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On-Line Optimization Using Steady State Models

by

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ABSTRACT

Many sectors of the chemical industry suffer from a production overcapacity. Efficient production strategies are important. This situation combines with dropping computer costs to form an excellent environment for on-line optimization. If the transient periods of an operation are short relative to the steady intervals, a major part of the operation economics is determined by the steady state. Therefore, an optimization limited to the steady state will cover the main part of the attainable profit of the plant.

A structure for an on-line optimizer is proposed. The optimization is conceived as a calculation of a set of optimal setpoints for the plant. The on-line optimizer is composed of a number of modules. The most important modules perform the optimization and identify the model. Although steady state models are much more readily available and accurate than dynamic mod 'ls, they still are approximate and contain parameters that have to be updated regularly to correct for the plant model mismatch and for slow changes in the plant. Sensitivity analysis of the optimization results and statistical analysis of the model identification results are combined in short-cut feasibility studies and on-line accuracy estimation. Data reconciliation improves the robustness of the application.

Two examples serve as illustrations. The first example concerns a propane-propylene splitter. This example shows many of the interesting issues on a system of reduced size. The results are therefore easier to interpret. The second example is a boiler load allocation problem. This example is more involved and shows a realistic application.

1. INTRODUCTION

An on-line optimizer is a system situated between process control loops and production scheduling. This optimizer adjusts the operation of a plant automatically in order to obtain an operation which approaches optimality with respect to a certain criterion and subject to possible constraints. The optimization criterion typically corresponds to the production profit. Constraints can occur from ecological (e.g. maximal concentration of salts in purge water), safety (e.g. maximal pressure in production loop) or operational limits (e.g. output reactor equals input separation section).

Technology and market situation combined, cause increased interest in on-line optimization. Large scale application of on-line optimization becomes more realistic as computing costs drop. Frequently the necessary hardware for data acquisition and processing is available in modern production facilities. While computer costs dropped, energy prices increased dramatically. This resulted in the heat integration of many plants. Efficiency of individual units was often improved significantly, and a logical next step considers the integration of a plant through the optimization of the interactions of the units. The optimization of this interaction can be automated. This trend towards on-line optimization is currently amplified by production overcapacities in various sectors of the chemical, petrochemical and petroleum industry. Efficient production strategies are of extreme importance.

This paper is restricted to continuous chemical plants with transient periods that are relatively short compared to periods of steady state operation. Under these circumstances the major part of the plant operation economics is determined by steady state conditions. Therefore, optimal steady state conditions will cover most of the optimal operation advantage. Steady state models are more readily available than dynamic models.

In this study, steady state on-line optimization is conceived as a calculation and implementation of optimal setpoints. Currently, setpoints are often updated off-line, using recent plant data. The setpoints are determined after an analysis of the many-sided environment with which the plant interacts. Economical, ecological, safety, maintenance and operational factors are of importance. The setpoints have to be updated on a regular basis. Changes in the plant and its environment occur. Prices of feedstock change, catalysts deactivate and heat exchangers foul or are in maintenance. Therefore, a set of desired values that at a given time were optimal, may not be optimal any more after a certain period of operation. Deviations and changes in plant operating conditions can be fast compared to off-line updating of setpoints. A significantly better result can be obtained by increasing the frequency of the adjustments of the setpoints. These setpoints are implemented in the control of the plant, and maintained until the next optimization run is executed.

This paper reports on some of the conclusions and results of a study of the more fundamental issues concerning on-line optimization. First the concept and structure of an on-line optimizer are described. Then several modules that make up part of the on-line optimizer are discussed : the data reconciliation, model identification, optimization and sensitivity analysis and the combination of sensitivity and statistical information on parameter estimates. Finally, some conclusions are presented.

2. STRUCTURE AND CONCEPT

The structure of an on-line optimizer is presented in figure 1. The two most important blocks in the on-line optimizer perform the optimization and the model updating.

