units. The plant data information flows via reconciliation, rectification, and interpretation to the plant model. The results of the model (i.e., troubleshooting, model building, or parameter estimation) are then used to improve plant operation through remedial action, control, and design.

Unit (Plant) Data Measurements supporting plant-performance analysis come from daily operating logs, specific plant tests, automatic data acquisition, and specific measurement requirements. Examples of these data include temperatures, pressures, flows, compositions, elapsed time, and charge volume. The data are all subject to random errors from a variety of sources ranging from plant fluctuations and sampling technique through instrument calibration to laboratory methodology. The random errors define the precision in the data.

The measurements are also subject to systematic errors ranging from sensor position, sampling methods, and instrument degradation

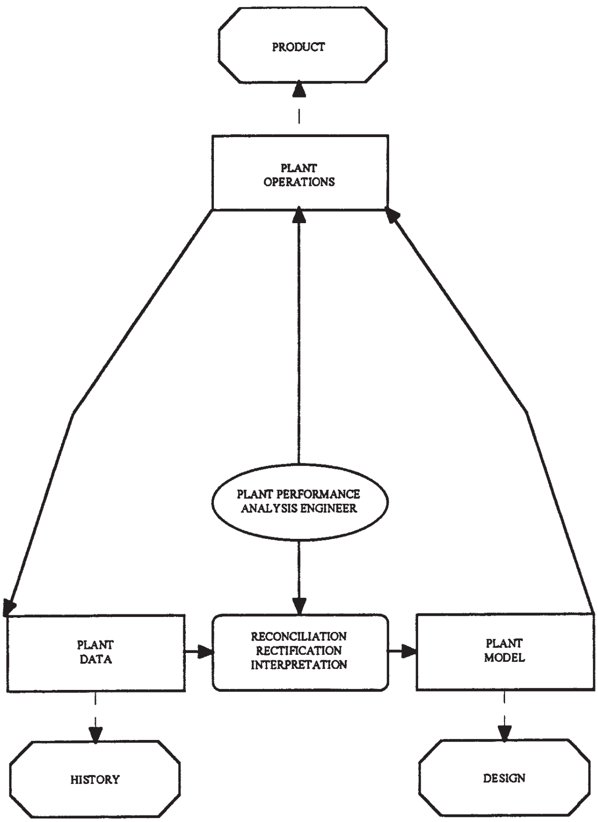

FIG. 30-1 Simplified plant performance analysis triangle.

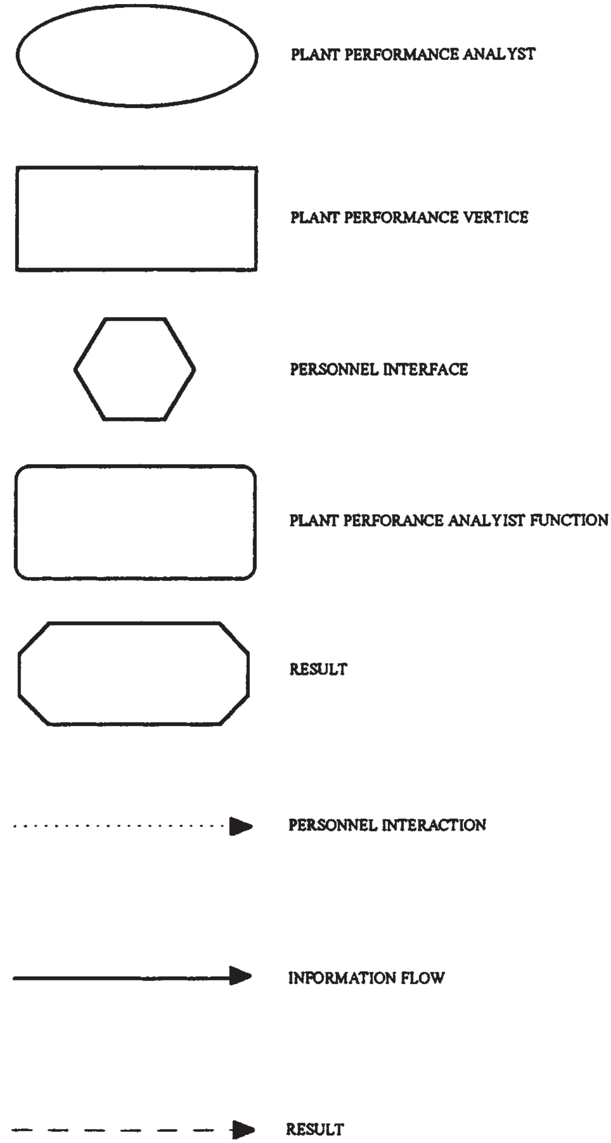

FIG. 30-2 Symbol key used in plant performance triangle.

to miscalibration in the field and laboratory. The systematic errors define the accuracy in the data.

These measurements with their inherent errors are the bases for numerous fault detection, control, and operating and design decisions. The random and systematic errors corrupt the decisions, amplifying their uncertainty and, in some cases, resulting in substantially wrong decisions.

Role of Plant-Performance Analysts In this simplified representation, the principal role of analysts is to recognize these uncertainties; to accommodate them in the analysis; and to develop more confident control, operating, or design decisions. The analysts recognize and quantify these uncertainties through repeated measurements and effective communication with equipment and laboratory technicians. They validate the data comparing them to known process and equipment information. They accommodate these errors through reconciliation—adjusting the measurements to close the process constraints. Example constraints include process constraints such as material balances, energy balances, equilibrium relations (occasionally), elapsed time, and so on; and equipment constraints or boundaries that define the limitations of equipment operation. The reconciliation literature focuses primarily on process constraints, but it is important to include equipment constraints and boundaries to ensure correct measurement adjustment.

During reconciliation, measurements in which the analysts have a high degree of confidence are adjusted little, if at all, to meet the constraints, while adjustments for less reliable measurements are greater. Correct reconciliation minimizes the impact of measurement error and results in adjusted measurements that represent plant operation better than the raw ones. Traditionally, analysts have adjusted the measurements intuitively, relying on their experience and engineering judgment. The purpose of mathematical and statistical algorithms developed over the past several years is to perform these adjustments automatically. However, algorithmic adjustment is subject to many of the same pitfalls that exist for intuitive adjustment. Both intuitive and algorithmic adjustment require correct estimates for uncertainty in the measurements. Both methods also require a correct implicit model of the plant. Without correct measurement error estimates and constraints, reconciliation will add bias to the adjusted measurements. For example, an unrecognized leak or vent invalidates the material-balance constraints developed from the implicit plant model, and either intuitive or algorithmic adjustment of data to meet invalid constraints adds systematic error to the adjusted measurements. Even when reconciliation is done algorithmically, the experience and judgment of the analysts are crucial.

The primary assumption in reconciliation is that the measurements are subject only to random errors. This is rarely the case. Misplaced sensors, poor sampling methodology, miscalibrations, and the like add systematic error to the measurements. If the systematic errors in the measurements are large and not accounted for, all reconciled measurements will be biased. During the measurement adjustment, the systematic errors will be imposed on other measurements, resulting in systematic error throughout the adjusted measurements.

Rectification accounts for systematic measurement error. During rectification, measurements that are systematically in error are identified and discarded. Rectification can be done either cyclically or simultaneously with reconciliation, and either intuitively or algorithmically. Simple methods such as data validation and complicated methods using various statistical tests can be used to identify the presence of large systematic (gross) errors in the measurements. Coupled with successive elimination and addition, the measurements with the errors can be identified and discarded. No method is completely reliable. Plant-performance analysts must recognize that rectification is approximate, at best. Frequently, systematic errors go unnoticed, and some bias is likely in the adjusted measurements.

The result of the reconciliation/rectification process is a set of adjusted measurements that are intended to represent actual plant operation. These measurements form the basis of the troubleshooting, control, operating, and design decisions. In order for these decisions to be made, the adjusted measurements must be interpreted. Interpretation typically involves some form of parameter estimation. That is, significant parameters—tray efficiency in a descriptive distillation model or linear model parameters in a relational model—are estimated. The model of the process coupled with the parameter estimates is used to control the process, adjust operation, explore other operating regimes, identify deteriorating plant and instrument performance or to design a new process. The adjusted measurements can also be interpreted to build a model and discriminate among many possible models. The parameter estimation and model building process is based on some form of regression or optimization analysis such that the model is developed to best represent the adjusted measurements. As with reconciliation and rectification, unknown or inaccurate knowledge of the adjusted measurement uncertainties will translate into models and parameter estimates with magnified uncertainty. Further, other errors such as those incorporated into the database will corrupt the comparison between the model and adjusted measurements. Consequently, parameters that appear to be fundamental to the unit (e.g., tray efficiency) actually compensate for other uncertainties (e.g., phase equilibria uncertainty in this case).

Extended Plant-Performance Triangle The historical representation of plant-performance analysis in Fig. 30-1 misses one of the principal aspects: identification. Identification establishes troubleshooting hypotheses and measurements that will support the level of confidence required in the resultant model (i.e., which measurements will be most beneficial). Unfortunately, the relative impact of the measurements on the desired end use of the analysis is frequently overlooked. The most important technical step in the analysis procedures is to identify which measurements should be made. This is one of the roles of the plant-performance engineer. Figure 30-3 includes identification in the plant-performance triangle.

The typically recorded measurements in either daily operations or specific plant-performance tests are not optimal. The sampling locations were not selected with troubleshooting, control, operations, or model building as the focus. Even if the designers analyzed possible sample locations to determine which might maximize the information contained in measurements, it is likely that the actual operation is different from that envisioned by the designers or control engineers. More often, the sample locations are based on historic rules of thumb whose origins were likely based on convenience. Thus, for a given measurement, the amount of information leading to accurate parameter estimates is limited. Greater model accuracy can be achieved if locations are selected with the end use of the information well defined. It is necessary to define the intended end-use of the measurements and then to identify measurement positions to maximize the value in testing hypotheses and developing model parameter estimates.

END USE

The goal of plant-performance analysis is to improve understanding, efficiency, quality, and safety of operating plants. The end use must be established to focus the analysis. Figure 30-3 shows the three principal categories of end use improvements. The criteria for accuracy may vary among the categories requiring different numbers and levels of accuracy in the measurements.

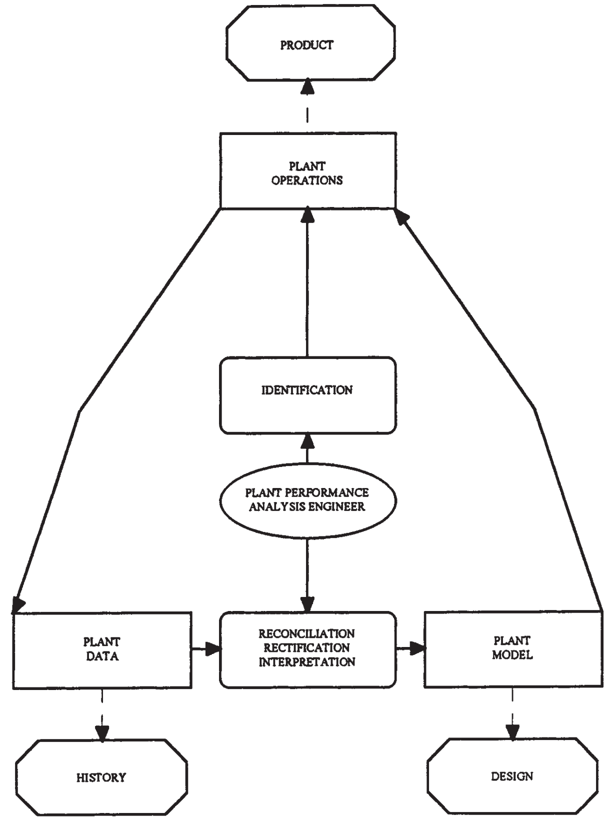

FIG. 30-3 Extended plant performance triangle.

Plant Operation The purpose is to maintain and improve performance (i.e., product quality, rate, efficiency, safety, and profits). Examples include identification of plant conditions that limit performance (troubleshooting, debottlenecking) and exploration of new operating regions.

History The history of a plant forms the basis for fault detection. Fault detection is a monitoring activity to identify deteriorating operations, such as deteriorating instrument readings, catalyst usage, and energy performance. The plant data form a database of historical performance that can be used to identify problems as they form. Monitoring of the measurements and estimated model parameters are typical fault-detection activities.

Design In this context, *design* embodies all aspects requiring a model of the plant operations. Examples can include troubleshooting, fault detection, control corrections, and design development.

TECHNICAL BARRIERS TO ACCURATE UNDERSTANDING

Limited Contained Information Data supporting the plant-performance analysis can come from daily operating logs, automatic or manual, or from formal plant tests. Daily logs consist of those measurements that the process and control designers and, subsequently, the plant engineers deem to be important in judging daily plant operation. No special operations (e.g., accumulating a constant-composition feed stock) are prerequisite for acquiring plant data of this caliber. While these data were intended to give sensitive insight into plant-performance, oftentimes they are recorded based on history and not formal analysis (i.e., their value has not been established or identified with respect to their end use). This presents the first technical hurdle—using data with limited contained information.

Formal unit (plant) tests (e.g., those developed for commissioning) usually last over a period of hours to weeks. The intent is to have the plant lined out in a representative operating regime. Feed stocks are typically accumulated in advance to ensure steady-state or controlled operation. Plant personnel are notified about the importance of the test so that they pay special attention to the operation, including charging rates, operating conditions, cycle times, and the like. Laboratory resources are dedicated beyond those normally required. A formal unit (plant) test requires significant coordination and investment. While it may give an indication of the plant capability, it is not representative of normal operation. During a unit (plant) test, greater attention and more personnel are dedicated to operation and data acquisition. Excursions in operating conditions are minimized. The data-acquisition effort should focus on sensitive measurements, providing insight beyond that gleaned from daily operations. However, oftentimes, little forethought is given to the end use of the information and the conclusions that will be drawn from it. Therefore, these additional data are not typically in the most sensitive regions of space and time. These data, too, contain less than optimal information.

There are significant technical barriers to accurate understanding from either source.

Limited Data First, plant data are limited. Unfortunately, those easiest to obtain are not necessarily the most useful. In many cases, the measurements that are absolutely required for accurate model development are unavailable. For those that are available, the sensitivity of the parameter estimate, model evaluation, and/or subsequent conclusion to a particular measurement may be very low. Design or control engineers seldom look at model development as the primary reason for placing sensors. Further, because equipment is frequently not operated in the intended region, the sensitive locations in space and time have shifted. Finally, because the cost-effectiveness of measurements can be difficult to justify, many plants are underinstrumented.

Plant Fluctuations Second, the plant is subject to constant fluctuations. These can be random around a certain operating mean; drift as feed stock, atmospheric, and other conditions change; or step change due to feed or other changes. While these fluctuations may be minimized during a formal unit (plant) test, nevertheless they are present. Given that each piece of equipment has time constants, usually unknown, these fluctuations propagate throughout the process, introducing error to assumed constraints such as material and energy balances.

Random Measurement Error Third, the measurements contain significant random errors. These errors may be due to sampling technique, instrument calibrations, and/or analysis methods. The error-probability-distribution functions are masked by fluctuations in the plant and cost of the measurements. Consequently, it is difficult to know whether, during reconciliation, 5 percent, 10 percent, or even 20 percent adjustments are acceptable to close the constraints.

Systematic Measurement Error Fourth, measurements are subject to unknown systematic errors. These result from worn instruments (e.g., eroded orifice plates, improper sampling, and other causes). While many of these might be identifiable, others require confidence in all other measurements and, occasionally, the model in order to identify and evaluate. Therefore, many systematic errors go unnoticed.

Systematic Operating Errors Fifth, systematic operating errors may be unknown at the time of measurements. While not intended as part of daily operations, leaky or open valves frequently result in bypasses, leaks, and alternative feeds that will add hidden bias. Consequently, constraints assumed to hold and used to reconcile the data, identify systematic errors, estimate parameters, and build models are in error. The constraint bias propagates to the resultant models.

Unknown Statistical Distributions Sixth, despite these problems, it is necessary that these data be used to control the plant and develop models to improve the operation. Sophisticated numerical and statistical methods have been developed to account for random errors, identify and eliminate gross errors, and develop parameter estimates. These methods require good estimates of the underlying uncertainties (e.g., probability distributions for each of the measurements). Because the probability distributions are usually unknown, their estimates are usually poor and biased. The bias is carried through to the resulting conclusions and decisions.

PERSONNEL BARRIERS TO ACCURATE UNDERSTANDING

Because the technical barriers previously outlined increase uncertainty in the data, plant-performance analysts must approach the data analysis with an unprejudiced eye. Significant technical judgment is required to evaluate each measurement and its uncertainty with respect to the intended purpose, the model development, and the conclusions. If there is any bias on the analysts' part, it is likely that this bias will be built into the subsequent model and parameter estimates. Since engineers rely upon the model to extrapolate from current operation, the bias can be amplified and lead to decisions that are inaccurate, unwarranted, and potentially dangerous.

To minimize prejudice, analysts must identify and deal effectively with personnel barriers to accurate understanding. One type of personnel barrier is the endemic mythologies that have been developed to justify decisions and explain day-to-day operation in the plant. These mythologies develop because time, technical expertise, or engineers' and operators' skills do not warrant more sophisticated or technical solutions.

Operators Operators develop mythologies in response to the pressure placed upon them for successful production quality and rates. These help them make decisions that, while not always technically supported, are generally in the correct direction. When they are not, convincing plant personnel of the deficiency in their decision structures is a difficult task.

Design and Control Engineers Equally important are the mythologies developed by the design or control engineers. Their models of plant performance are more technically sound, but may be no more accurate than the operators' mythology. Consequently, the mythology passed along by the design and control engineers can also add bias to the foundation upon which the analyst relies.

Finally, with the current developments in control technology, there is a reliance by the operating engineer on, what is in most cases, an approximate model. While the control and design engineers might fully recognize the limitations inherent in projecting beyond the narrow confines of current operation, the operating engineer will frequently believe that the control model is accurate. This leads to bias in the operation and subsequent decisions regarding performance.

Analysts The above is a formidable barrier. Analysts must use limited and uncertain measurements to operate and control the plant and understand the internal process. Multiple interpretations can result from analyzing limited, sparse, suboptimal data. Both intuitive and complex algorithmic analysis methods add bias. Expert and artificial intelligence systems may ultimately be developed to recognize and handle all of these limitations during the model development. However, the current state-of-the-art requires the intervention of skilled analysts to draw accurate conclusions about plant operation.

The critical role of analysts introduces a potential for bias that overrides all others—the analysts' evaluation of the plant information. Analysts must recognize that the operators' methods, designers' models, and control engineers' models have merit but must also beware they can be misleading. If the analysts are not familiar with the unit, the explanations are seductive, particularly since there is the motivation to avoid antagonizing the operators and other engineers.

Analysts must recognize that the end use as well as the uncertainty determines the value of measurements. While the operators may pay the most attention to one set of measurements in making their decisions, another set may be the proper focus for model development and parameter estimation. The predilection is to focus on those measurements that the operators believe in or that the designers/controllers originally believed in. While these may not be misleading, they are usually not optimal, and analysts must consciously expand their vision to include others.

In most situations, the plant was designed to be controlled and operated in a certain regime. It is likely that this has changed due to differences between the design basis and actual operation, due to operating experience and wholesale changes in purpose. Further, when developing sample, control, and measurement points, the designers/controllers may have had a model in mind for the operation. It is likely that that model is not accurate. Alternatively, they may have only used rules of thumb. Focusing only on previously selected points is limiting.

Each of the above can reduce analysts' opportunity for full understanding of the plant. Analysts must recognize that the plant operates by well-defined but not always obvious rules. It is important to identify these fundamental rules. If the analyst uses incorrect rules, the results will be further biased.

For the plant-performance analysis to be effective, the identified variables must be measured, the laboratory analysis must be correct, the simulation programs must accurately model the plant and the control recommendations must be implemented. In many settings, these aspects are not performed by plant-performance analysts. Analysts may be viewed as outsiders and operators are reluctant to modify their time-tested decision process. Laboratories geared to focusing on feed stock and product quality view unit (plant) tests as an overload. Simulation programs are not easily modified and proposed changes may not receive high priority attention. Control engineers may view modifications as an invasion of their responsibility. The plant-performance analysis milieu is much more complicated than that presented in Fig. 30-3 because of the personnel and communication barriers to implementation.

Figure 30-4 presents a more complete representation of plant-performance analysis. The information flow always faces barriers of personnel interactions. The operator must be convinced that the proposed changes and measurements will work using his/her language. The laboratory personnel must be convinced that the measurements are necessary, occasionally convinced that greater accuracy is required and that methods used are not giving results needed. Again, communication in their language must be effective. The software interaction is typically direct. However, the general nature of commercial simulators limits their effectiveness in particular situations. Occasionally, modifications are required. The software engineer is not familiar with the process and likely cannot be made aware because of proprietary considerations. This impedes communication. Finally, control engineers have been successful in establishing a control scheme which for all appearances works. Modifying the performance implies that they have not been as successful as appearances might indicate. While in all of these situations, teamwork should override these personnel considerations, it often doesn't. Consequently, communication is the paramount skill for plant-performance analysts.

OVERALL GUIDELINES

There are four overall guidelines that analysts should keep in mind. They must recognize the difficulties associated with the limited number and accuracy of the data, overcome the plant operation mythologies, overcome the designers' and controllers' biases and, finally, override the analysts' own prejudices. The following four overall guidelines assist in overcoming the hurdles to proper plant performance.

First, any analysis must be coupled with a technically correct interpretation of the equipment performance soundly rooted in the fundamentals of mass, heat, and momentum transfer; rate processes; and thermodynamics. Pseudotechnical explanations must not be substituted for sound fundamentals. Even when the development of a relational model is the goal of the analysis, the fundamentals must be at the forefront.

Second, any analysis must recognize the nonlinearities of equipment capability. Model development must recognize that equipment fundamentals will affect conclusions and extrapolations. These

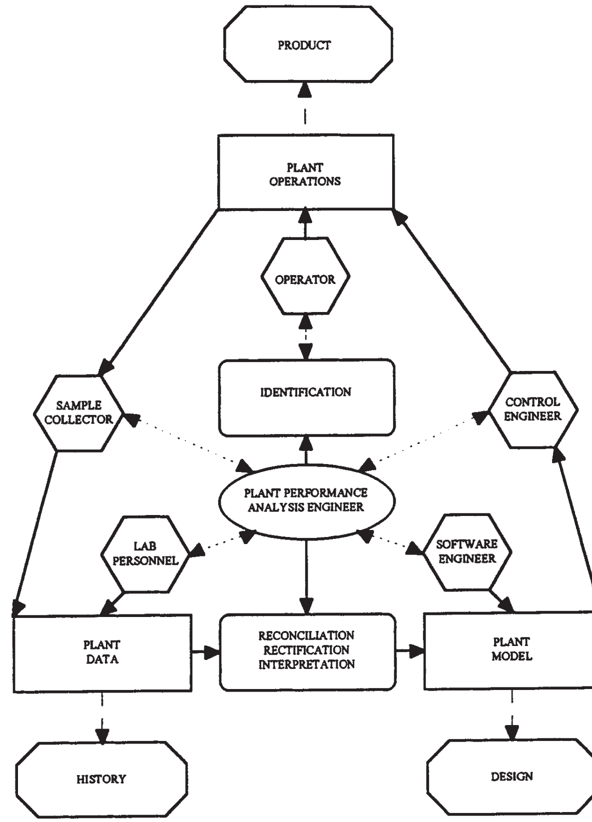

FIG. 30-4 Complete plant performance triangle including personnel interaction.

boundaries and nonlinearities of equipment performance overlay the chemical engineering fundamentals and temper the conclusions.

Third, any analysis must recognize that the measurements have significant uncertainty, random and systematic. These affect any conclusions drawn and models developed. Multiple interpretations of the same set of measurements, describing them equally well, can lead to markedly different conclusions and, more significantly, extrapolations.

Fourth, communication is paramount, since successful analysis requires that those responsible for measurement, control, and operation are convinced that the conclusions drawn are technically correct and the recommended changes will enhance their performance. This is the most significant guideline in implementing the results of the analysis.

Analysis of plant performance has been practiced by countless engineers since the beginning of chemical-related processing. Nevertheless, there is no body of knowledge that has been assembled called "analysis of plant performance." The guidelines given herein are effective in plant-performance applications. There are many more practiced by others that are also effective and should be employed whenever the challenges arise. Therefore, the material discussed in this section is the initial point for analysis and should not be considered all-inclusive. The particular equipment, operations, and problems associated with any plant spawn a myriad of effective methods to approach analysis of plant performance. They should not be ignored in preference to material in this section but should be added to these to improve the accuracy of conclusions and the efficiency of approach.

PLANT-ANALYSIS PREPARATION

MOTIVATION

These are a few of the reasons to justify analysis of plant performance. Units come on-line too slowly or with extreme difficulty because heat exchangers cannot add or remove heat, venting is inadequate, or towers do not produce quality product. Units come on-line and do not meet nameplate capacity and/or quality. Unit efficiency, quality, and/or yield are below expectations because energy or catalyst usage appears too high, product compositions are below that required, or raw material usage is excessive. Unit safety is questioned because operation appears too close to equipment control limitations. Unit environmental specifications are unfulfilled. Unit operations have deteriorated from historical norms. Alternate feed stocks are available, but their advantages and disadvantages if fed to the unit are unknown. Product demand exceeds the apparent capacity of the unit requiring modifications in operating conditions, in equipment configuration, or in equipment size. Unit operation is stable, and understanding of the operation is desired.

Troubleshooting start-up, quality and capacity problems, detecting faults in deteriorating effectiveness or efficiency performance, unit modeling to examine alternate feed stocks and operating conditions, and debottlenecking to expand operations are all aspects of analysis of plant performance. Conclusions drawn from the analyses lead to piping and procedure modifications, altered operating conditions including setpoint modifications and improved designs. Analyzing plant performance and drawing accurate conclusions is one of the most difficult and challenging responsibilities of the chemical engineer (Gans, M., D. Kohan, and B. Palmer, “Systematize Troubleshooting Techniques,” *Chemical Engineering Progress*, April 25–29, 1991). Measurements and data are incomplete and inaccurate. Identical symptoms come from different causes. Aspects of unit response are not readily quantified and modeled, requiring inductive, investigative reasoning. According to Gans et al. (1991), 75 percent of all plant problems are due to unidentified, inefficient plant performance ultimately traced to simple equipment problems and limitations. Another 20 percent are due to inadequate design such as those encountered in startup and quality/quantity limitations. The remainder is due to a process failure. The goal of the plant-performance analyst is to identify correctly the problems and the opportunities for changes and to quantify the potential improvements.

The opportunities leading to false conclusions and inadequate recommendations are extreme. The probability of successful completion of analysis of plant performance is greatly enhanced if the preparatory work is complete. Analysts must define the detail of study required. Analysts must understand the operation of the unit. This includes the chemical engineering fundamentals and the operator’s perspective and control response. Analysts must understand historical unit performance, developing a model commensurate with the measurements available and the detail of study required. Should a unit test, short-cut or exhaustive, be required, the unit personnel must understand the goals and their responsibilities. The laboratory must be prepared to handle the overload of samples that may be necessary and be able to produce data of required quality. Personnel and the supporting supplies must be available to make measurements, gather samples, and solve problems during the course of the test.

The purpose of this section is to provide guidelines for this preparation. General aspects are covered. Preparations for the specific units can be drawn from these. Topics include analyst, model, plant, and laboratory preparation. Since no individual analyst can be responsible for all of these activities, communication with other personnel is paramount for the success of the analysis.

ANALYST PREPARATION

Analysts must have a strong foundation in plant operations and in the unit under study. The hurdles thrown at analysts increase the probability that the conclusions drawn will be incorrect. A lack of understanding in the operation of the unit increases the likelihood that the conclusions will be inaccurate. An understanding of the chemical engineering fundamentals, the equipment flowsheets, the equipment plot, the operators’ understanding and interpretations, and the operators’ control decisions is essential to minimize the likelihood for drawing false conclusions. Reaching this understanding prior to undertaking a unit test and the measurement interpretation will increase the success and efficiency of the analysis.

The analyst must necessarily rely on the expertise and efforts of others to operate, gather, and analyze samples and record (automatically or manually) readings. Communication of the goals, measurement requirements, and outcome to all involved is critical. It is imperative that all involved understand their responsibilities, the use of the information that they gather, and the goals of the test.

Measurement locations and methods may be different from those used daily. Analysts and the sample-gatherers must be intimately familiar with the locations, difficulties, and methods. Analysts must ensure that the methods are safe, that the locations are as indicated on the flow sheets, and that the sample-gatherers will be able to safely obtain the necessary samples.

Process Familiarization The analysts’ first step in preparation for analyzing plant performance is to become completely familiar with the process. Analysts should review:

- Process flow diagrams (PFDs)
- Operating instructions and time-sequence diagrams
- Piping and instrumentation diagrams (P&IDs)
- Unit installation
- Operator perspectives, foci, and responses

The review should emphasize developing an understanding of the processing sequence, the equipment, the equipment plot, the operating conditions, instrument and sample locations, the control decisions, and the operators’ perspectives. While the preparation effort may be less for those who have been responsible for the unit for a long period of time, the purpose of the test requires that the types and locations of the measurements be different from those typically recorded and typically used. The condition of these locations must be inspected. Operating specifications may be different. Therefore, refreshment is always necessary.

The intensity of the situation requiring the analysis may not allow analysts to develop a formal preparatory review of the unit as described below. Analysts must recognize that the incomplete preparation may result in a less efficient analysis of plant performance.

PFDs (process flow diagrams) display the processing sequence for the unit, the principal pieces of equipment in the unit, and the operating conditions and control scheme. The equipment sequence should represent the sequence found in the unit. The operating conditions shown on the flow sheet may be those envisioned by the designer and may not properly reflect the current conditions. These should be verified during the subsequent discussions with operators and studied through review of the shift and daily logs. Where differences are substantial, these need to be understood, as they may indicate that operating philosophy has changed significantly from that proposed by the designers. It is particularly important to verify that the control scheme represents the current control philosophy. The purpose of each piece of equipment must be understood. This understanding should include understanding of key components, temperature specifications, elapsed time constraints, and the like. The basis of the operating conditions must be understood with respect to these constraints. The PFD review is completed by developing a material balance of sufficient detail for analysts to understand the reactions and separations.

Operating instructions and time-sequence diagrams provide insight into the basis for the operating conditions. They will also provide a foundation for the subsequent discussion with operators. The time sequence diagrams may provide insight into any difficulties that will arise during the unit test.

P&IDs (piping and instrumentation diagrams) should identify instruments, sample locations, the presence of sample valves, nozzle blinding, and control points. Of particular importance are the bypasses and alternate feed locations. The isolation valves in these lines may leak and can distort the interpretation of the measurements.

Understanding the positions of sample and other measurement locations within the equipment is also important. The presence or absence of isolation valves needs to be identified. While isolation valves may be too large for effective sampling, their absence will require that pipe fitters add them such that sample valves can be connected. This must be done in advance of any test. If analysts assume that samples are from a liquid stream when they are vapor or that temperature measurements are within a bed instead of outside it, interpretation of results could be corrupted. Analysts should also develop an understanding of control transmitters and stations. The connection between these two may be difficult to identify at this level in fully computer-controlled units.

Unit layout as installed is the next step of preparation. This may take some effort if analysts have not been involved with the unit prior to the plant-performance analysis. The equipment in the plant should correspond to that shown on the PFDs and P&IDs. Where differences are found, analysts must seek explanations. While a line-by-line trace is not required, details of the equipment installation and condition must be understood. It is particularly useful to correlate the sample and measurement locations and the bypasses shown on the P&IDs to those actually piped in the unit. Gas vents and liquid (particularly water-phase) discharges may have been added to the unit based on operating experience but not shown on the P&IDs. While these flows may ultimately be small within the context of plant-performance analysis, they may have sufficient impact to alter conclusions regarding trace component flows, particularly those that have a tendency to build in a process.

Discussion with operators provide substantial insight. The purpose of the discussion should be to develop an understanding of operators' perspectives of the unit, their foci for the operation, and their decision sequence in response to deviations and off-specification products. Two additional, albeit nontechnical, goals of this discussion are to establish rapport with the operators and to learn their language. The operators will ultimately be required to implement recommendations developed by analysts. Their confidence is essential to increase the likelihood of success. The following topics should be included in the discussion.

The operators have been given instructions on unit operation. Most of these are written and should have been studied prior to the meeting. Others may be verbal or implied. While this is not optimal, verbal instructions and operating experience are still part of every unit. It is not unusual that different shifts will have different operation methods. While none of the shift operations may be incorrect, they do lead to variability in operation and different performance. "What-if" questions posed to the operators can lead to insight into operator response. This will lead to analysts gaining better understanding of the unit (Block, S.R., "Improve Quality with Statistical Process Control," *Chemical Engineering Progress,* November 1990, 38–43). The discussion with the operators must provide insight into their view of the unit operation, their focus on the operation, and their understanding of equipment limitations.

One topic of discussion is the measurements to which the operators pay the most attention (their foci). Of the myriad of measurements, there is a limited set that they find most important. These are the measurements that they use to make the short-cycle decisions. The important points to glean are the reasons they focus on these, the values and trends that they expect, and their responses to the deviations from these.

With respect to their response, the discussion should emphasize why these are important and why they adjust certain control settings. Among the deviations on which analysts should focus the discussion are the high and low alarm settings. Some alarms will require rapid response. Alarms may give insight into equipment-operation boundaries as well as process constraints.

Operators typically have long cycle measurements upon which they focus. These may be part of morning reports giving production rates, compositions, yields, and so on. They may also have some recorded measurements that they examine once per shift. Analysts should understand the importance that the operators place on these measurements and the operators' responses to them.

Analysts are typically not totally prepared to discuss the purpose of the impending test at this meeting. Therefore, this topic may be premature. There is typically a sequence of meetings between operators and analysts. The information flow in the first is typically from the operators to analysts as analysts develop their understanding and learn to communicate in the operators' language. After the analysts study the process further based on the first meeting and preliminary simulations of the unit, another meeting is useful to test the analysts' understanding and communication methods. A third meeting to discuss the impending test purpose, focus, measurements, and procedures completes this phase of the preparation.

Data Acquisition As part of the understanding, the measurements that can be taken must be understood. A useful procedure to prepare for this is to develop a tag sheet for the process (Lieberman, N.P., *Troubleshooting Refinery Processes,* PennWell Books, Tulsa, 1981, 360 pp). An example of a simplified sheet is given in Fig. 30-5.

This sheet will be used ultimately to record readings during the

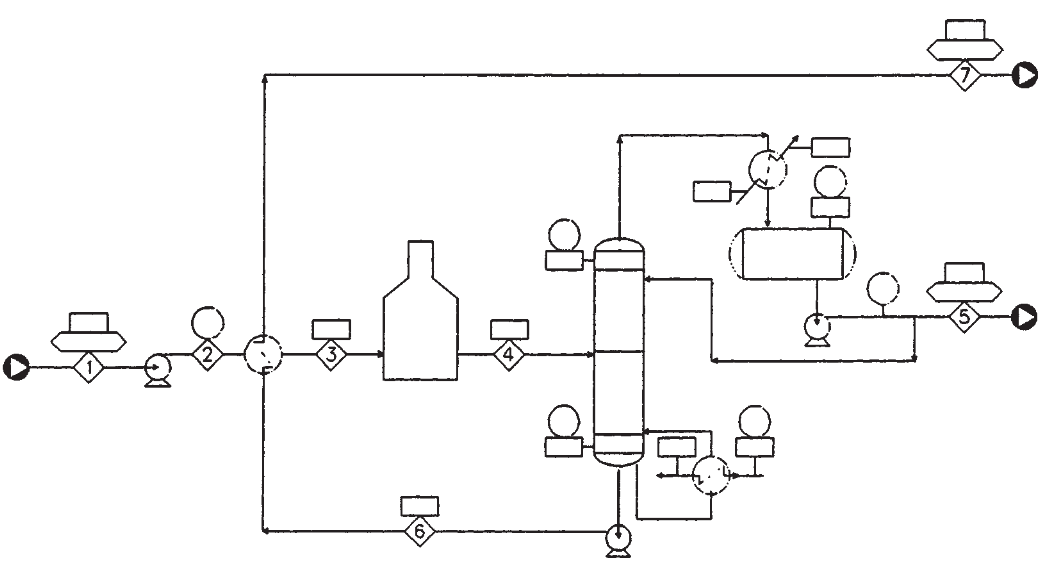

FIG. 30-5 Simplified tag-sheet for a distillation process.

plant test. It will help to develop a consistent set of measurements for the plant and help validate the measurements (identify inconsistencies). At this stage, however, it gives the analyst a visual representation of what measurements can be made. If there are sample locations, these must be added. Also, differential pressure measurements, additional flows, and utilities can be added as the unit instrumentation allows and as identified as being important during the identification step. Since identification has not been completed at this point, the measurements shown on these sheets are the ones already available on the board and in the field. The tag sheet also provides a visual point for discussion with the operators to confirm that certain measurements are made or can be made.

As part of this step, the analyst needs to develop an understanding of the uncertainty in the measurements and typical fluctuations experienced in daily operation. The uncertainties are functions of the instruments and their condition. Qualitatively, dial thermometers are less certain than thermocouples. On-line analyzers tend to be less accurate than lab analyses (assuming that the sample-gathering methodology is correct). Readings using different pressure gauges are less reliable than readings using a single pressure gauge. These random errors may be negligible in a unit that exhibits large fluctuations. The relative importance of plant fluctuations and random measurement error should be established. Multiple, rapid readings, control samples, or confirming measurements with other instruments will help establish the measurement uncertainty. Operating data will provide insight into the plant fluctuations, which can then be compared to the instrument uncertainty.

Operators frequently have insight into which instruments are accurate and which are not. If those instruments subsequently prove critical, recalibration must be done prior to the unit test. Preliminary analysis of daily measurements and practice measurements will help to identify which are suspect and require instrument recalibration prior to the unit test.

Analysts should discuss sample-collection methods with those responsible. Frequently, the methods result in biased data due to venting, failure to blow down the sample lines, and contamination. These are limitations that must either be corrected or accepted and understood. Sampling must be conducted within the safety procedures established for the unit. Since samples may be hot, toxic, or reactive in the presence of oxygen, the sample gatherers must be aware of and implement the safety procedures of the unit.

Material Balance Constraint There are two types of constraints for the unit. These are the process constraints and the equipment constraints. In each of these, there are equality constraints such as material balances and inequality constraints such as temperature limits. Analysts must understand the process and equipment constraints as part of the preparation for the unit analysis.

The most important of the process constraints is the material balance. No test or analysis can be completed with any degree of certainty without an accurate material balance. The material balance developed during this preparation stage provides the foundation for the analysts' understanding of the unit and provides an organizational tool for measurement identification. Analysts should develop a material balance for the process based on typical operating measurements. This can be compared to the design material balance. Estimates of tower splits, reactor conversions, elapsed times, and stream divisions help to identify the operating intent of the unit. Analysts must focus on trace as well as major components. The trace components will typically provide the most insight into the operation of the unit, particularly the separation trains.

During this preparation stage, analysts will frequently find that there is insufficient quantity or quality of measurements to close the material balance. Analysts should make every effort to measure all stream flows and compositions for the actual test. They should not rely upon closing material balances by back-calculating missing streams. The material balance closure will provide a check on the validity of the measurements. This preparatory material balance will help to identify additional measurements and schedule the installation of the additional instruments.

A typical material-balance table listing the principal components or boiling ranges in the process as a function of the stream location should be the result of this preliminary analysis. An example shown as a spreadsheet is given in the validation discussion (Fig. 30-18).

Energy Balance Many of the principal operating problems found in a plant result from energy-transfer problems such as fouled or blanketed exchangers, coked furnaces, and exchanger leaks. Consequently, developing a preliminary energy balance is a necessary part of developing an understanding of the unit. A useful result of the energy-balance analysis is the identification of redundant measurements that provide methods to obtain two estimates for unit performance. For example, reflux-flow and steam-flow measurements provide two routes to identifying heat input to a tower. These redundant measurements are very useful; both should be taken to provide the redundancy, and one or the other should not be ignored.

The material balance table can be supplemented with temperatures, pressures, phases, and stream enthalpies (or internal energies). Utility flows and conditions should be added to the process information.

Other Process Constraints Typical of these constraints are composition requirements, process temperature limits, desired recoveries, and yields. These are frequently the focus of operators. Violation of these constraints and an inability to set operating conditions that meet these constraints are frequently the motivation for the unit analysis.

Equipment Constraints These are the physical constraints for individual pieces of equipment within a unit. Examples of these are flooding and weeping limits in distillation towers, specific pump curves, heat exchanger areas and configurations, and reactor volume limits. Equipment constraints may be imposed when the operation of two pieces of equipment within the unit work together to maintain safety, efficiency, or quality. An example of this is the temperature constraint imposed on reactors beyond which heat removal is less than heat generation, leading to the potential of a runaway. While this temperature could be interpreted as a process constraint, it is due to the equipment limitations that the temperature is set.

Developing an understanding of these constraints provides further insight into unit operation.

Database The database consists of physical property constants and correlations, pure component and mixture, that are necessary for the proper understanding of the operation of the unit. Examples of the former are molecular weights, boiling curves, and critical properties. Example pure-property correlations are densities versus temperature, vapor pressures versus temperature, and enthalpies versus temperature and pressure. Example mixture-property correlations are phase equilibria versus composition, temperature, and pressure; kinetic rate constants versus temperature; and interfacial tension versus composition and temperature. While the material balance can be developed without most of these, the energy balance and any subsequent model cannot. Therefore, an accurate database is critical to accurate understanding of plant operation. Very often, unit model parameters will interact with database parameters. The most notable example is the distillation tower efficiency and the phase equilibria constants. If the database is inaccurate, the efficiency estimate will also be inaccurate. Therefore, whenever the goal of the unit analysis is to develop a model for operation and design, care must be taken to minimize errors in the database that can affect the accuracy of the model parameters. Inaccurate models cannot be used for sensitivity studies or extrapolation to other operating conditions.

Analysts should not rely on databases developed by others unless citations and regression results are available. Many improper conclusions have been drawn when analysts have relied upon the databases supplied with commercial simulators. While they may be accurate in the temperature, pressure, or composition range upon which they were developed, there is no guarantee that they are accurate for the unit conditions in question. Pure component and mixture correlations should be developed for the conditions experienced in the plant. The set of database parameters must be internally consistent (e.g., mixture-phase equilibria parameters based on the pure-component vapor pressures that will be used in the analysis). This ensures a consistent set of database parameters.

It is not unusual for 30–40 percent of the process design effort to be spent in developing a new database. The amount of time required at this stage in the analysis of plant performance for analysis of the unit should be equivalent. The amount of effort devoted to database development becomes more intensive as the interaction between the model parameters and the database increases.

PLANT MODEL PREPARATION

Focus For the purposes of this discussion, a model is a mathematical representation of the unit. The purpose of the model is to tie operating specifications and unit input to the products. A model can be used for troubleshooting, fault detection, control, and design. Development and refinement of the unit model is one of the principal results of analysis of plant performance. There are two broad model classifications.

The first is the relational model. Examples are linear (i.e., models linear in the parameters and neural network models). The model output is related to the input and specifications using empirical relations bearing no physical relation to the actual chemical process. These models give trends in the output as the input and specifications change. Actual unit performance and model predictions may not be very close. Relational models are useful as interpolating tools.

The second classification is the physical model. Examples are the rigorous modules found in chemical-process simulators. In sequential modular simulators, distillation and kinetic reactors are two important examples. Compared to relational models, physical models purport to represent the actual material, energy, equilibrium, and rate processes present in the unit. They rarely, however, include any equipment constraints as part of the model. Despite their complexity, adjustable parameters bearing some relation to theory (e.g., tray efficiency) are required such that the output is properly related to the input and specifications. These models provide more accurate predictions of output based on input and specifications. However, the interactions between the model parameters and database parameters compromise the relationships between input and output. The nonlinearities of equipment performance are not included and, consequently, significant extrapolations result in large errors. Despite their greater complexity, they should be considered to be approximate as well.

Preliminary models are required to identify significant measurements and the complexity of model required and to test the analysis methods that will be used during the unit analysis. Effort must be devoted during the preparation stage to develop these preliminary models.

It must be recognized that model building is not the only outcome of analysis of plant performance. Many troubleshooting activities do not require a formal mathematical model. Even in these circumstances, analysts have developed through preliminary effort or experience a mental model of the relation between specifications, input, and output that provides a framework for their understanding of the underlying chemical engineering. These mental models generally take longer to develop but can be more accurate than mathematical models.

Intended Use The intended use of the model sets the sophistication required. Relational models are adequate for control within narrow bands of setpoints. Physical models are required for fault detection and design. Even when relational models are used, they are frequently developed by repeated simulations using physical models. Further, artificial neural-network models used in analysis of plant performance including gross error detection are in their infancy. Readers are referred to the work of Himmelblau for these developments. [For example, see Terry and Himmelblau (1993) cited in the reference list.] Process simulators are in wide use and readily available to engineers. Consequently, the emphasis of this section is to develop a preliminary physical model representing the unit.

Required Sensitivity This is difficult to establish *a priori.* It is important to recognize that no matter the sophistication, the model will not be an absolute representation of the unit. The confidence in the model is compromised by the parameter estimates that, in theory, represent a limitation in the equipment performance but actually embody a host of limitations. Three principal limitations affecting the accuracy of model parameters are:

- Interaction between database and model parameters
- Interaction between measurement error and model parameters
- Interaction between model and model parameters

Three examples are discussed.

Tray efficiency is one example of the first interaction. Figure 30-6 is a representation of a distillation tray.

Defining tray efficiency as the difference between the actual and the equilibrium vaporization, the efficiency is:

$$\theta_{i,j} = \frac{y_{i,j} - x_{i,j}}{y^*_{i,j} - x_{i,j}}$$

where $$y^*_{i,j} = K_{i,j} x_{i,j}$$

Tray efficiency $\theta_{i,j}$ is supposed to represent a measure of the deviation from equilibrium-stage mass transfer assuming backmixed trays. However, the estimate of tray efficiency requires accurate knowledge of the equilibrium vaporization constant. Any deviations between the actual equilibrium relation and that predicted by the database will be embodied in the tray efficiency estimate. It is a tender trap to accept tray efficiency as a true measure of the mass transfer limitations when, in fact, it embodies the uncertainties in the database as well.

As another example of the first interaction, a potential parameter in the analysis of the CSTR is estimating the actual reactor volume. CSTR shown in Fig. 30-7. The steady-state material balance for this CSTR having a single reaction can be represented as:

$$0 = X_{i,1} - X_{i,2} - V_r k f(\vec{\mathbf{X}}_2, S_2, \rho_2)$$

where X_i is the flow of component i, V_r is the reactor volume, k is the rate constant at the reactor temperature, $\vec{\mathbf{X}}_2$ is the vector of component flows in stream 2, S_2 is the stream-2 flow, and ρ_2 is the stream-2 density. Any effort to estimate the reactor volume and therefore also the volume efficiency of the reactor depends upon the database estimate of the rate constant. Any errors in the rate constant will result in errors in the reactor volume estimate. Extrapolations to other operating conditions will likely be erroneous. Estimating the rate constant based on reactor volume will have the same difficulties.

The second interaction results in compromised accuracy in the parameter estimate due to the physical limitations of the process as

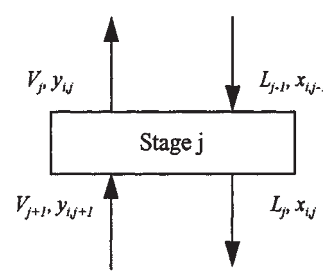

FIG. 30-6 Representation of a distillation tray numbering from the top of the column.

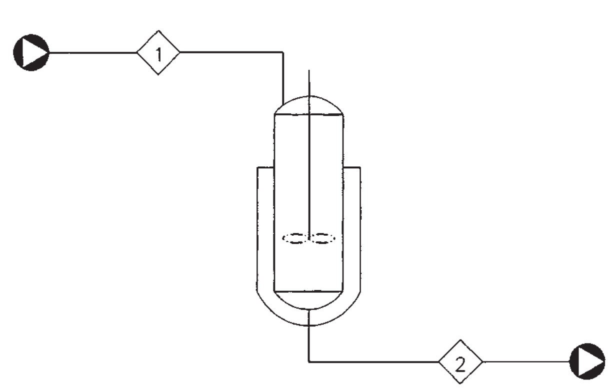

FIG. 30-7 Flow sheet of a single feed and single product CSTR.

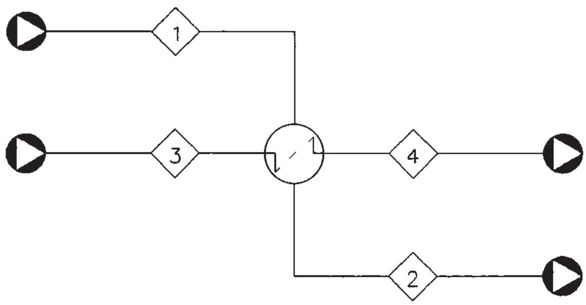

FIG. 30-8 PFD of Shell and tube heat exchanger.

embodied in the measurement uncertainties. Figure 30-8 shows a simple shell and tube heat exchanger. Many plant problems trace back to heat-transfer-equipment problems. Analysts may then be interested in estimating the heat-transfer coefficient for the heat exchanger to compare to design operation. However, this estimation is compromised when stream temperature changes are small, amplifying the effect of errors in the heat-transfer estimation. For example, the heat transfer could be calculated from the energy balance for Stream 1.

$$Q = S_1 C_p (T_2 - T_1)$$

The error in estimating the temperature difference is

$$\sigma_{\Delta T} = \sqrt{2}\sigma_T$$

The percentage error in the temperature difference translates directly to the percentage error in the estimate Q. As temperature-measurement error increases, so does the heat transfer coefficient error.

The third interaction compromising the parameter estimate is due to bias in the model. If noncondensables blanket a section of the exchanger such that no heat transfer occurs in that section, the estimated heat-transfer coefficient based on a model assuming all of the area is available will be erroneous.

The first two examples show that the interaction of the model parameters and database parameters can lead to inaccurate estimates of the model parameters. Any use of the model outside the operating conditions (temperature, pressures, compositions, etc.) upon which the estimates are based will lead to errors in the extrapolation. These model parameters are effectively no more than adjustable parameters such as those obtained in linear regression analysis. More complicated models may have more subtle interactions. Despite the parameter ties to theory, they embody not only the uncertainties in the plant data but also the uncertainties in the database.

The third example shows how the uncertainties in plant measurements compromise the model parameter estimates. Minimal temperature differences, very low conversions, and limited separations are all instances where errors in the measurements will have a greater impact on the parameter estimate.

The fourth example shows how improper model development will lead to erroneous parameter estimates. Assuming that the equipment performs in one regime and developing a model based on that assumption could lead to erroneous values of model parameters. While these values may imply model error, more often the estimates appear reasonable, giving no indication that the model does not represent the unit. More complicated examples like the kind given by Sprague and Roy (1990) emphasize the importance of the accuracy of the underlying model in parameter estimation, troubleshooting, and fault detection. In these situations, the model may describe the current operation reasonably well but will not actually describe the unit operation at other operating conditions.

Preliminary Analysis The purpose of the preliminary analyses is to develop estimates for the model parameter values and to establish the model sensitivity to the underlying database and plant and model uncertainties. This will establish whether the unit test will actually achieve the desired results.

The model parameter estimation follows the methods given in the interpretation subsection of this chapter. Analysts acquire plant measurements, adjust them to close the important constraints including the material and energy balances and then through repeated simulations, adjust parameter values to obtain a best description of the adjusted measurements. Not only does this preliminary analysis provide insight into the suitability of the model but also it tests the analysis procedures. The primary emphasis at this stage should be on developing preliminary parameter estimates with less emphasis on rigorously developing the measurement error analysis.

Once the model parameters have been estimated, analysts should perform a sensitivity analysis to establish the uniqueness of the parameters and the model. Figure 30-9 presents a procedure for performing this sensitivity analysis. If the model will ultimately be used for exploration of other operating conditions, analysts should use the results of the sensitivity analysis to establish the error in extrapolation that will result from database/model interactions, database uncertainties, plant fluctuations, and alternative models. These sensitivity analyses and subsequent extrapolations will assist analysts in determining whether the results of the unit test will lead to results suitable for the intended purpose.

PLANT PREPARATION

Intent Plant personnel, supplies, and budget are required to successfully complete a unit test. Piping modifications, sample collection, altered operating conditions, and operation during the test require advance planning and scheduling. Analysts must ensure that these are accomplished prior to the actual test. Some or all of the following may be necessary for a successful unit test.

Communication Analysts will require the cooperation of the

- Unit operators
- Unit supervisors
- Plant management
- Maintenance personnel
- Laboratory personnel

Operators are primarily concerned with stable operation and may be leery of altering the operation; they may fear that operation will drift into a region that cannot be controlled. Supervision may be reluctant despite their recognizing that a problem exists: Any deficiencies with the operation or operating decisions is their responsibility. Permission for conducting the test from the supervisor and the operators will be required. Management cooperation will be required, particularly if capital is ultimately needed. Maintenance will be called upon to make modifications to sample locations and perform a sequential pressure measurement. The laboratory personnel, discussed in detail in the next subsection, may view the unit test as an overload to available resources. These concerns must be addressed to ensure accurate sample interpretation.

Permission Analysts must have the permission of the operators and the supervisors to conduct even the most straightforward tests. While this is part of the analysts' preparation, it is important for all involved to know that analysts have that permission.

Schedule Complex tests should be done over a period of days. This provides the opportunity for the unit to be nearly steady. The advantages are that confirming measurements can be made. Scheduling a multiday test should be done when there is a likelihood that the feed stock supply and conditions will be nearly constant. The cooperation of upstream units will be required. The multiday test also requires that the downstream units can take the unit products.

The schedule should be set well in advance so that support services can provide the necessary personnel and supplies.

Simpler tests will not require this amount of time. However, they should be scheduled to minimize disruption to normal operations.

Piping Modifications One result of the inspection of the sample locations is a list of sample locations that will require modifications. The mechanical department will be required to make these modifications before the unit test is run. It is likely that the locations that are not typically used will be plugged with debris. The plugs will have to be drilled out before the test begins. Drilling out plugs presents a safety hazard, and those involved must be aware of this and follow the plant safety protocols.

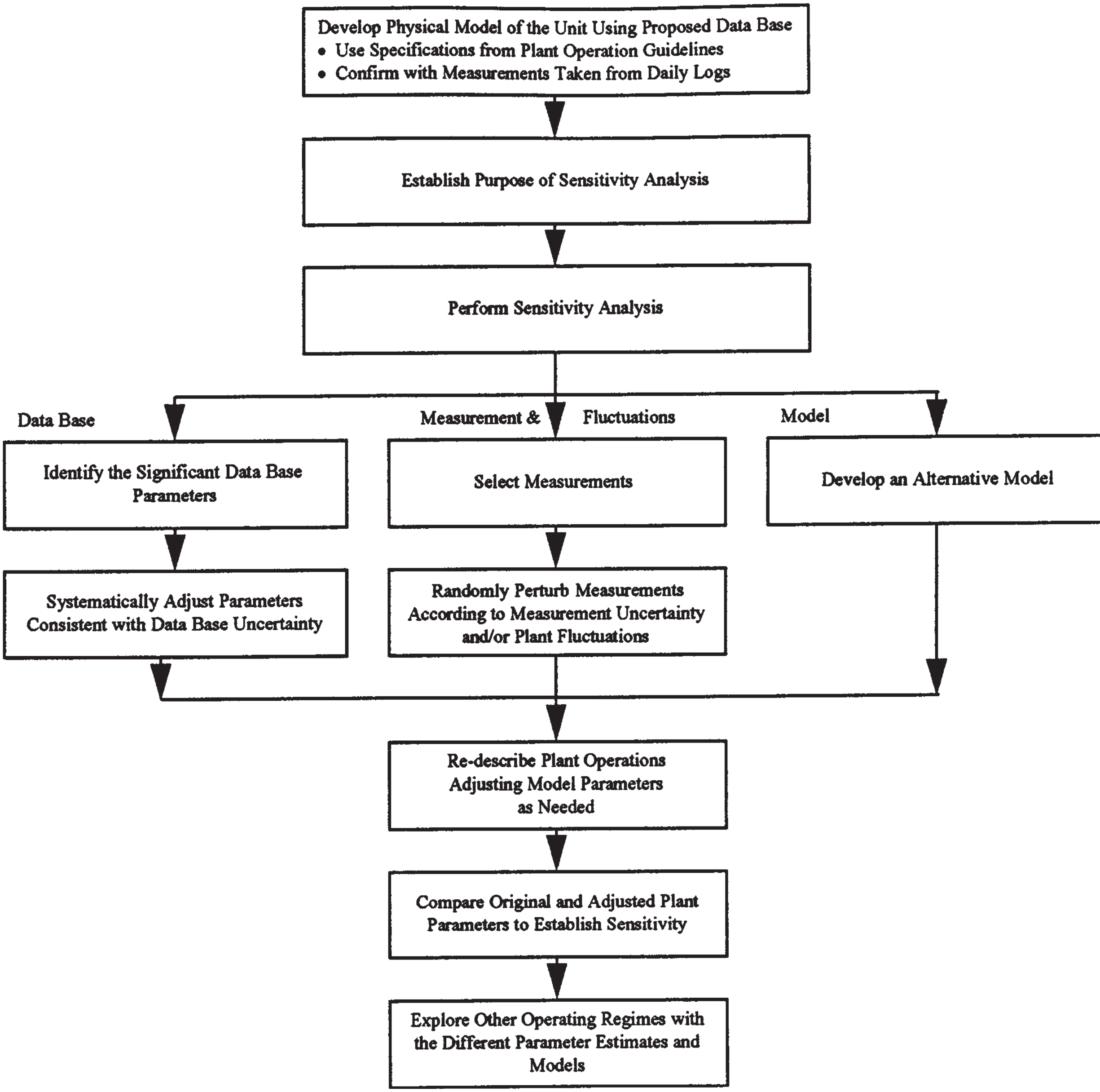

FIG. 30-9 Logic diagram for plant sensitivity analysis.

Instrumentation Calibration may be required for the instruments installed in the field. This is typically the job of an instrument mechanic. Orifice plates should be inspected for physical condition and suitability. Where necessary, they should be replaced. Pressure and flow instruments should be zeroed. A preliminary material balance developed as part of the preliminary test will assist in identifying flow meters that provide erroneous measurements and indicating missing flow-measurement points.

When doing a hydraulic test, a single pressure gauge should be used and moved from location to location. This gauge must be obtained in advance. The locations where this pressure will be measured should be tagged to assist the pipe fitter who will be responsible for moving the gauge from location to location. A walk-through with the pipe fitter responsible can be instructive for both the analysts and the fitter.

Thermocouples tend to be reliable, but dial thermometers may need to be pulled and verified for accuracy.

Sample Containers More sample containers will be required for a complex test than are typically used for normal operation. The number and type of sample containers must be gathered in advance, recognizing the number of measurements that will be required. The sample containers should be tagged for the sample location, type, and conditions.

Field Measurement Conditions Those gathering samples must be aware of the temperature, pressure, flammability, and toxic characteristics of the samples for which they will be responsible. This is particularly important when samples are taken from unfamiliar locations. Sample ports will have to be blown down to obtain representative samples. Liquid samples will have to be vented. Temperatures above

330 K (140° F) can cause burns. Pressures above atmospheric will result in flashing upon pressure reduction during venting. Venting to unplug the sample port and the sample bomb must be done properly to minimize exposure. A walk-through may be useful so that sample-gatherers are familiar with the actual location for the sample.

Operating Guidelines The test protocol should be developed in consultation with the principal operators and supervisor. Their cooperation and understanding are required for the test to be successful. Once the protocol is approved, analysts should distribute an approved one-page summary of the test protocol to the operators. This should include a concise statement of the purpose of the test, the duration of the test, the operating conditions, and the measurements to be made. The supervisor for the unit should initial the test protocol. Attached to this statement should be the tag sheet that will be used to record measurements.

Upstream and Downstream Units Upstream and downstream units should be notified of the impending test. If the unit test will last over a period of days, analysts should discuss this with the upstream unit to ensure that they are not scheduling activities that could disrupt feed to the unit under study. Analysts should seek the cooperation of the upstream units by requesting as consistent feed as possible. The downstream units should also be notified to ensure that they will be able to absorb the product from the unit under study. For both units, measurements from their instruments will be useful to confirm those for the unit under study. If this is the case, analysts must work with those operators and supervisors to ensure that the measurements are made.

Preliminary Test Operation of the unit should be set at the test protocol conditions. A preliminary set of samples should be taken to identify problems with instruments, measurements, and sample locations. This preliminary set of measurements should also be analyzed in the same manner that the full-test results will be analyzed to ensure that the measurements will lead to the desired results. Modifications to the test protocol can be made prior to exerting the effort and resources necessary for the complete test.

LABORATORY PREPARATION

Communication Laboratory services are typically dedicated to supporting the daily operation of the unit under study as well as other units in the plant. Their purpose is the routine confirmation that the unit is running properly and the determination of the quality of feed stocks. Laboratory staffing is normally set based on these routine service requirements. Consequently, whenever a plant test is conducted to address deterioration in efficiency, yield, or specifications or to develop a unit model, the additional samples required to support the test, place laboratory services in overload (Gans, M., and B. Palmer, "Take Charge of Your Plant Laboratory," *Chemical Engineering Progress,* September 1993, 26–33). If the laboratory cannot handle the analysis quickly, the likelihood of the samples reacting, leaking, or being lost markedly increases with subsequent deterioration in the accuracy of the conclusions to be drawn from the test. Therefore, adequate laboratory personnel must be accounted for early in the preparation process.

Plant-performance analysts must understand:

- Laboratory limitations
- Laboratory organization
- Laboratory measurement uncertainties
- Measurement cost
- Additional personnel requirements

The laboratory supervision and personnel must supply this information so that analysts gain this understanding.

Laboratory supervision and personnel must understand:

- Type of samples required
- Level of detail, accuracy, and precision of the samples
- Flammability, toxicity, and conditions of samples
- Anticipated schedule and duration of the test
- Justification for the overload assignments

Analysts provide this information.

The laboratory may need time to prepare for the unit test. This must be accounted for when the test is scheduled. The analysis of samples required for the unit test may focus on different composition ranges and different components than those done on a routine basis. Laboratory personnel may need to modify their methods or instruments to attain the required level of accuracy and detail. The modification, testing, and verification of the methods are essential parts of the preparation process. A practice run of gathering samples will help identify any deficiencies in the sample handling, storage, and analyses.

Without forethought, planning, and team-building, the sample analyses during the unit test may be delayed, lost, or inaccurate. The laboratory is an essential part of the unit test and must be recognized as such.

Confidence The accuracy of the conclusions drawn from any unit test depends upon the accuracy of the laboratory analyses. Plant-performance analysts must have confidence in these analyses including understanding the methodology and the limitations. This confidence is established through discussion, analyses of known mixtures, and analysis of past laboratory results. This confidence is established during the preparation stage.

Discussing the laboratory procedures with the personnel is paramount. Routine laboratory results may focus on certain components or composition ranges in the sample. The routine analyses narrow the laboratory personnel's outlook. The succinct and often misleading daily logs are the result of this focus. Analysts who have little daily interaction with the laboratory and plant may interpret daily results differently than intended. A typical example is laboratory analyses of complex streams where components are often grouped and identified as a single component. Consequently, important trace components are unanalyzed or masked. The impending plant test may require that these components be identified and quantified. The masking in the routine results can only be identified through discussion.

Even within a single sample analysis, it is likely that some of the reported concentrations are known with greater accuracy than others. Laboratory personnel will know which concentrations can be relied upon and which should be questioned. The plant-performance analyst should know at this stage which of the concentrations are of greatest importance and direct the discussion to those components.

Should the additional component compositions be required to fully understand the unit operation, the laboratory may have to develop new analysis procedures. These must be tested and practiced to establish reliability and minimize bias. Analysts must submit known samples to verify the accuracy.

Known samples should also be run to verify the accuracy and precision of the routine methods to be used during the unit test. Poor quality will manifest itself as poor precision, measurements inconsistent with plant experience or laboratory history, and disagreement among methods. Plotting of laboratory analysis trends will help to determine whether calibrations are drifting with time or changing significantly. Repeated laboratory analyses will establish the confidence that can be placed in the results.

If the random errors are higher than can be tolerated to meet the goals of the test, the errors can be compensated for with replicate measurements and a commensurate increase in the laboratory resources. Measurement bias can be identified through submission and analysis of known samples. Establishing and justifying the precision and accuracy required by the laboratory is a necessary part of establishing confidence.

Sampling Despite all of the preparation inside the laboratory, by far the greatest impact on successful measurements is the accuracy of the sampling methods. The number of sample points for a unit test are typically greater than the number required for routine sampling. It is likely that some of the sample locations, characteristics, and properties are unfamiliar to the sample-gatherers responsible for the routine ones. This unfamiliarity could lead to improper sampling, such that samples are not representative of the unit, and accidents, such that the sample gatherers are placed at risk. Part of the preparation process is to reduce this unfamiliarity to ensure safety and accuracy. The safety of the sample-gatherers is paramount and should not be compromised. Proper sampling methods accounting for volatility, flash points, toxicity, corrosivity, and reactivity should be written down for each plant and unit within the plant. The methodology must be understood and practiced.

Plant-performance analysts should be involved in reviewing the entire sampling procedure. The procedures for review are:

- Sampling locations
- Sampling safety
- Containers
- Sample transport, storage, and discharge system
- In-laboratory sampling
- Sample container cleaning

Each plant has established methods. The following should be considered during this preparation stage. Problems identified, typically during a pretest, should be solved prior to the initiation of the unit test.

Sampling locations for the unit test should be readily and safely accessible. The sample gatherer should be able to easily access the sample point. An isolation valve should be installed at the location. If a blind is installed, this should be modified in advance of the test. The sample locations shown on the P&IDs must be compared against the actual locations on the equipment. Experienced operators may provide insight into the suitability of the location in question.

The integrity and suitability of the sample containers must be established during the preparation stage. This is particularly important for those sample containers that will be used for the nonroutine measurements. Leaks jeopardize personnel and distort the resultant composition. Dirty containers contaminate samples. Open containers used for high boiling samples are unsuitable for volatile, high-temperature, pressurized samples. Trace components may preferentially adsorb onto either the container surface or the residue left in the container. Since trace components provide the greatest insight into unit operation and are the most difficult to quantify, this adsorption could lead to distorted conclusions.

Dead legs in the sample line must be discharged safely to ensure that the sample will actually be representative of the material in the unit. Without blowing down the dead leg, samples taken will be erroneous, as they may be representative of some past operating conditions. If the location is nonroutine, the sample leg may have accumulated debris. The debris could partially or totally block the line. Opening the isolation valve to blow down the line could result in a sudden, uncontrolled release, presenting a hazard to the sample gatherer.

Sample temperatures may be below ambient. If the sample vessel is liquid-full, a hazard results due to overpressurization as the liquid expands. Venting may be required, but it can distort the results. This safety hazard must be accounted for in the procedure and in interpreting the laboratory results.

Sample temperatures may be above ambient. If the temperature is significantly above ambient, personnel must be protected against burns.

Samples may separate into two or more phases as they cool in the sample line: precipitate, coagulate, and freeze. Laboratory sampling may result in nonrepresentative compositions. Heat tracing may be required and may not be installed on the nonroutine sample locations.

Validation of the measurements may require the simultaneous measurement of pressure and temperature. Typical sample locations do not have thermowells and pressure indicators. Consequently, modifications will be required to facilitate validation.

The efficient analysis will be required to minimize compromise of the analysis due to degradation (e.g., dimerization, polymerization, reactions, leaks, and contamination).

Samples will form multiple phases. The laboratory secondary sampling methods must recognize the presence of vapor, liquid, and solid phases. Improper secondary sampling methods will result in distorted measurements. These limitations must be clearly communicated to the laboratory.

Cataloging and storage of samples may inundate the laboratory, resulting in storage and retrieval problems. Mislabeled and lost samples are frequent problems. The longer the special samples remain in the laboratory, the greater the likelihood that some will be lost or mislabeled.

These potential sampling problems must be solved in advance of the unit test. The conclusions drawn from any unit test are strongly affected by the accuracy of the sampling methods and the resultant analyses. Methods should be discussed and practiced before the actual unit test. Analysts should use the trial measurements in preliminary plant-performance analysis to ensure that the results will be useful during the actual unit test.

PREPARATION GUIDELINES

Overall Everyone involved in the unit test and the analysis of measurements must understand:

- The purpose of the test
- The expectations of plant-performance analysts
- Each individual's personal responsibility to the successful outcome

Analyst Analysts must have a firm understanding of the operation of the unit. If they are not involved in the day-to-day operation or responsible for the unit, more preliminary work including process familiarization, equipment familiarization, operator interviews, and constraint limitations will be required. Even when an analyst is responsible, a review is necessary. Analysts must firmly establish the purpose of the unit test. Different levels require different budgets, personnel, and unit commitment. Additional resources beyond that required for routine measurements must be justified against the value of the measurements to the establishment of the understanding of the plant operation.

Model The level of sophistication needs to be identified. Preliminary usage of the model should identify the uniqueness of parameter estimates and conclusions to be drawn.

Plant Sufficient personnel and supplies will be required for the test. Personnel may include additional operators, sample-gatherers, pipe fitters, and engineers. Upstream and downstream units need notification so that feed and product rates can be maintained.

Laboratory The laboratory requirements and responsibilities need to be identified and accepted. The laboratory supervisor must be aware of the impending test and the likely demands placed on his/her area of responsibility. Agreement as to error levels and expected turnaround must be reached. Proper sampling methodology and storage must be established and practiced.

PLANT-PERFORMANCE ANALYSIS

THE PROBLEM

Consider Fig. 30-10. This is a single unit process with one input and two output streams. The goal for plant-performance analysis is to understand accurately the operation of this unit.

Plant-performance analysis requires the proper analysis of limited, uncertain plant measurements to develop a model of plant operations for troubleshooting, design, and control.

Measurements The potential set of data can be identified by the matrix

$$\mathbf{X}_1$$

The rows represent the type of measurement (e.g., compositions, flows, temperatures, and pressures). The columns represent streams, times, or space position in the unit. For example, compositions, total flows, temperatures, and pressures would be the rows. Streams 1, 2, and 3 would be columns of the matrix of measurements. Repeated measurements would be added as additional columns.

For more complex equipment, the columns might contain measurements for internal distillation, batch-reactor intermediate conditions, or tubular-reactor between-bed conditions. Some of these

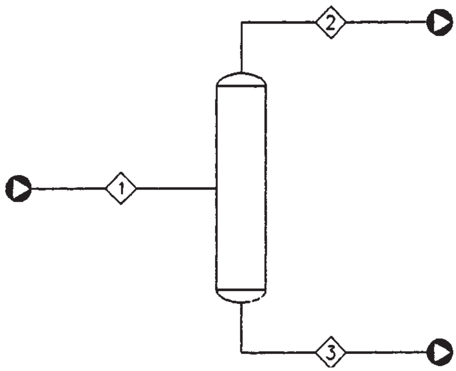

FIG. 30-10 Flow sheet of single unit process.

measurements might be recorded regularly, while others may be recorded only for the specific unit test analysis.

This matrix will necessarily be sparse. First, not all measurements can be taken for a given stream or position (e.g., a chromatographic analysis may only measure a subset of the component compositions). Second, not all streams or positions are included. Third, some of the measurements are inadequate due to bias and are discarded.

Equipment Limitations The plant-performance engineer might also have a matrix of equipment information that must be accounted for in the analysis.

$$\mathbf{X}_2$$

This matrix will contain information regarding loading characteristics such as flooding limits, exchanger areas, pump curves, reactor volumes, and the like. While this matrix may be adjusted during the course of model development, it is a boundary on any possible interpretation of the measurements. For example, distillation-column performance markedly deteriorates as flood is approached. Flooding represents a boundary. These boundaries and nonlinearities in equipment performance must be accounted for.

The purpose of the plant-performance analysis is to operate on the set of measurements obtained, subject to the equipment constraints to troubleshoot; to develop models; or to estimate values for model parameters.

$$g\langle \mathbf{X}_1^m;\mathbf{X}_2\rangle \Rightarrow \vec{\beta}$$

where $g\langle\rangle$ is an operator on the measurements and data. The vector $\vec{\beta}$ is a representation of the conclusions, model, and/or equipment parameters.

Measurement Selection The identification of which measurements to make is an often overlooked aspect of plant-performance analysis. The end use of the data interpretation must be understood (i.e., the purpose for which the data, the parameters, or the resultant model will be used). For example, building a mathematical model of the process to explore other regions of operation is an end use. Another is to use the data to troubleshoot an operating problem. The level of data accuracy, the amount of data, and the sophistication of the interpretation depends upon the accuracy with which the result of the analysis needs to be known. Daily measurements to a great extent and special plant measurements to a lesser extent are rarely planned with the end use in mind. The result is typically too little data of too low accuracy or an inordinate amount with the resultant misuse in resources.

If the problem were accurately known, identification of which measurements should be taken would be exact. When the problem is initially not accurately known, the identification, measurement, and analysis procedure is iterative. Familiarity with the plant will help in identifying the measurements most likely to provide insight.

When building a model for the plant either in terms of a set of relations or in terms of a set of parameters for an existing model, it is important that the measurements contain a maximum amount of information. If the model is embodied in the symbol of the parameters, $\vec{\beta}$, then the measurements should be made such that the measurement matrix $\mathbf{X}_1^m$ has the greatest impact on $\vec{\beta}$**.** This maximizes the plant information contained in the parameters. The process is necessarily iterative. Measurements are analyzed to refine the model and optimal locations for new measurements are defined.

Analysts must recognize the above sensitivity when identifying which measurements are required. For example, a typical use of plant data is to estimate the tray efficiency or HTU of a distillation tower. Certain tray compositions are more important than others in providing an estimate of the efficiency. Unfortunately, sensor placement or sample port location are usually not optimal and, consequently, available measurements are, all too often, of less than optimal use. Uncertainty in the resultant model is not minimized.

Plant Operations Each of the elements x_{ij} in $\mathbf{X}_1^m$ have inherent error. Consequently, x_{ij} is only an estimator of the actual plant value. Or,

$$x_{ij} = \tilde{x}_{ij} + \varepsilon$$

It is useful to recognize the contributions to this error.

First, plant operations are rarely exactly as intended. While the designer may have developed all operating specifications as if the plant would operate at steady state, the plant fluctuates and drifts with time. Changes occur because of changes in feed stock, atmospheric conditions, operating conditions, controller response, and any number of factors, both known and unknown. The actual value then fluctuates around some mean operation. For example, Fig. 30-11 is a typical plant strip chart recording. The lower trace shows that the measurement is fluctuating around a mean value. The upper trace also shows fluctuation, but the mean value is changing with time.

While the random fluctuations apparent are a function of the scaling factor for the traces, the two show different amplitudes. The top trace has a relatively small fluctuation, while the bottom trace shows a larger one.

Mathematically, the mean value is the desired value for further analysis.

$$\tilde{x}_{ij} = \bar{x}_{ij} + \varepsilon_{ij}^P$$

The plant drift makes all measurements functions of time. The upper trace in the above figure shows some evidence of drift. Figure 30-12 shows a larger drift.

This drift can be represented mathematically as:

$$\tilde{x}_{ij}(t) = \bar{x}_{ij}(t) + \varepsilon_{ij}^P$$

This time dependence is different for each measurement. The fluctuation may also be a function of time.

In addition to the drift with time, step changes due to operating decisions, atmospheric changes, or other conditions result in additional time dependence. Not only is there a sudden change due to the actual decision, but also the plant changes due to the time constants. For example, Fig. 30-13 shows measurements with step changes in the operation.

Data Limitations The process of measuring $\tilde{x}_{ij}(t)$ adds additional error due to the random error of measurement. Or,

$$x_{ij}(t) = \tilde{x}_{ij}(t) + \varepsilon_{ij}^M$$

$$x_{ij}(t) = \bar{x}_{ij}(t) + \varepsilon_{ij}^P + \varepsilon_{ij}^M$$

Consequently, if these random errors are assumed to be normal, the total uncertainty including fluctuations is:

$$\sigma_{ij}^T = \sqrt{(\sigma_{ij}^P)^2 + (\sigma_{ij}^M)^2}$$

where σ replaces ε to represent a normal distribution. Therefore,

$$x_{ij}(t) = \bar{x}_{ij}(t) + \sigma_{ij}^{\mathbf{T}}$$

The problem with plant data becomes more significant when sampling, instrument, and calibration errors are accounted for. These errors result in a systematic deviation in the measurements from the actual values. Descriptively, the total error (mean square error) in the measurements is

$$\text{MSE} = (\sigma_{ij}^{\mathbf{T}})^2 + (b^M)^2$$

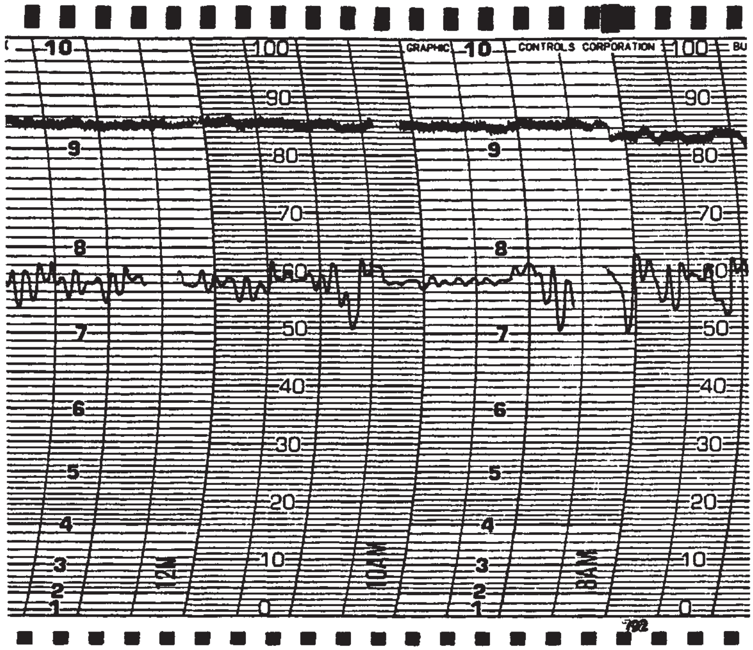

FIG. 30-11 Plant measurements showing fluctuations around a mean value.

The above assumes that the measurement statistics are known. This is rarely the case. Typically a normal distribution is assumed for the plant and the measurements. Since these distributions are used in the analysis of the data, an incorrect assumption will lead to further bias in the resultant troubleshooting, model, and parameter estimation conclusions.

Constraints Limitations Typically, the plant performance is assumed to be subject to process constraints.

$$\vec{\mathbf{f}}\langle \mathbf{X}_1 \rangle = \vec{\mathbf{0}}$$

where $\vec{\mathbf{f}}\langle\,\rangle$ is a vector of constraints. For the process shown in Fig. 30-10, these constraints could be, using the component flows and total flows and temperatures as the measurements:

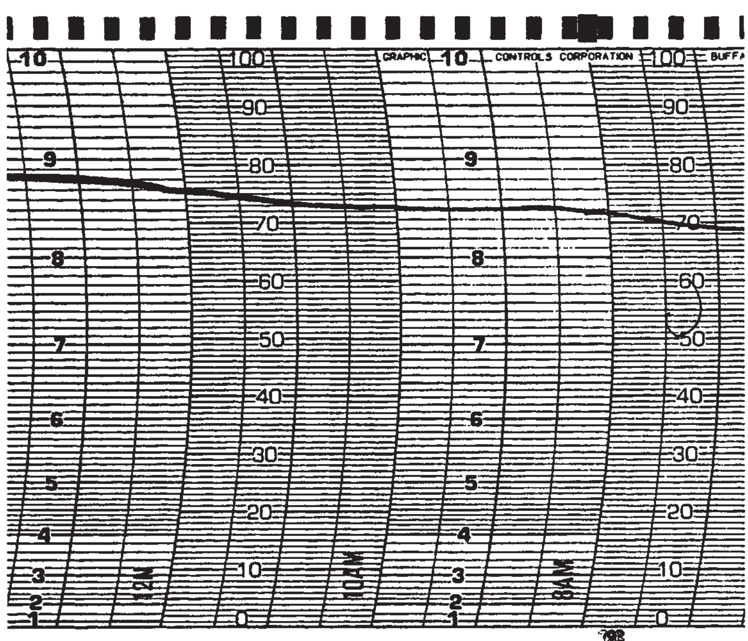

FIG. 30-12 Plant measurements showing drift with time.

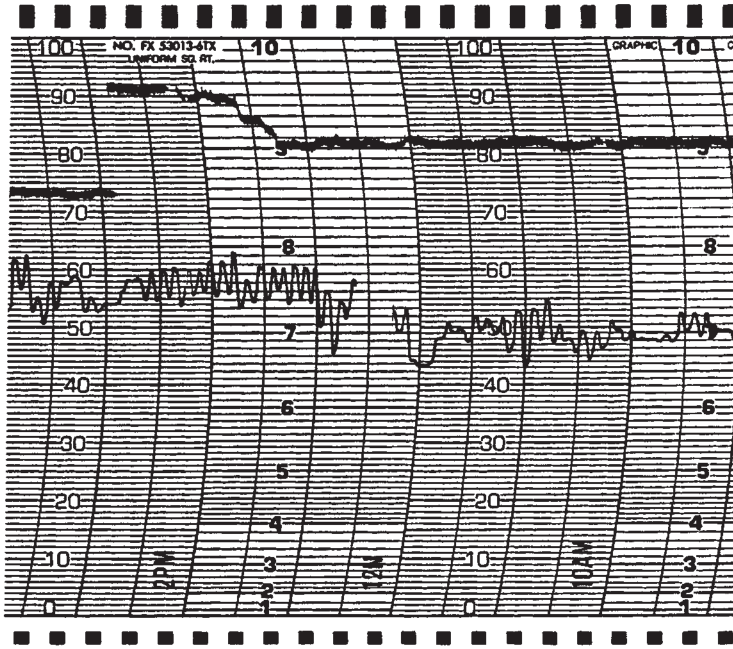

FIG. 30-13 Plant measurements exhibiting step changes, drift, and random fluctuations.

$$x_{i,1} - x_{i,2} - x_{i,3} = 0 \qquad i = 1 \ldots c$$

where c is the number of components

$$x_{c+1,1} - x_{c+1,2} - x_{c+1,3} = 0$$

$$x_{c+1,1}H_1 - x_{c+1,2}H_2 - x_{c+1,3}H_3 = 0$$

where the $c + 1$th position is the total flow. Only c of the material balance constraints are independent. Of course, the actual measurements do not close the constraints.

$$\vec{\mathbf{f}}\langle \mathbf{X}_1^m \rangle \neq \vec{\mathbf{0}}$$

To complicate matters further, because of the time dependence, leaks, or accumulation, the constraints might not actually apply such that there is a vector of unknown plant bias' associated with the constraints.

$$\vec{\mathbf{f}}\langle \mathbf{X}_1^m \rangle = \vec{\mathbf{b}}^P$$

Assuming $\vec{\mathbf{b}}^P = 0$ will potentially add bias to the interpretation of plant measurements. Further, the plant bias may to some extent mask the error in the measurements. While the designer may have envisioned a constant set of conditions or a specified time dependence, it is likely that the actual operation changes due to external factors.

The technical problem becomes one of:

$$g\langle \mathbf{X}_1^m ; \mathbf{X}_2 \rangle \overset{b^e}{\Rightarrow} \vec{\boldsymbol{\beta}}$$

subject to $\qquad \vec{\mathbf{f}}\langle \mathbf{X}_1^m \rangle = \vec{\mathbf{b}}^P$

This is a formidable analysis problem. The number and impact of uncertainties makes normal plant-performance analysis difficult. Despite their limitations, however, the measurements must be used to understand the internal process. The measurements have limited quality, and they are sparse, suboptimal, and biased. The statistical distributions are unknown. Treatment methods may add bias to the conclusions. The result is the potential for many interpretations to describe the measurements equally well.

Personnel Bias Because of the possibility of several interpretations of the plant-performance problem, the judgment of analysts plays a critical role. Any bias in the analysts' judgments will carry through the data analyses. To minimize this, analysts must develop an implicit model based on the fundamental rules of the plant and not on the prejudices of the operators, designer engineers, control engineers, or the analyst's own perceptions.

The following presents guidelines for identifying, validating, reconciling, rectifying, and interpreting plant measurements to remove some of the bias from the conclusions.

IDENTIFICATION

Motivation Unit tests require a substantial investment in time and resources to complete successfully. This is the case whether the test is a straightforward analysis of pump performance or a complex analysis of an integrated reactor and separation train. The uncertainties in the measurements, the likelihood that different underlying problems lead to the same symptoms, and the multiple interpretations of unit performance are barriers against accurate understanding of the unit operation. The goal of any unit test should be to maximize the success (i.e., to describe accurately unit performance) while minimizing the resources necessary to arrive at the description and the subsequent recommendations. The number of measurements and the number of trials should be selected so that they are minimized.

Often, analysts will want to run special short-term tests with the operating unit in order to identify the cause of the trouble being experienced by the unit. Operators are naturally leery of running tests outside their normal operating experience because their primary focus is the stable control of the unit, and tests outside their experience may result in loss of control. Multiple tests with few results may decrease their cooperation.

Modern petro/chemical processes provide the opportunity for gathering a large number of measurements automatically and frequently. Most are redundant and provide little additional insight into unit performance. The difficulties in handling a large amount of information with little intimate knowledge of the operation increases the likelihood that some of the conclusions drawn will be erroneous.

Therefore, the identification of appropriate tests and measurements most important to understanding the unit operation is a critical step in the successful analysis of plant performance.

Limitations Identifying the appropriate test to troubleshoot a unit problem requires hypothesis development and testing. Hypotheses are based on the observed problem in current operation and the historical performance. It is the skill of analysts to develop the minimum number of hypotheses and unit tests to identify what is typically a well-hidden problem.

Identifying the minimum number of specific measurements containing the most information such that the model parameters are uniquely estimated requires that the model and parameter estimates be known in advance. Repeated unit tests and model building exercises will ultimately lead to the appropriate measurements. However, for the first unit test in absence of a model, the identification of the minimum number of measurements is not possible.

The methodology of identifying the optimum test and number of measurements has received little attention in analysis of plant performance and design literature.

Measurement Error Uncertainty in the interpretation of unit performance results from statistical errors in the measurements, low levels of process understanding, and differences in unit and modeled performance (Frey, H.C., and E. Rubin, "Evaluate Uncertainties in Advanced Process Technologies," *Chemical Engineering Progress,* May 1992, 63–70). It is difficult to determine which measurements will provide the most insight into unit performance. A necessary first step is the understanding of the measurement errors likely to be encountered.

An example adapted from Verneuil, et al. (Verneuil, V.S., P. Yan, and F. Madron, "Banish Bad Plant Data," *Chemical Engineering Progress*, October 1992, 45–51) shows the impact of flow measurement error on misinterpretation of the unit operation. The success in interpreting and ultimately improving unit performance depends upon the uncertainty in the measurements. In Fig. 30-14, the material balance constraint would indicate that $S_3 = -7$, which is unrealistic. However, accounting for the uncertainties in both S_1 and S_2 shows that the value for S_3 is -7 ± 28. Without considering uncertainties in the measurements, analysts might conclude that the flows or model contain bias (systematic) error.

Analysts should review the technical basis for uncertainties in the measurements. They should develop judgments for the uncertainties based on the plant experience and statistical interpretation of plant measurements. The most difficult aspect of establishing the measurement errors is establishing that the measurements are representative of what they purport to be. Internal reactor CSTR conditions are rarely the same as the effluent flow. Thermocouples in catalyst beds may be representative of near-wall instead of bulk conditions. Heat leakage around thermowells results in lower than actual temperature measurements.

These measurement uncertainties must be accounted for in developing hypotheses used to explain unit performance and in identifying measurements which will provide the best model of the unit.

Hypothesis Development Successful, efficient development of hypotheses and operating conditions to test them require design, operation, control, and troubleshooting experience. Understanding the relation of the fundamentals of chemical engineering, the specifications and their intent for operation, the response of equipment to upsets, and the identification of the unusual are all essential tools for developing and testing hypotheses during troubleshooting exercises. Hypothesis development is typically iterative with unit operating conditions adjusted to test a hypothesis. The results lead to other hypotheses and other operating conditions. This is an essential part of troubleshooting and model development.

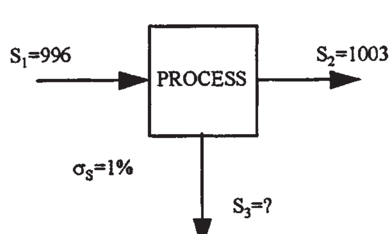

FIG. 30-14 Material balance measurements with error.

Troubleshooting is usually based on checklists developed by analysts specific to the unit and types of equipment in the unit. These checklists assist in hypothesizing the cause of observed problems based on past experience and in developing tests or measurements to confirm the hypotheses. Few published checklists exist in the literature. Most analysts develop their own based on experience. As engineers move from assignment to assignment with little direct, continued experience in the design, operation, control, and troubleshooting, the checklists are lost. The skill resides with the engineer and not with the unit. Consequently, individual checklists are developed repeatedly with little continuity unless current analysts seek out those who were once responsible for the unit. One notable exception is the set of checklists for refinery operations published by Lieberman (1981). Many of his experiences arise in and apply to other chemical engineering applications. His lists give the observed problem and possible explanations. Harrison and France (Harrison, M.E. and J.J. France, "Auxiliary Equipment: Troubleshooting Distillation Columns," *Chemical Engineering*, June 1989, 130–137) list a series of problems with corresponding causes. Symptoms in one piece of equipment may appear as a problem in another; therefore, checklists should include the potential that other equipment in the unit is the cause of the observed problem.

A proposed checklist form is given in Table 30-1. The descriptive example concerns a problem observed with distillation performance in a specific unit. It is included for descriptive purposes only and does not provide an exhaustive list of possible explanations for the observed problem. The important aspects are a clear statement of the problem; recognized changes in unit operation at the time of the observation and hypothesized causes under the categories of erroneous instrument readings; changes upstream and downstream from the unit and within the unit itself. Typical explanations under each cause category could be substantially longer than ones included in the table.

History is important is establishing hypotheses. When a problem arises in a unit, something has changed. The first step in developing a hypothesis explaining the cause of the problem is to establish that the operation has clearly changed from some earlier operation. Easily identified alterations in operation such as those that result from changes in operating specifications, equipment installations, or operator responses should be listed.

The observations may be erroneous due to misleading measurements. The basis of the observations should be examined. Instruments may have degraded. Sample lines may have become plugged. Trip settings may have changed. Where possible, these causes should be eliminated before moving to more complex explanations and tests. Many unit problems are caused by upstream or downstream units. This interaction should be identified before performing extensive tests with the unit. In the table, a sudden increase in light ends could flood the upper section of the tower. Pump cavitation may be the result of fluctuating discharge pressures in the downstream units. Corrosion in the unit may be caused by carryover from an upstream unit. Insufficient pump capacity could be caused by a changed fluid density from changed feed stock.

With the problem being identified as real and other units being eliminated as the cause, the focus can move to identifying whether the problem is with capacity or efficiency within the unit.

The following are guidelines for establishing checklists used to identify the cause of observed problems.

TABLE 30-1 Example Checklist Form

Observed problem	Increased pressure drop in the distillation column
Unit changes	Steam header pressure increase, no equipment changes
Instrument cause	DP meter reading is misleading due to failed instrument, plugged ports, etc.
Upstream cause	Increased percentage of light components fed to column resulting in flooding in rectifying section
Downstream cause	Not applicable
Capacity cause	Steam reboiler flow set above column jet flood limit
Efficiency cause	Trays plugged with polymer buildup

- Establish the timeline of the problem hypothesizing that changes in operation, equipment, or response are the root cause of the problem.
- Establish the observed problem is real by hypothesizing potential problems with instruments and instrument installations.
- Establish that the observed problem could not be caused by upstream or downstream unit performance.
- Establish that the problem is one with capacity of the unit by hypothesizing causes for the decreased unit production.
- Establish that the problem is one with efficiency of the unit by hypothesizing causes to explain the decreased performance of the unit.

Any set of guidelines must be tempered by the analysts' experience. This is an investigative process. The explanations are rarely simple. However, many exhaustive tests have been run to identify that a bypass valve or alternative feed valve had been mistakenly left open. Plant resources were misused because the simple was overlooked.

Since hypothesis development and testing frequently require alternative operating conditions, safety considerations must be paramount. The operators' concerns about loss of control are justified. When tests are planned, it must be recognized that adjustments should be slow and stepwise with time allowed for the unit to line out. All possible outcomes of the adjustments should be thought through to minimize the potential for moving the unit into an unstable operating regime.

Model Development Preliminary modeling of the unit should be done during the familiarization stage. Interactions between database uncertainties and parameter estimates and between measurement errors and parameter estimates could lead to erroneous parameter estimates. Attempting to develop parameter estimates when the model is systematically in error will lead to systematic error in the parameter estimates. Systematic errors in models arise from not properly accounting for the fundamentals and for the equipment boundaries. Consequently, the resultant model does not properly represent the unit and is unusable for design, control, and optimization. Cropley (1987) describes the erroneous parameter estimates obtained from a reactor study when the fundamental mechanism was not properly described within the model.

Verneuil et al. (Verneuil, V.S., P. Yan, and F. Madron, "Banish Bad Plant Data," *Chemical Engineering Progress,* October 1992, 45–51) emphasize the importance of proper model development. Systematic errors result not only from the measurements but also from the model used to analyze the measurements. Advanced methods of measurement processing will not substitute for accurate measurements. If highly nonlinear models (e.g., Cropley's kinetic model or typical distillation models) are used to analyze unit measurements and estimate parameters, the likelihood for arriving at erroneous models increases. Consequently, resultant models should be treated as approximations.

Recognition of measurement error, model nonlinearities, interactions, and potential fundamental oversights are an important part of the identification stage of analysis of plant performance. Repeated simulations using different models extrapolated to other operating conditions will provide insight into model viability. Model accuracy can be verified by operating the unit at different operating conditions and making appropriate measurements. Identification of these conditions and measurements is one aspect of the identification step. These model building studies to identify possible alternative models and operating conditions are useful in minimizing the impact of erroneous model development and subsequent parameter estimation.

Measurement Selection Along with the hypothesis development, the principal result of the identification step is determining which measurements will provide insight into the unit operation. This often-overlooked aspect of analysis of plant performance deserves greater attention in the plant operations and research literature. The potential resource savings resulting from minimizing the number of measurements, repeated unit tests, and associated personnel are enormous. Coupled with the benefit of developing a more robust model of the unit, this overlooked aspect of analysis of plant performance potentially outweighs the benefits of all other aspects.

The goal of measurement selection is to identify a set of measurements that, when interpreted, will lead to unique values for the model parameters, insensitive to uncertainties in the measurements. This is an iterative process where:

- A group of measurements are proposed based on preliminary model predictions
- Values for parameters are estimated using the interpretation procedures
- Simulated unit performance sensitivity to the parameter estimates is evaluated
- Alternative measurements are proposed
- The process is repeated

The optimum measurements are those taken in the unit test. Figure 30-15 provides one procedure for identifying which measurements should be taken within the plant.

A preliminary model is developed during the preparation stage. Preliminary values of the model parameters are estimated based on adjusted plant measurements. Simulations of the unit are then run to develop values for the temperatures, pressures, flows, compositions, and the like, that are representative of the unit operation. A group of measurements that could possibly be taken in the unit test is then selected. At that point, analysts have two options. In option A, the parameter estimates are perturbed, the unit resimulated, and the group of measurements compared to the set corresponding to the perturbed parameters. If the comparison is such that the simulated measurements are different beyond the experimental error, then the parameter values are unique and the group of measurements are appropriate. If they are not, the proposed measurements should be changed and the process repeated. In option B, the process is similar. The group of measurements are perturbed according to the measurement error, the parameters re-estimated, and the parameter values compared. If there is relatively little change in the parameter values, the selected measurements are acceptable. If there is a large change, the measurements do not provide a unique set of parameter estimates. Consequently, the model would be unsuitable. The measurement set needs to be modified. Once the set of measurements have been selected, the model should be examined and modified if necessary. There are two primary indications that the model may be inadequate. First, the preliminary model with the estimated parameters provide descriptions of one or more measurements representing unit behavior, particularly internal to individual pieces of equipment. Second, the values of the parameters are unrealistic.

With respect to selecting measurements, emphasis should include measurements within the equipment such as tower internal temperatures and compositions, internal reactor conditions, and intermediate exchanger temperatures in multipass exchangers. Trace component compositions provide particular insight into distillation-column performance. Those components that fall between the heavy and light keys and distribute in the products can usually be described by a variety of models and parameter estimates: They provide little insight into the column performance.

The procedure given in Fig. 30-15 leaves much to analysts. Criteria for selecting the number and location of measurements for a particular piece of equipment or unit have not been established in the literature. Therefore, there is heavy reliance on examining alternative models at the bottom of the procedure. The creativity of analysts to develop alternative explanations for performance or hypotheses explaining why the present model might be wrong is a particularly important skill.

VALIDATION

Initial Measurement Examination The process of reconciling data to constraints; rectifying data to detect and identify systematic errors; and interpreting data to troubleshoot, model-build, and estimate parameters is a time-consuming, often unnecessary, and, many times, inaccurate series of steps. Even under the most controlled circumstances, the methods often provide estimates of plant operation that are no better than that provided by the actual plant measurements. If the adjusted measurements contain significant error, the resultant conclusions could be significantly in error and misleading. Prescreening can identify measurements containing significant error and can provide insight into the plant operation.

Validation is the procedure of comparing measurements to known relations between the measurements and equipment settings (May,

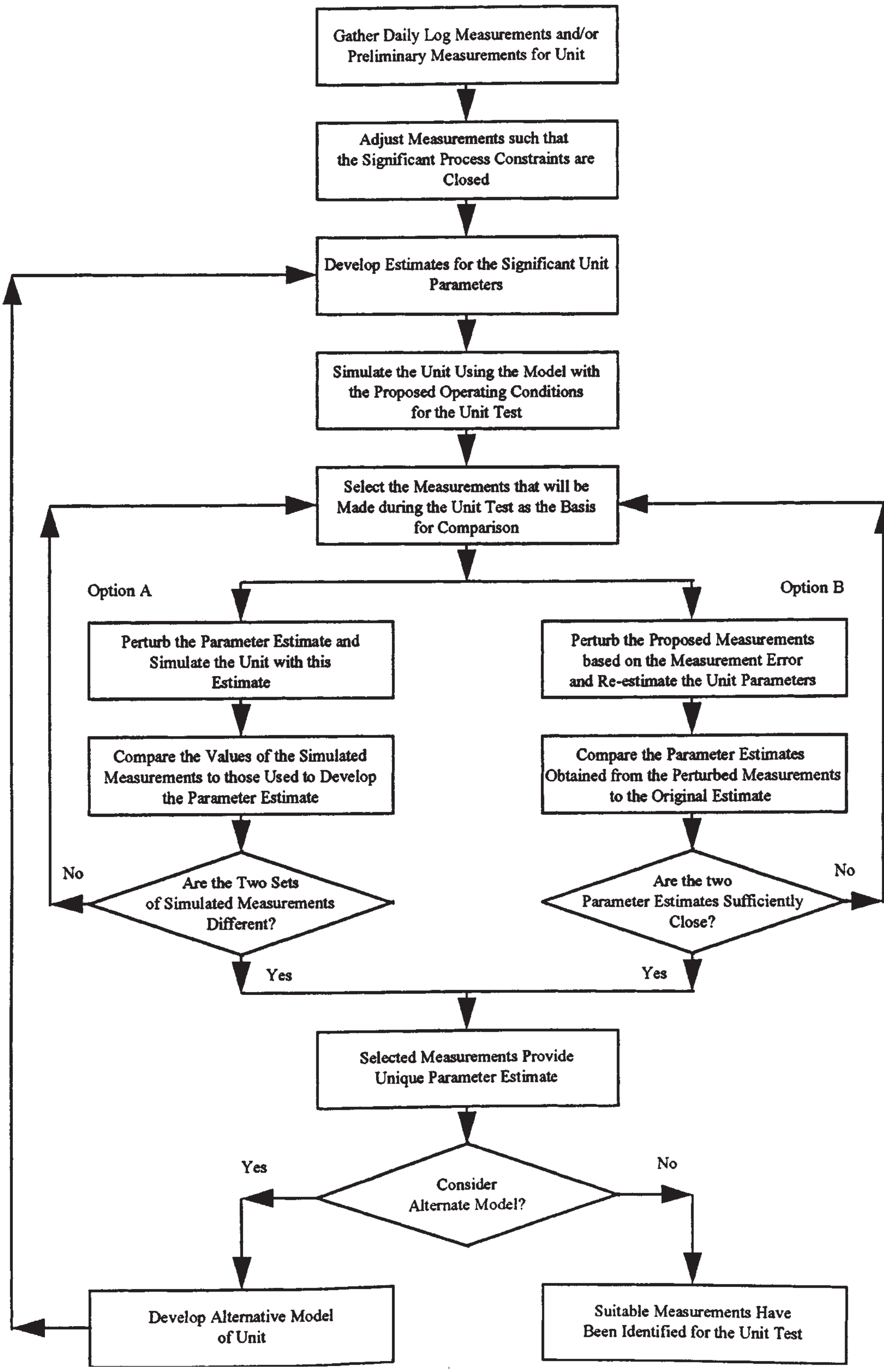

FIG. 30-15 Procedure for identifying measurements.

D.L. and J.T. Payne, "Validate Process Data Automatically," *Chemical Engineering*, June 1992, 112–116). If a measurement is clearly inconsistent with equipment operation that is known to be true, the measurement must then be deemed suspect. Validation is the procedure of comparing a measurement to one or more of the following.

- Another measurement
- An expected range
- Equipment status
- Equipment relations

If the comparison shows that the measurement is inconsistent with the comparison information, the measurement is considered suspect. If a measurement can be compared to more than one set of information and found to be inconsistent with all, it is likely that the measurement is in error. The measurement should then be excluded from the measurement set. In this section, validation is extended to include comparison of the measurements to the constraints and initial adjustment in the measurements. Validation functions as an initial screening procedure before the more complicated procedures begin. Oftentimes, validation is the only measurement treatment required prior to interpretation.

It is important to note that validation typically only brings a measurement under suspicion. It does not verify that the measurement is incorrect. Safety is paramount. Some validation analysis could result in concluding that the measurement is invalid when, in fact, the comparison information is invalid. It is not difficult to extrapolate that actions could result from this erroneous conclusion which would place maintenance and operating personnel in jeopardy. Validation merely raises suspicion; it does not confirm errors of measurement.

The greater the number of validation comparisons between the measurement and the list above, the greater the likelihood that the measurement can be identified as valid or invalid.

Measurement versus Measurement In this type of validation, a process measurement is compared against another. For example, if a separate high-level alarm indicates that a tank is overflowing but the level gauge indicates that it is in the expected range, one of these measurements is wrong. As another example, if a light component suddenly appears in the bottoms of a distillation tower and no other light components contained in the feed appear in the bottoms, the first measurement is suspect.

Measurement versus Expected Range If a steam flow is expected to vary in a relatively narrow range and the flow measurement indicates that it is twice the high value, the flow measurement is then suspect and should be reviewed. A frequent occurrence is when a measurement remains unchanged for a period of time when normal plant fluctuations should result in oscillations around a setpoint. The constant measurement would indicate that this reading is suspect.

Measurement versus Equipment State A pump off-line should have no flow. If the pump is off and the flow meter indicates that there is flow, the flow measurement is suspect.

Measurement versus Equipment Performance Pumps that are in reasonable condition typically operate within 5 percent of their pump curve. Consequently, pressures and flows that are inconsistent with the pump curve imply that the indicated flow and/or pressure are incorrect. Figure 30-16 shows a single impeller curve plotted as head versus flow. The point shown is inconsistent with the pump operation. Therefore, that pair of flow and pressure measurements is not validated and should not be used in the subsequent steps.

Validation versus Rectification The goal of both rectification and validation is the detection and identification of measurements that contain systematic error. Rectification is typically done simultaneously with reconciliation using the reconciliation results to identify measurements that potentially contain systematic error. Validation typically relies only on other measurements and operating information. Consequently, validation is preferred when measurements and their supporting information are limited. Further, prior screening of measurements limits the possibility that the systematic errors will go undetected in the rectification step and subsequently be incorporated into any conclusions drawn during the interpretation step.

INITIAL CONSTRAINT ANALYSIS AND ADJUSTMENTS

Spreadsheet Analysis Once validation is complete, prescreening the measurements using the process constraints as the comparison statistic is particularly useful. This is the first step in the global test discussed in the rectification section. Also, an initial adjustment in component flows will provide the initial point for reconciliation. Therefore, the goals of this prescreening are to:

- Pretreat raw measurements
- Estimate the overall and component constraint deviations
- Identify missing measurements
- Adjust (initially) the measurements to close the constraints

The principal focus of this validation is the material and energy bal-

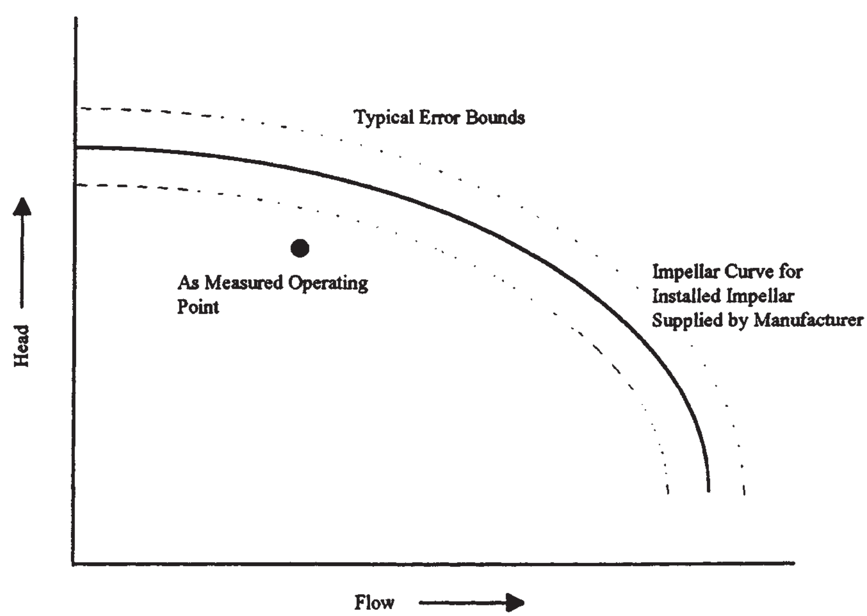

FIG. 30-16 Typical pump curve showing inconsistency between measurement and curve.

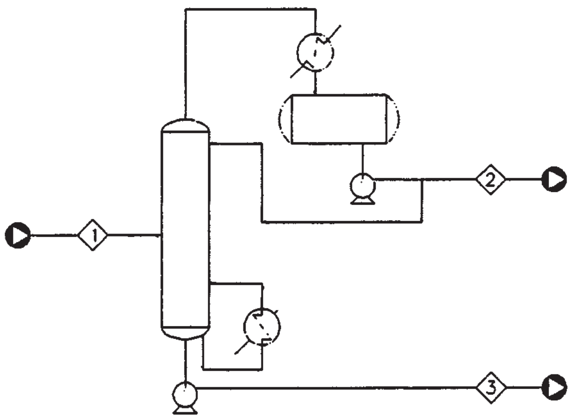

FIG. 30-17 Distillation tower example.

ances for the unit. Specifically designed spreadsheets are particularly useful during this step. The level of sophistication depends upon the analysts' goals. Spreadsheets can be used for pretreatment of measurements, constraint analysis, and measurement adjustment. Oftentimes, the more sophisticated reconciliation and rectification methods are not warranted or will not provide any better results, particularly when a single unit is under analysis.

For the purposes of this discussion, consider a single distillation tower with one feed, a distillate, and bottoms, as shown in Fig. 30-17.

A straightforward, generic analysis spreadsheet for this tower is shown in Fig. 30-18. For this example, the three stream compositions and the total flows have all been measured. Also, since this is a column in a purification train, the bottoms flow rate has been measured independently as the feed to the next tower.

Spreadsheet Structure There are three principal sections to the spreadsheet. The first has tables of as-reported and normalized composition measurements. The second section has tables for overall and component flows. These are used to check the overall and component material balance constraints. The third has adjusted stream and component flows. Space is provided for recording the basis of the adjustments. The structure changes as the breadth and depth of the analysis increases.

The example spreadsheet covers a three-day test. Tests over a period of days provide an opportunity to ensure that the tower operated at steady state for a period of time. Three sets of compositions were measured, recorded, normalized, and averaged. The daily compositions can be compared graphically to the averages to show drift. Scatter-diagram graphs, such as those in the reconciliation section, are developed for this analysis. If no drift is identified, the scatter in the measurements with time can give an estimate of the random error (measurement and fluctuations) in the measurements.

The second section of the spreadsheet contains the overall flows, the calculated component flows, and the material balance closure of each. The weighted nonclosure can be calculated using the random error calculated above, and a constraint test can be done with each component constraint if desired. Whether the measurement test is done or not, the nonclosure of the material balance for each component gives an indication of the validity of the overall flows and the compositions. If particular components are found to have significant constraint error, discussions with laboratory personnel about sampling and analysis and with instrument personnel about flow-measurement errors can take place before any extensive computations begin.

The measurements and flows can be adjusted to close the constraints. These adjustments can then be compared to the measurements to determine whether any are reasonable. Statistical routines or hand adjustments are possible. These adjusted flows and compositions might form the basis for the interpretation step bypassing any deeper reconciliation and rectification. This is particularly appropriate where many compositions are left unmeasured and those that are measured have different levels of error. More sophisticated routines will not compensate for incomplete, imprecise, and potentially inaccurate measurements.

Recommendations Once measurements are made, validation is the most important step for establishing a sound set of measurements. The comparisons against other measurements or other known pieces of information quickly identify suspect measurements. Spreadsheet analysis of constraints, particularly material and energy balances, identifies other weaknesses in the measurements and provides the opportunity for discussions with those responsible before considerable analysis effort is expended. Finally, initial adjustments provide the beginnings of the interpretation analysis.

RECONCILIATION

Single-Module Analysis Consider the single-module unit shown in Fig. 30-10. If the measurements were complete, they would consist of compositions, flows, temperatures, and pressures. These would contain significant random and systematic errors. Consequently, as collected, they do not close the constraints of the unit being studied. The measurements are only estimates of the actual plant operation. If the actual operation were known, the analyst could prepare a scatter diagram comparing the measurements to the actual values, which is a useful analysis tool. Figure 30-19 is an example.

If the measurements were completely accurate and precise (i.e., they contained neither random nor systematic error), all of the symbols representing the individual measurements would fall on the zero deviation line. Since the data do contain error, the measurements should fall within ± 2 on this type of diagram. This example scatter diagram shows that some of the measurements do not compare well to the actual values.

Unfortunately, the actual plant operation is unknown. Therefore, the actual value of each of the measurements is unknown. The purpose of reconciliation is to adjust the measurements so that they close the process constraints. The implicit hypothesis is that the resultant adjusted measurements better represent the actual unit operation than do the actual measurements.

Statistical Approach Ignoring any discrepancies between the implicit model used to establish the constraints and the actual unit, the measurements are adjusted to close the constraints. This adjustment effectively superimposes the known process operation embodied in the constraints onto the measurements. Minimum adjustments are made to the measurements.

The matrix of measurements is rearranged into a stacked vector where each subsequent set of stream measurements follows the one above. As an example, the component flows in the $\mathbf{X}_1^m$ matrix are placed in the vector of measurements as follows:

$$\vec{\mathbf{X}}^m = \begin{bmatrix} x_{1,1} \\ x_{2,1} \\ \cdot \\ \cdot \\ x_{c,1} \\ x_{2,1} \\ \cdot \\ \cdot \\ x_{c-1,3} \\ x_{c,3} \end{bmatrix}$$

Defining, $$\delta\vec{\mathbf{X}}_1 = \hat{\vec{\mathbf{X}}}_1^m - \vec{\mathbf{X}}_1^m$$

Minimize: $$\delta\vec{\mathbf{X}}_1^T \delta\vec{\mathbf{X}}_1$$

Such that: $$\vec{\mathbf{f}}(\hat{\vec{\mathbf{X}}}_1^m) = \vec{\mathbf{0}}$$

If the constraints are linear (e.g., the component flow material balances) or can be linearized, then

$$\mathbf{B}\hat{\vec{\mathbf{X}}}_1^m = \vec{\mathbf{0}}$$

In the material balance example, the matrix **B** contains the material balance coefficients for the component flows based on the implicit model of the process. These adjustments can be done by hand or by

ANALYSIS OF TOWER DATA

Measured compositions reported on lab logs

Component	Feed composition			Distillation composition			Bottoms composition		
	Date 1 wt%	Date 2 wt%	Date 3 wt%	Date 1 wt%	Date 2 wt%	Date 3 wt%	Date 1 wt%	Date 2 wt%	Date 3 wt%
Component 1									
Component 2									
Component 3									
•									
•									
•									
Component c-1									
Component c									
Total									

Average compositions for period

Component	Stream compositions		
	Feed wt%	Ovhd wt%	Btms wt%
Component 1			
Component 2			
Component 3			
•			
•			
•			
Component c-1			
Component c			
Total			

Normalized compositions for single date

Component	Stream compositions		
	Feed wt%	Ovhd wt%	Btms wt%
Component 1			
Component 2			
Component 3			
•			
•			
•			
Component c-1			
Component c			
Total			

Stream flowrates for single date

Stream	lb/hr	
Feed		
Distillate		
Bottoms		As measured
Bottoms		Back-calculated from next unit
Bottoms		Back-calculated to close

Projected stream flows—next tower basis

Component	Stream flows			Closure	
	Feed lb/hr	Ovhd lb/hr	Btms lb/hr	lb/hr	%
Component 1					
Component 2					
Component 3					
•					
•					
•					
Component c-1					
Component c					
Total					

Projected single date flows—next tower basis

Component	Stream flows			Closure	
	Feed lb/hr	Ovhd lb/hr	Btms lb/hr	lb/hr	%
Component 1					
Component 2					
Component 3					
•					
•					
•					
Component c-1					
Component c					
Total					

Possible material balance adjustment

Component	Stream flows						
	Feed		Ovhd product		Btms product		
	lb/hr	wt%	lb/hr	wt%	lb/hr	wt%	Descriptive notes
Component 1							
Component 2							
Component 3							
•							
•							
•							
Component c-1							
Component c							
Total							

FIG. 30-18 Generic spreadsheet for analyzing measurement validity.

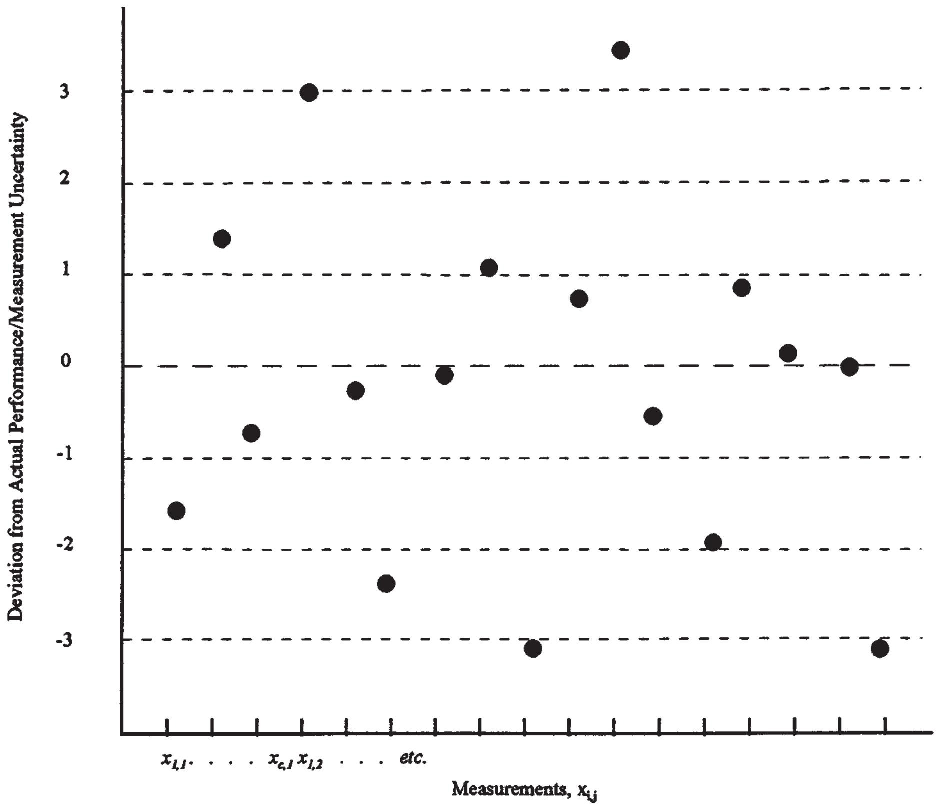

FIG. 30-19 Scatter diagram of measurements before reconciliation.

using computer aids. They can be made without consideration of measurement errors in the data (Leibovici, C.F., et al., "Improve Prediction with Data Reconciliation," *Hydrocarbon Processing,* October, 1993, 79–80) as above or can be done by accounting for the random errors (MacDonald, R.J. and C.S. Howat, "Data Reconciliation and Parameter Estimation in Plant Performance Analysis," *AIChE Journal,* **34**(1), 1988, 1–8.) For the latter, the problem becomes:

Minimize: $\delta\vec{\mathbf{X}}_1^{\mathbf{T}}\mathbf{J}^{-1}\delta\vec{\mathbf{X}}_1$

Such that: $\vec{\mathbf{f}}(\hat{\mathbf{X}}_1^m) = \vec{\mathbf{0}}$

where **J** is the variance-covariance of the measurements. If the number of measurements is limited for a stream, the adjustments can be made on the limited number of measurements. The constraints can also be used to estimate missing or discarded measurements: This use of the constraints is defined as *coaptation* in the literature. However, this propagates errors and should be done with caution.

Analysis of Measurement Adjustments Once reconciliation has been completed, the adjusted measurements can be compared to the actual measurements using a scatter diagram. Figure 30-20 presents an example. In this figure, the weighted residuals in the adjustments are plotted. The weighting factor is a measure of the random error in that particular measurement. In this visualization, the value of the residual should be between ±2. The scatter has improved from the previous figure, but numerical studies have indicated that the analyst can expect only 60 percent of the measurements to be adjusted toward the actual value. Consequently, while the scatter may have improved, there is no guarantee that a particular adjusted measurement is better than the actual measurement. This is one of the principal shortcomings of any automatic data adjustment method.

Adjustments outside this range could be suspect, either because of measurement error or error in the estimated uncertainty. These will be evaluated in the rectification step. Weighted residual values of 0 do not necessarily indicate that the measurement is correct. While this is a possible explanation, a more likely one is that the selected constraints used in the reconciliation are not sensitive functions of this measurement. Therefore, in the interpretation step, caution is recommended in using these adjusted measurements to compare against the model estimate.

At this point, analysts have a set of adjusted measurements that may better represent the unit operation. These will ultimately be used to identify faults, develop a model, or estimate parameters. This automatic reconciliation is not a panacea. Incomplete data sets, unknown uncertainties and incorrect constraints all compromise the accuracy of the adjustments. Consequently, preliminary adjustments by hand are still recommended. Even when automatic adjustments appear to be correct, the results must be viewed with some skepticism.

Complex Flow Sheets Operating plants do not consist of single flashes, heat exchangers, distillation towers, or reactors. As the number of pieces of equipment increases within the unit under study, the reconciliation becomes more difficult. For example, Fig. 30-21 presents a more complicated, three-module unit.

There are now constraints for each of the modules within the unit. For example, the material and energy balances must close for each module. The overall material and energy balances must also close, but they are not independent. There are three approaches to close these constraints.

First, the reconciliation can be done separately around each module. Each module is studied alone. The measurements are reconciled to the individual module constraints without consideration of any other module with common streams. For example, the first module in the figure is reconciled, and the measurements corresponding to

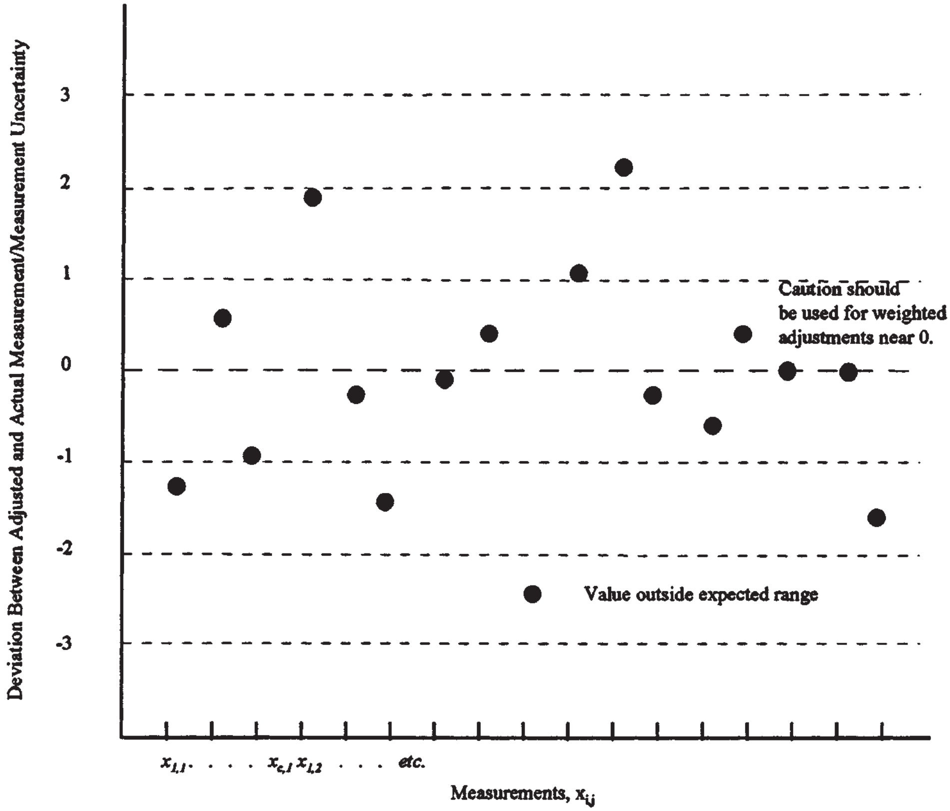

FIG. 30-20 Scatter diagram showing results of reconciliation.

stream 3 are adjusted to close the constraints around the first module. The reconciliation process moves to the second. The stream-3 measurements are adjusted again to close the module-2 constraints. This adjustment does not take into account any previous adjustments done for module 1. The adjustments will not be the same. The adjusted stream-3 compositions and flows will be different for module 1 and module 2. Consequently, the overall constraints will not close. This method provides the best estimate for the actual operation for a specific module, but each stream joining two units is reconciled twice yielding two differing estimates.

In the second approach, the reconciliation is done sequentially from module to module within the unit under study. This is done typically following the primary direction of material flow. This approach reconciles the measurements for each module in turn, progressing through the entire unit under study. Consequently, the reconciled measurements from the first module are used in the reconciliation of

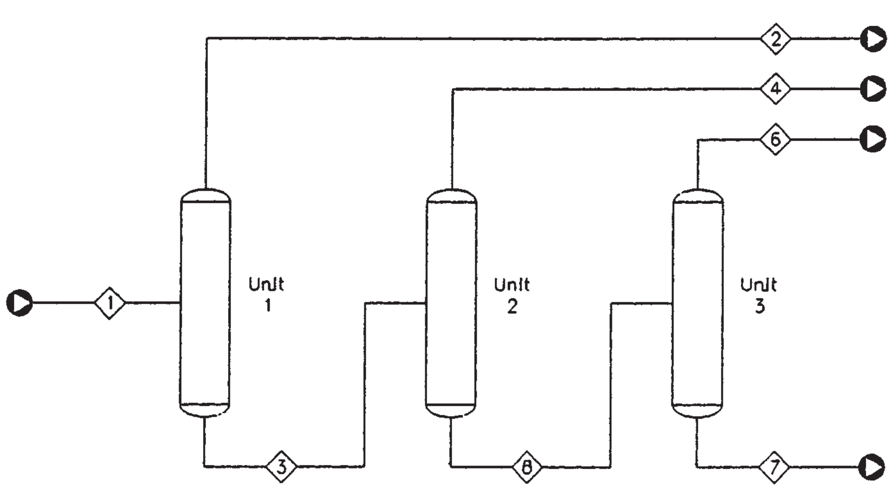

FIG. 30-21 Three-module unit.

the measurements for the second. Each stream is reconciled only once. This ensures overall closure upon completion. Errors in the reconciliation from the first are propagated to subsequent modules. Given that numerical studies of plant data show that the reconciliation methods only improve the estimate of actual performance 60–70 percent of the time, this method introduces significant errors that propagate to an ever greater extent as the complexity of the flow sheet increases. This method should be avoided.

In the third approach, the reconciliation is done simultaneously for all of the modules in the entire unit. This provides a consistent set of adjusted measurements for the entire flow sheet, ensuring individual module and entire unit constraint closure. However, each module's adjustments are poorer than those obtained by a separate reconciliation.

If the focus of the analysis is on an individual module or piece of equipment, the separate method is recommended.

References A variety of mathematical methods are proposed to cope with linear (e.g., material balances based on flows) and nonlinear (e.g., energy balances and equilibrium relations) constraints. Methods have been developed to cope with unknown measurement uncertainties and missing measurements. The reference list provides ample insight into these methods. See, in particular, the works by Mah, Crowe, and Madron. However, the methods all require more information than is typically known in a plant setting. Therefore, even when automated methods are available, plant-performance analysts are well advised to perform initial adjustments by hand.

Recommendations Plant measurements should be adjusted to close the constraints of the process. This adjustment should be done on a component or subcomponent (e.g., atomic) basis. The adjustments should be done recognizing (at a minimum) the uncertainty in the measurements. While sophisticated routines have been developed for reconciliation, the vagaries of plant measurements may make them unsuitable in most applications. The routines are no substitute for accurate, precise measurements. They cannot compensate for the uncertainties and limited information typically found in plant data.

RECTIFICATION

Overview Reconciliation adjusts the measurements to close constraints subject to their uncertainty. The numerical methods for reconciliation are based on the restriction that the measurements are only subject to random errors. Since all measurements have some unknown bias, this restriction is violated. The resultant adjusted measurements propagate these biases. Since troubleshooting, model development, and parameter estimation will ultimately be based on these adjusted measurements, the biases will be incorporated into the conclusions, models, and parameter estimates. This potentially leads to errors in operation, control, and design.

Some bias is tolerable in the measurements. This is the case when:

- The bias is insignificant compared to the random error
- The bias does not have significant impact on the measurement adjustment
- The bias does not contribute significantly to the errors in the constraints
- The biased measurement is of little value during interpretation

Consequently, these biases are not of concern.

However, other bias errors are so substantial that their presence will significantly distort any conclusions drawn from the adjusted measurements. *Rectification* is the detection of the presence of significant bias in a set of measurements, the isolation of the specific measurements containing bias, and the removal of those measurements from subsequent reconciliation and interpretation. Significant bias in measurements is defined as *gross error* in the literature.

The methods discussed in the technical literature are not exact. Numerical simulations of plant performance show that gross errors frequently remain undetected when they are present, or measurements are isolated as containing gross errors when they do not contain any.

Consequently, analysts must take a skeptical view of rectification results. The detection and isolation methods are computationally intensive and better suited for automatic procedures. Simulation studies show that the best interpretation occurs when entire measurement sets found containing gross errors are discarded. Therefore, the emphasis in this section is on detection. Citations are given for the detection and isolation of measurements containing gross errors.

Reconciliation Result The actual measurements do not close the constraint equations. That is,

$$\vec{\mathbf{f}}(\vec{\mathbf{X}}_1^m) \neq \vec{\mathbf{0}}$$

or, in the linear case,

$$\mathbf{B}\vec{\mathbf{X}}_1^m \neq \vec{\mathbf{0}}$$

Note that nonlinear constraints can be treated in this manner through linearization. Consequently, adjustments to the measurements are required. The result from the reconciliation process is this set of adjusted measurements,

$$\hat{\vec{\mathbf{X}}}_1^m$$

such that

$$\mathbf{B}\hat{\vec{\mathbf{X}}}_1^m = \vec{\mathbf{0}}$$

These were developed using constrained regression analysis or other suitable methods such that the following objective function is minimized.

$$\delta\vec{\mathbf{X}}_1^{\mathbf{T}}\mathbf{J}^{-1}\delta\vec{\mathbf{X}}_1$$

which can be expressed in algebraic form as:

$$\sum_i \left(\frac{\hat{x}_i^m - x_i^m}{\sigma_{x_i}}\right)^2$$

These adjusted measurements are examined as part of the rectification procedure.

There are three principal categories of rectification tests according to Mah (*Chemical Process Structures and Information Flows,* Butterworths, Boston, 1989, p. 414). These are the global test, the constraint test (nodal test), and the measurement test. There are variations published in the literature, and the reader is referred to the references for discussion of those.

Global Test The measurements do not close the constraints of the process. In the linear, material balance constraint example used above,

$$\mathbf{B}\vec{\mathbf{X}}_1^m = \vec{\mathbf{r}}$$

where $\vec{\mathbf{r}}$ is a vector of residuals for the constraints. The purpose of the global test is to test the null hypothesis:

$$H_0\text{: } \vec{\mathbf{r}} = \vec{\mathbf{0}}$$

$$H_a\text{: } \vec{\mathbf{r}} \neq \vec{\mathbf{0}}$$

The variance-covariance matrix for $\vec{\mathbf{r}}$ is:

$$\mathbf{R} = \mathbf{BJB}^{\mathbf{T}}$$

The test statistic

$$\mathbf{r}^{\mathbf{T}}\mathbf{R}^{-1}\mathbf{r}$$

is a chi-squared (χ^2) random variable with degrees of freedom equal to the number of constraints, assuming all measurements are made in the constraint equations.

This test does not require reconciliation before it is applied. However, should the null hypothesis be rejected, it only indicates that a gross error might be present. It does not isolate which of the measurements (or constraints) are in error. Consequently, gross-error isolation must be done subsequently.

Constraint Test In this test, each individual constraint is tested based on the measurements. The test statistic is

$$\frac{r_j}{\sqrt{R_{jj}}}$$

with

$$H_0\text{: } r_j = 0$$

$$H_a\text{: } r_j \neq 0$$

This statistic is normal. As with the global test, the constraint test is based on the actual measurements before reconciliation. Reconciliation is not required in advance of the application of this test. Also, the constraint test does not isolate which of the measurements contains gross error. Subsequent isolation is required.

Measurement Test This test compares the adjusted measurements to the actual measurements. In so doing, each measurement is tested for gross error. From the reconciliation development,

$$\delta\vec{\mathbf{X}}_1 = \hat{\vec{\mathbf{X}}}_1^m - \vec{\mathbf{X}}_1^m$$

where the vector $\delta\vec{\mathbf{X}}_1$ is the adjustments made to each of the measurements. Premultiplying this vector by the inverse of the variance-covariance matrix of the measurements gives a test of maximum power (assuming that $\mathbf{J}$ is diagonal). Define,

$$\vec{\mathbf{d}} = \mathbf{J}^{-1}\delta\vec{\mathbf{X}}_1$$

Define the variance-covariance matrix for this vector to be

$$\mathbf{Q} = \mathbf{B}^{\mathrm{T}}(\mathbf{BJB}^{\mathrm{T}})^{-1}\mathbf{B}$$

Thus, the $N(0,1)$ test statistic is

$$\frac{|d_j|}{\sqrt{Q_{jj}}}$$

Unlike the other two tests, this is associated with each measurement. Reconciliation is required before this test is applied, but no further isolation is required. However, due to the limitations in reconciliation methods, some measurements can be inordinately adjusted because of incorrectly specified random errors. Other adjustments that do contain gross errors may not be adjusted because the selected constraints are not sensitive to these measurements. Therefore, even though the adjustment in each measurement is tested for gross error, rejection of the null hypothesis for a specific measurement does not necessarily indicate that that measurement contains gross error.

Gross-Error Isolation Gross-error detection methods do not isolate which measurements contain gross error. The Global and Constraint Tests work only with the process constraints. While they detect gross errors in one or more constraints, they do not isolate the measurements. The measurement test does isolate those measurements that were adjusted to a larger-than-expected extent. These adjustments may be in error, as discussed above. Once the presence of gross errors has been detected, the actual measurements need to be isolated. Rosenberg et al. (Rosenberg, J., R.S.H. Mah, and C. Iordache, "Evaluation of Schemes for Detecting and Identifying Gross Errors in Process Data," *Industrial and Engineering Chemistry, Research,* **26**(3), 1987, 555–564) review methods for isolation of gross errors.

The authors test two methods coupled with the measurement test. In one, they sequentially eliminate measurements and rearrange the constraints to isolate the specific measurements that contain gross errors. In the other, streams are added back as the search continues.

Both of these schemes require substantial computing effort and are focused on networks of modules (i.e., complex units). The reader is referred to the article for the details of these isolation procedures as they are beyond the scope of this section.

Statistical Power There are two types of errors. In the type-I error, gross errors are isolated as present when none are. In the type-II error, no errors are isolated when they are actually present. A third measure of error is selectivity taken from Rosenberg et al. (cited above), which is the normalized probability of detecting a gross error in a stream when there is error in that stream only. The power of the detection methods is defined as the probability of detecting gross errors when present. The probability of making a false detection must be minimized. The selectivity should also be high. A balance among these competing goals must be established.

Results of simulation studies of different types of flow sheets and measurement-error levels show that the performance of these schemes depends on the magnitude of the gross error relative to the measure of the random error. The larger the gross error, the greater the power and lower the probability of committing a type-II error. The complexity of the flow sheet contributes in the form of the constraint equations. Flowsheets with parallel streams have identical constraint equations, giving equal statistical performance. For the cases studied, the power ranges from 0.1 to 0.8 (desired value 1.0), the probability of making type-II errors ranges from 0.2 to 0.7 (desired value 0.0), and the selectivity ranges from 0.1 to 0.8 (desired value 1.0). These statistics depend on random and gross error magnitudes and flow sheet configuration. These ranges of statistics show that the tests are not exact.

This inexact performance leads to the recommendation that measurement sets should be discarded in their entirety when gross errors are detected. Therefore, actual isolation of which measurements contain error is not necessary when entire sets are discarded.

Recommendation When all measurements were recorded by hand, operators and engineers could use their judgment concerning their validity. Now with most acquired automatically in enormous numbers, the measurements need to be examined automatically. The goal continues to be to detect correctly the presence or absence of gross errors and isolate which measurements contain those errors. Each of the tests has limitations. The literature indicates that the measurement test or a composite test where measurements are sequentially added to the measurement set are the most powerful, but their success is limited. If automatic analysis is required, the composite measurement test is the most direct to isolation-specific measurements with gross error.

However, given that reconciliation will not always adjust measurements, even when they contain large random and gross error, the adjustments will not necessarily indicate that gross error is present. Further, the constraints may also be incorrect due to simplifications, leaks, and so on. Therefore, for specific model development, scrutiny of the individual measurement adjustments coupled with reconciliation and model building should be used to isolate gross errors.

INTERPRETATION

Overview Interpretation is the process for using the raw or adjusted unit measurements to troubleshoot, estimate parameters, detect faults, or develop a plant model. The interpretation of plant performance is defined as a discreet step but is often done simultaneously with the identification of hypotheses and suitable measurements and the treatment of those measurements. It is isolated here as a separate process for convenience of discussion.

The activities under interpretation are divided into four categories. Troubleshooting is a procedure to identify and solve a problem in the unit. Hypothesized causes for the observed problems are developed and then tested with appropriate measurements or identification of changes in operating conditions.

Parameter estimation is a procedure for taking the unit measurements and reducing them to a set of parameters for a physical (or, in some cases, relational) mathematical model of the unit. Statistical interpretation tempered with engineering judgment is required to arrive at realistic parameter estimates. Parameter estimation can be an integral part of fault detection and model discrimination.

Fault detection is a monitoring procedure intended to identify deteriorating unit performance. The unit can be monitored by focusing on values of important unit measurements or on values of model parameters. Step changes or drift in these values are used to identify that a fault (deteriorated performance in unit functioning or effectiveness) has occurred in the unit. Fault detection should be an ongoing procedure for unit monitoring. However, it is also used to compare performance from one formal unit test to another.

Model discrimination is a procedure for developing a suitable description of the unit performance. The techniques are drawn from the mathematics literature where the goodness-of-fit of various proposed models are compared. Unfortunately, the various proposed models will usually describe a unit's performance equally well. Model discrimination is better accomplished when raw or adjusted measurements from many, unique operating conditions provide the foundation for the comparisons.

These procedures are not mutually exclusive and are divided here as a matter of convenience for discussion. The identification, measurement treatment, and interpretation are typically embodied into a single effort with testing and retesting as analysts search for the cause of the observed symptoms.

Troubleshooting The initial steps of troubleshooting have been discussed in the identification section. Successful troubleshooting requires the acquisition and organization of a large amount of observations from diverse sources. Analysts rely heavily on the observations of operators and supervisors along with the interpretation of unit measurements. In troubleshooting, a complete unit test is usually the last resort to identify the cause of the observed problem. Therefore, the measurements and observations are usually incomplete, and analysts must hypothesize causes, identify measurements or alternative operating conditions, and interpret the results based on the analysts' understanding of the unit operation.

Hasbrouck et al. (Hasbrouck, J.F., J.G. Kunesh, and V.C. Smith, "Successfully Troubleshoot Distillation Towers," *Chemical Engineering Progress,* March 1993, 63–72) provide guidelines for those practicing troubleshooting. These have been incorporated into much of the preparation and identification discussion. Analysts must understand the objectives of the troubleshooting activities established by unit supervision, plant management, and the analysts' management. Analysts must be able to communicate with and have the cooperation of the unit operators and supervision. Analysts must understand the unit. Discussions with operators and supervision should emphasize the symptoms and not their conclusions. Analysts should observe unit operation both in the control room and in the unit to establish whether the observations of those involved are accurate. Analysts should obtain log-sheet measurements to provide the foundation for establishing the hypotheses explaining the unit problems. As part of this collection, log sheets from a period when the unit operated correctly should also be obtained. At this point, the interpretation process can begin.

The current and past operation should be compared so that the timing of the observed problems is established. The possible causes (hypotheses) can be compared against the measurements found on the log sheets. The number of possible causes can then be reduced. When the quantity or quality of measurements is insufficient to further reduce the set of causes, additional measurements are required. These may require special instruments (e.g., gamma-ray scanning) not routinely used in the plant. Alternative operating conditions may also be required to further reduce the number of causes. As part of the problem identification, it is always important to look for measurements that are inconsistent with the proposed explanation. They will be more informative than the ones justifying the hypothesized cause. Ultimately, with appropriate additional measurements, the cause can be identified. This is not an exact science and, as stated above, relies heavily upon the communication, technical, and investigative skills of analysts.

Figure 30-22 is an expanded flowchart for troubleshooting activities incorporating the recommendations for hypothesis development as well as interpretation laid out in Table 30-1. The figure is adapted from Hasbrouck et al. but expanded and rearranged to make it germane to units beyond distillation. Following the guidelines from Table 30-1, the changes in the unit equipment, instrumentation, and operating conditions that coincide with the observed problems are listed. Instrument readings are verified to ensure that the problem is valid and not an aberration of poor instruments or calibrations. Hasbrouck et al. recommend establishing the magnitude of the problem and verifying that it is significant enough to justify further troubleshooting activities. In this step, analysts monitor unit operations to verify the observations of operators and unit supervisors. Hypothesis development continues with establishing whether the problem is with the unit under study or with an upstream unit, downstream unit, auxiliary equipment, or control. If it is outside the unit under study, attention should turn to troubleshooting that equipment. If it is within the unit, then analysts should establish whether the operating conditions are inappropriately set, causing capacity or efficiency problems, or whether the equipment itself is the cause of the problem. Troubleshooting continues by acquiring measurements from logs or, if necessary, from special instrumentation to reduce the number of possibilities and ultimately identify the cause of the problems. The process concludes with the alternative operating conditions or equipment identified with supporting economic justification. Analysts then communicate the results to the management, unit supervision, and the operators. If necessary, the analysts oversee the implementation of the changes.

Figure 30-22 should be interpreted as a guideline for successful troubleshooting and not a recipe to be followed exactly. Any one of the steps can be bypassed as the ground rules for the activity dictate and the insight into the problem develops. Since troubleshooting is not an exact science, analysts are well advised to look always for the alternative causes recognizing that symptoms' underlying causes are not unique.

Parameter Estimation Relational and physical models require adjustable parameters to match the predicted output (e.g., distillate composition, tower profiles, and reactor conversions) to the operating specifications (e.g., distillation material and energy balance) and the unit input, feed compositions, conditions, and flows. The physical-model adjustable parameters bear a loose tie to theory with the limitations discussed in previous sections. The relational models have no tie to theory or the internal equipment processes. The purpose of this interpretation procedure is to develop estimates for these parameters. It is these parameters linked with the model that provide a mathematical representation of the unit that can be used in fault detection, control, and design.

The purpose is to develop estimates of significant model parameters that provide the best estimate of unit operation. The unit operation is embodied in the measurements.

$$\vec{\mathbf{X}}_1^m$$

If reconciliation and rectification procedures were applied to the measurements, either statistically or judgmentally, to close the constraints, the unit operation is also embodied in the adjusted measurements.

$$\hat{\vec{\mathbf{X}}}_1^m$$

Each of these have corresponding uncertainties.

The object, then, is to develop a set of predicted values for the measurements based on the model

$$\hat{\vec{\mathbf{X}}}_1^M$$

such that the differences between these model predictions and the raw or adjusted measurements are minimized.

Define: $$\delta\vec{\mathbf{X}}_1^M = \hat{\vec{\mathbf{X}}}_1^M - \vec{\mathbf{X}}_1^m$$

or $$\delta\vec{\mathbf{X}}_1^M = \hat{\vec{\mathbf{X}}}_1^M - \hat{\vec{\mathbf{X}}}_1^m$$

and minimize: $$\delta\vec{\mathbf{X}}_1^{M\,\mathbf{T}}\delta\vec{\mathbf{X}}_1^M$$

This minimization can be unweighted as above, or it can be weighted using the statistical uncertainty $\mathbf{J}^{-1}$ with respect to the measurements or engineering judgment.

While the statistical weighting is elegant and rigorous if the uncertainties are known, its applicability is limited because the uncertainties are seldom known. Commercial simulator models are yet unable to iterate on the parameter estimates against the unit measurements. And, the focus should be on a limited subset of the complete measurements set.

The parameter adjustment procedure is most often done with analysts performing the adjustments by comparing model predictions to the raw or adjusted measurements. The spreadsheet given in Fig. 30-18 is extended to include comparisons between the predictions and basis. Figure 30-23 presents one possible extension. The spreadsheet contains two principal sections. First, there is a section for the comparison of component flows. The component flows for the comparisons are the raw or adjusted measurements. The predicted values come from the model with the current estimates for the parameters. The deviations are summarized as a root mean square error between the measurements and predictions, weighted if appropriate. The second section includes a comparison between measured and predicted values that are of particular interest, like the measurements upon which the operators focus, trace component concentrations, ratios of one group of components to another, or a special product. This section of the spreadsheet is repeated as often as necessary to provide a running comparison, as the parameter values are adjusted to improve the description of the unit operation. The adjustment of the parameter values is accomplished through finite-difference approximation of the sensitivity of the performance criteria to the parameter values.

The hurdles to arriving at a unique set of parameter values are large.

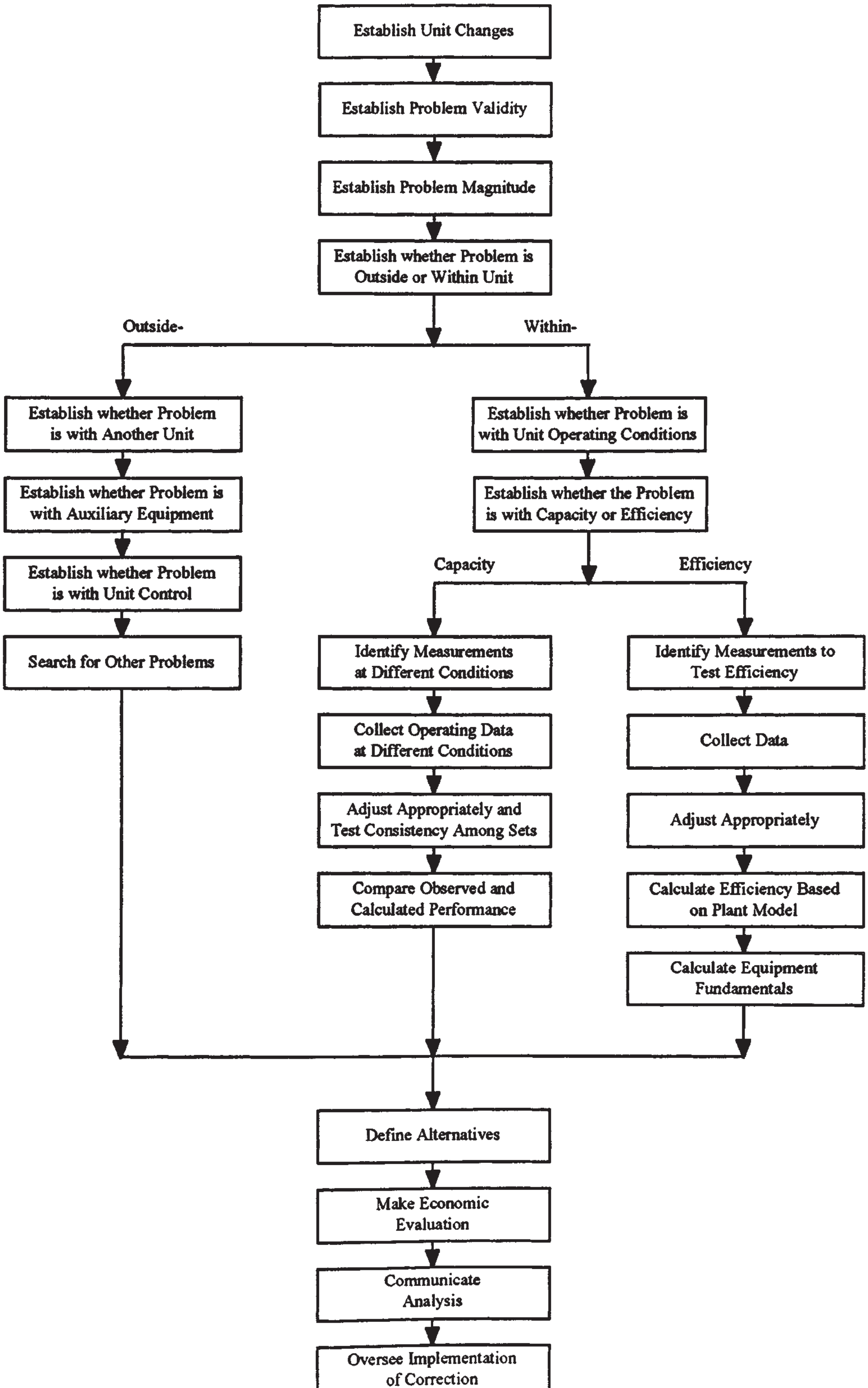

FIG. 30-22 Flowchart for troubleshooting.

Comparison between plant and calculated material balance for tower

Component	Stream flows								
	Feed, lb/hr			Ovhd product, lb/hr			Btms product, lb/hr		
	Plant	Calc	Δ (Delta)	Plant	Calc	Δ (Delta)	Plant	Calc	Δ (Delta)
Component 1									
Component 2									
Component 3									
•									
•									
•									
Component c-1									
Component c									
Total									

RMSE lb/hr lb/hr
RMSE % %

	Plant	Calc
Temperatures Overhead, F Bottoms, F		
Duties MM Btu/hr		
Targets Target 1 Target 2 Target 3		

FIG. 30-23 Spreadsheet extension to Fig. 30-17 to compare measurements or adjusted measurements to predicted values.

• *The measurements do not close the constraints.* Estimation of the parameter values against the actual measurements results in parameter values that are not unique.

• *The adjusted measurements are not unique and may be no better than the actual measurements.* Simulation studies testing reconciliation methods in the absence of gross error show that they arrive at a better estimate of the actual component and stream flows 60 percent of the time; 40 percent of the time, the actual measured values better represent the unit performance.

• *Gross-error-detection methods detect errors when they are not present and fail to detect the gross errors when they are.* Coupling the aforementioned difficulties of reconciliation with the limitations of gross-error-detection methods, it is likely that the adjusted measurements contain unrecognized gross error, further weakening the foundation of the parameter estimation.

• *Few simulation studies of parameter estimation in analysis of plant-performance are given in the literature.* Those that are reported show that, for the levels of measurement errors expected in a plant, the uncertainty in estimated parameter values is very large, much larger than that needed for design. For example, MacDonald and Howat (1988) show that, for a simple flash vessel with an actual simulated value of 75 percent flash efficiency, the 95 percent confidence interval in the interpretation of simulated operation is 75% ± 12%. Verneuil et al. (1992) point out that interpretation of unit data using highly nonlinear models should be done with the recognition that the results must be treated as an approximation.

• *The presence of errors within the underlying database further degrades the accuracy and precision of the parameter estimate.* If the database contains bias, this will translate into bias in the parameter estimates. In the flash example referenced above, including reasonable database uncertainty in the phase equilibria increases the 95 percent confidence interval to ±14. As the database uncertainty increases, the uncertainty in the resultant parameter estimate increases as shown by the trend line represented in Fig. 30-24. Failure to account for the database uncertainty results in poor extrapolations to other operating conditions.

• *The models that require parameter estimates are approximate.* Much of the theoretical basis of the parameter definition is lost. Equipment nonlinearities and boundaries are not accounted for in the analysis.

Despite these hurdles, models with accurate parameter estimates are required for analysis, control, and design. The effectiveness of parameter estimation can be improved by following these guidelines.

• *Increase the number of measurements included in the measurement set by using measurements from repeated sampling.* Including repeated measurements at the same operating conditions reduces the impact of the measurement error on the parameter estimates. The result is a tighter confidence interval on the estimates.

• *Include measurements that represent the internal conditions of equipment.* Including internal measurements such as tray compositions, between-catalyst-bed measurements or spatial measurements in a CSTR improve the likelihood that the parameter estimates are accurate. These measurements are particularly useful when product compositions (e.g., principal component composition in superfractionation) are not a sensitive measure of the parameter estimate.

• *Increase the number of operating conditions in the measurement set.* Measurement sets from different operating conditions have the same effect as increasing the number of measurements. They have the added benefit identifying weaknesses in the model when it cannot accurately describe all of the conditions.

• *Focus on specific measurements of particular sensitivity during the parameter adjustment.* Analysts should focus on the primary measurements upon which the operation, control, or design are based during the parameter adjustment step. This guideline suggests the artificial weighting of particular measurements. For example, in superfractionation, the nondistributed component product compositions provide little insight into evaluating the accuracy of the estimate of the tray efficiency. Including the deviation in these when developing a new parameter estimate provides little value and potentially masks the impact that the parameters have on the trace component compositions. Monitoring the deviations in the internal tray compositions of these nondistributed components in the region where they drop from the feed-tray composition to zero composition is important, but it is not where these compositions are at their limiting values on the other side of the feed tray.

• *Use additional measurement sets that were not included in the development of the parameter estimates to test their accuracy.* A certain subset of the raw or adjusted measurements is used to adjust the parameter estimate. Once the optimal values are attained, the model is used to predict values to compare against other measurement sets or subsets. These additional measurements provide an independent check on the parameter estimates and the model validity.

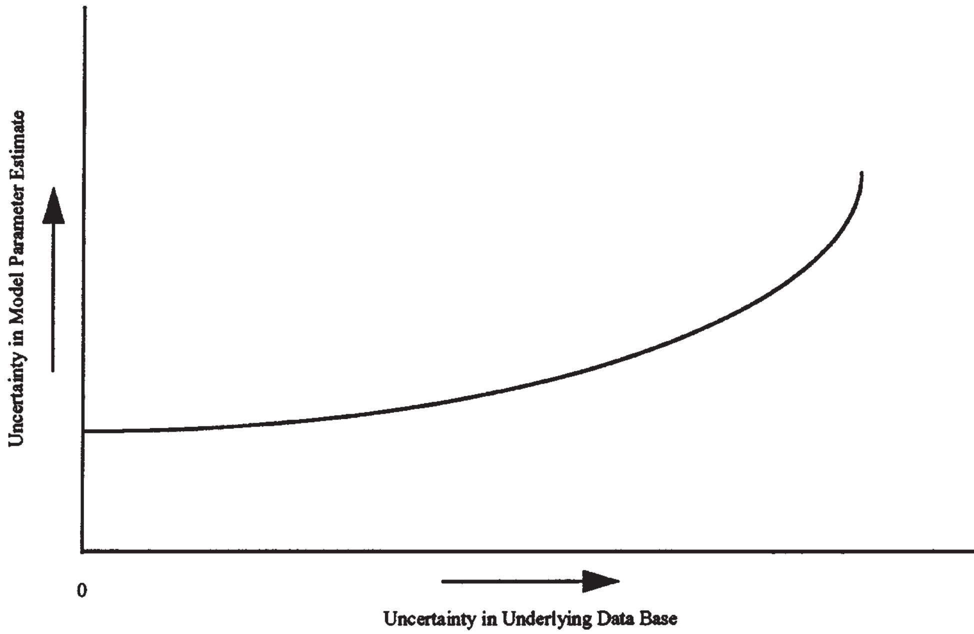

FIG. 30-24 Trend in parameter estimate uncertainty as the database uncertainty increases.

As with troubleshooting, parameter estimation is not an exact science. The facade of statistical and mathematical routines coupled with sophisticated simulation models masks the underlying uncertainties in the measurements and the models. It must be understood that the resultant parameter values embody all of the uncertainties in the measurements, underlying database, and the model. The impact of these uncertainties can be minimized by exercising sound engineering judgment founded upon a familiarity with unit operation and engineering fundamentals.

Fault Detection Measurements for units operating at steady-state fluctuate around mean values. The means tend to drift with time. Dynamic processes necessarily have time fluctuations in the measurements. These fluctuations and drifts make it difficult to determine readily the level of unit performance. Along with the process measurements, utility, raw material, and catalyst usage are monitored through the course of operation. The efficiency or economics of the unit are strong functions of these usages. These too change with time, and it is difficult to determine if the efficiency of the unit operation has changed. Control of the unit depends upon the accuracy of unit instrument readings. Should the instruments deteriorate, input signals to the controllers deteriorate and consequently control actions deteriorate. The validity of the instrument readings must be monitored to ensure that readings and the resultant actions are appropriate for efficient control.

These observations lead to the principal questions toward which fault detection is addressed.

- Has the unit operation effectiveness changed due to the input conditions, ambient conditions, or the state of the equipment?
- Has the unit operation efficiency deteriorated resulting in poorer performance?
- Has one or more of the instruments deteriorated such that the readings no longer represent the unit operation?

A fault may interfere with the effectiveness or the functioning of the unit (Watanabe, K., and D.M. Himmelblau, "Incipient Fault Diagnosis of Nonlinear Processes with Multiple Causes of Faults," *Chemical Engineering Science,* **39**(3), 1984, 491–508). The first question addresses the effectiveness. The second two address the functioning. Fault detection is a unit monitoring activity, done automatically or periodically, to determine whether the unit operation has changed.

Figures 30-11 through 14 provide typical traces of unit operations. Figure 30-12 shows a drift in the measurement, but it does not readily justify a conclusion that the unit operation is changing from one state to another. The apparent step changes shown in Fig. 30-13 may be due to instrument failure, input changes to the unit, operator-induced changes, and an aberration of the chart scaling. It is not readily clear whether the unit functioning or effectiveness has changed in either of these traces. The complex interactions defined by the chemical engineering and equipment fundamentals within the unit appear as changes in the measurements. The changes do not necessarily mean that the functioning or effectiveness of the unit has changed in any significant way.

The purpose of fault detection is to interpret the set of measurements to determine whether the operation of the unit has changed. This interpretation is done by monitoring the set of the measurements or by monitoring values for the significant unit parameters. It is done automatically as part of the computer control of the unit or periodically as when comparing one unit test to a subsequent one.

Automatic fault detection and diagnosis relies upon the interpretation of the unit measurements as they are gathered by the computer control/data acquisition system. The goal is to identify faults before they jeopardize the unit operation that could ultimately pose product, equipment, and safety problems if they are not corrected. The difficulty is that high-frequency data acquisition systems obtain a large amount of measurements. Automatic filtering methods and data compression are required to retain the unit trends without treating and archiving all the measurements. Readers are referred to Watanabe and Himmelblau (Watanabe, K. and D.M. Himmelblau, "Incipient Fault Diagnosis of Nonlinear Processes with Multiple Causes of Faults," *Chemical Engineering Science,* **39**(3), 1984, 491–508) and their citation list for a discussion of filtering methods. Narashimhan et al. propose that recording and analysis be done only when the process steady state has changed (Narashimhan, S., R.S.H. Mah, A.C. Tamhane, J.W. Woodward, and J.C. Hale, "A Composite Statistical Test for Detecting Changes of Steady States," *AIChE Journal,* **32**(9), 1986, 1409–1418). They develop a method for testing whether the unit is in steady state.

Periodic fault detection is readily done by analysts without extensive software support. Process monitoring such as the examination of the traces discussed above are one example. However, the number of measurements in a single set have such complex interactions that it is difficult to determine whether the unit operation has changed. A better approach for periodic fault detection is to estimate the parameter values based on the measurements. The parameters, assuming that the model is accurate, embody the entire operation of the unit as well as the uncertainties in the measurements. Since their number is small for any unit, it is easier to monitor the parameter values. Figure 30-25 presents a typical trend in unit parameter values. Two difficulties arise with this approach, however.

First, the parameter estimate may be representative of the mean operation for that time period or it may be representative of an extreme, depending upon the set of measurements upon which it is based. This arises because of the normal fluctuations in unit measurements. Second, the statistical uncertainty, typically unknown, in the parameter estimate casts a confidence interval around the parameter estimate. Apparently, large differences in mean parameter values for two different periods may be statistically insignificant.

A change in the measurements or parameters indicates a change in the unit operation. The diagnosis (interpretation) of the cause for the change requires troubleshooting skills.

Watanabe and Himmelblau (1984) present a discussion of their simulation studies of the dehydrogenation of heptane to toluene. Incomplete reaction, deterioration of catalyst performance, and fouling the heat exchange surface are specified as the source of the faults. These manifest themselves in the outlet concentration of toluene, the values of the Arrhenius equation frequency factor and activation energy, and the heat-transfer coefficient, respectively. If the toluene concentration falls, the reaction completion has decreased. If the frequency decreases and the activation energy increases, the catalyst has chemically degraded. If the frequency decreases with no change in the activation energy, the catalyst has physically degraded. If the heat-transfer coefficient decreases, the exchanger has fouled. They note, however, that model-formulation difficulties will mask problems such that the problems do not appear as symptoms in the parameter values.

Wei (Wei, C.-N., "Diagnose Process Problems," *Chemical Engineering Progress,* September 1991, 70–74) discusses his success in monitoring production rates and selectivity to identify faults in a moving bed adsorber. Continuous monitoring resulted in a time trace of values for his parameters, clearly indicating that the operation had changed. The cause of the change in the parameter values was then diagnosed using troubleshooting methods discussed above. It is important to be able to compare operation before and after control, equipment, and other unit modifications. The history of the parameter values provides valuable insight into the effectiveness of the modifications.

In Fig. 30-25, representation of the fault detection monitoring activity, there appears to be two distinct time periods of unit operation with a transition period between the two. The mean parameter value and corresponding sample standard deviation can be calculated for each time. These means can be tested by setting the null hypothesis that the means are the same and performing the appropriate *t*-test. Rejecting the null hypothesis indicates that there may have been a shift in operation of the unit. Diagnosis (troubleshooting) is the next step.

When the number of measurement sets is substantially less than that indicated Fig. 30-25, the interpretation becomes problematic. One option is to use the parameter values from one period to describe the measurements from another. If the description is within measurement error, the operation has not changed. If there is a substantial difference between the predictions and the measurements, it is likely that the operation has changed. Methods such as those developed by Narasimhan et al. (1986) can be used when the number of measurements are large. When implementing automatic methods to treat a large number of measurements, analysts should ensure that the unit is at steady state for each time period.

Model Discrimination Relational and physical models should be robust (i.e., able to describe the operation of the unit over a reasonable range of operating conditions). Relational models used in control do not necessarily describe the operation exactly. At any given operating condition, they exhibit bias from the actual operation. However, their intended purpose is to predict accurately trends in response to operating specification changes or deviations from setpoints. Physical models, particularly those used in incipient fault detection and diagnosis, must be unbiased, accurately reflecting the unit operation.

The parameters of these models must also be unique for the unit. Only one set of parameters should describe the operation over a wide range.

The models must be considered to be approximations. Therefore, the goals of robustness and uniqueness are rarely met. The nonlinear nature of the physical model, the interaction between the database and the parameters, the approximation of the unit fundamentals, the equipment boundaries, and the measurement uncertainties all contribute to the limitations in either of these models.

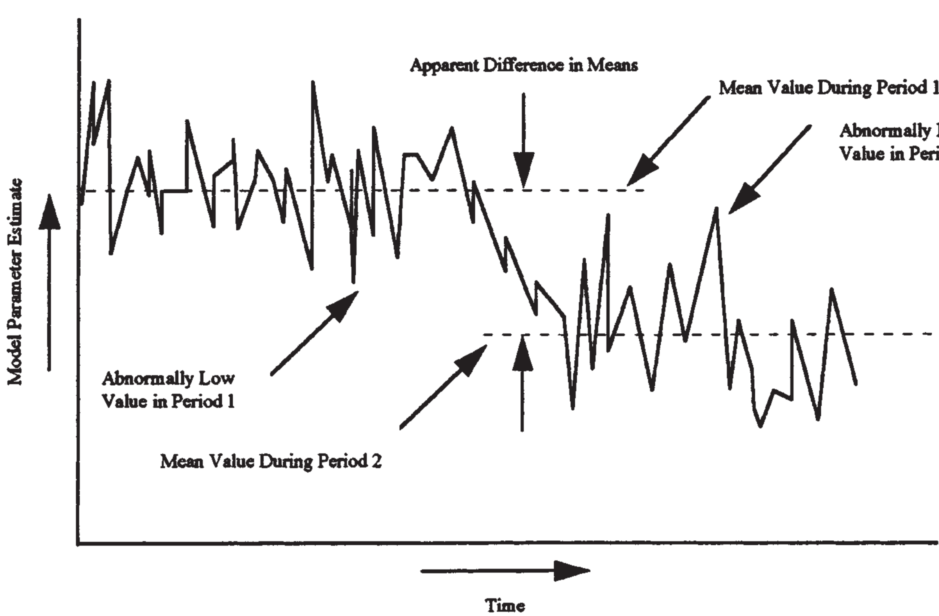

FIG. 30-25 Trend in model parameter developed during fault detection parameter estimation.

Because of these limitations, different models may appear to describe the unit operation equally well. Analysts must discriminate among various models with the associated parameter estimates that best meet the end-use criteria for the model development. There are three principal criteria for judging the suitability of one model over another. In addition, there are ancillary criteria like computing time and ease of use that may also contribute to the decision but are not of general concern.

The three principal criteria in order of importance are:

- Chemical engineering and equipment fundamentals foundation within the model
- Interpolation and extrapolation performance to other operating conditions
- Statistical representation of the raw or adjusted measurements

These criteria form the guidelines for discriminating among competing models. The principal reason for developing a model of the unit operation is to reliably predict unit performance under different operating conditions. Troubleshooting, fault detection, control, and design all fall under this purpose for developing a model. Different levels of accuracy may be required for each of these activities based on the end use criteria, but the choice of model within one of these activities should be that which best describes the unit operation. Models of limited accuracy have been used for operation and design with disappointing results. The developer of the model may recognize the model's limitations, but frequently these are not passed along to other analysts. Accurate predictions under different operating conditions is the primary goal and the foundation for the guidelines.

- The model that best describes the chemical engineering fundamentals including transport phenomena, rate mechanisms, and the thermodynamics; and includes contributions due to equipment nonlinearities and boundary conditions should be the model of choice.

This guideline is paramount. If the model is accurate in its fundamentals and equipment performance description, it should be able to describe the unit operation over a wide range of conditions. Its only limitations are the weaknesses of underlying database used in the model calculations and the errors in the unit measurements upon which the parameter estimates are based. An accurate description of the chemical engineering fundamentals incorporating the equipment nonlinearities with theory-based adjustable parameters is difficult to obtain. Analysts' knowledge of the transport and rate mechanisms is approximate under the best of circumstances. When the fundamentals are known, the mathematics may be so complex as to make the model unusable in the plant setting. Unless the model is specially developed for the analysis of plant performance, commercial simulators with their inherent inflexibility and limitations must be relied upon. They rarely allow changes to their model structure and do not incorporate the nonlinearities of equipment performance. Consequently, the model that is the best approximation of the fundamentals and equipment limitations and is computationally tractable should be the choice. It should have the greatest likelihood for extrapolation to other operating conditions.

- The model that best describes operating conditions other than those upon which its parameter estimates are based; i.e., the model that best interpolates among and extrapolates from its development conditions, should be the model of choice.

The best test for the suitability of the models is to develop their respective parameter estimates at one set of conditions and then test the accuracy of the models using measurements for other sets of conditions. The other conditions can be as relatively close to those used to establish the parameter estimates as might be experienced in routine operations. They may also be far different with different feed conditions and operating specifications.

Aside from the fundamentals, the principal compromise to the accuracy of extrapolations and interpolations is the interaction of the model parameters with the database parameters (e.g., tray efficiency and phase equilibria). Compromises in the model development due to the uncertainties in the data base will manifest themselves when the model is used to describe other operating conditions. A model with these interactions may describe the operating conditions upon which it is based but be of little value at operating conditions or equipment constraints different from the foundation. Therefore, it is good practice to test any model predictions against measurements at other operating conditions.

- The model that best describes the raw or adjusted measurements should be the model of choice.

The statistics literature presents numerous reviews of comparing the description of one model against another. Watanabe and Himmelblau (1984) present a list of review articles. The judgment criterion is based on a comparison of the model predictions against the measurements. These comparisons are related to the general statistic given below, developed for each model with its corresponding parameter set.

$$S^2 = \delta\vec{\mathbf{X}}_1^{M\,\mathbf{T}}\delta\vec{\mathbf{X}}_1^M$$

where $$\delta\vec{\mathbf{X}}_1^M = \hat{\vec{\mathbf{X}}}_1^M - \hat{\vec{\mathbf{X}}}_1^m$$

Appropriate weighting and focus on a subset of measurements can be introduced as statistical knowledge of the measurements, end-use focus, and engineering judgment warrant. When weighted with the uncertainties in the adjusted measurements, the statistic is χ^2. Two models can be compared using an F-statistic. With appropriate hypothesis testing, the best model can be chosen. These statistical comparisons are not a replacement for sound measurements and sound model fundamentals. They should be used as a guide only. The difficulties are:

- The statistical distributions of the measurements are unknown.
- The resultant distribution of the parameter estimates are also unknown.
- The weighting is usually arbitrary with only a subset of the measurements used.
- The statistical test provides no insight into the accuracy of the engineering fundamentals, equipment nonlinearities, or parameter interactions.

Unfortunately, models are rarely exact. The semblance of sophistication inherent in the model and used to develop parameter estimates frequently masks their deficiencies. Models are only approximate, and their predictions when the parameter estimates are based on analysis of plant performance must be considered as approximate. Validation of the model and the parameter estimates using other operating conditions will reduce the likelihood that the conclusions have significant error.