The optimization routine calculates a set of optimal setpoints with respect to an optimization objective and subject to certain constraints. The objective as well as the constraints have to be provided by the operating staff. The steady state model is also a constraint. The optimization task is conceptually the most important. The optimization combines the plant model and the operational objective in obtaining an optimal operation. Research in optimization theory made numerous stable and efficient optimization algorithms available. An excellent nonlinear programming algorithm with capabilities for solving large optimization problems is successive quadratic programming (SQP). Added to the actual optimization is an on-line sensitivity analysis of the optimization result. An advantage of SQP is that some of the results necessary for a sensitivity analysis become available as a "by-product" of the optimization. Sensitivity of the optimization result and solution for various factors such as the value of the model parameter estimates is calculated. The sensitivity analysis describes the status of the solution. It becomes clear which are the most limiting constraints, how flat or steep the objective is as a function of various variables of interest, what the possible gain or loss is if a constraint is relaxed or tightened. It is improbable that optimization will become an important technique for closed loop application

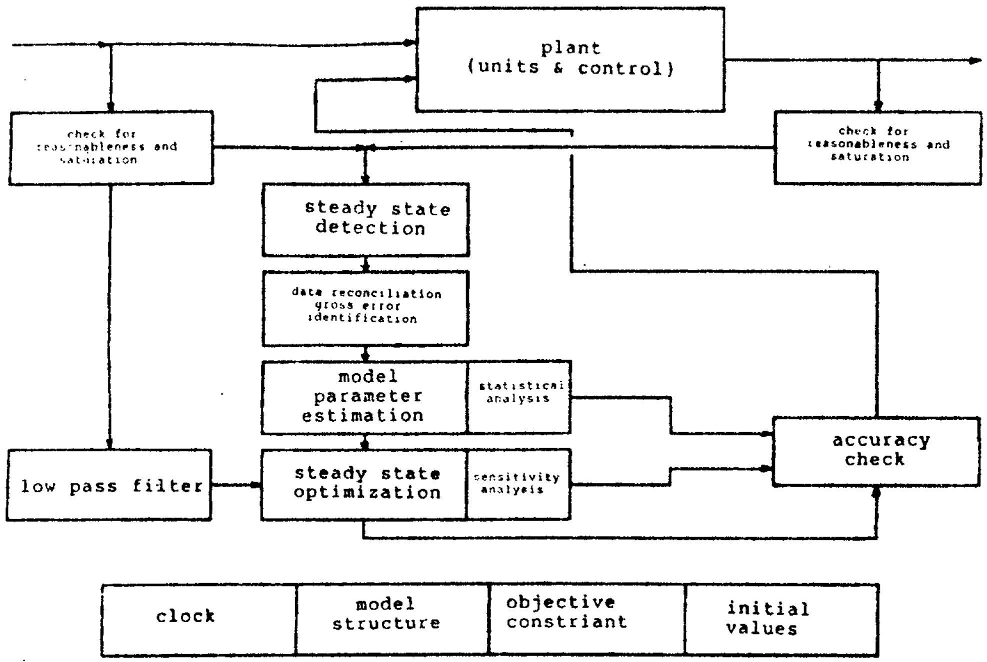

Fig.1 - *Schematic Structure of an On-line Optimizer*

without the status description a sensitivity analysis offers. Sensitivity analysis and its applications in on-line optimization are discussed briefly in sections 5 and 6. The accuracy check is an important on-line application that will be discussed later. It allows one to build in some protection in the on-line optimizer scheme.

The steady state model that is used as a constraint by the optimization algorithm is in general nonlinear. The model has to be updated periodically because of changing operating conditions. The model structure has to be provided by the operating staff. The model updating routine estimates the model parameters. Together with the data validation, the model identification task is the most challenging. It is a very critical step towards a judicious optimisation. The data validation section has to detect steady states and check data consistency. Data validation and model identification are probably the most critical tasks. The quality of the data often determines the feasibility of an on-line optimisation application.

Steady state detection can be very important and difficult. In general, units have to be checked one by one for steady state, and not the entire plant. Only certain key measurements have to be checked. The actual detection criterion form depends upon such things as noise level, stationarity etc. Checks for reasonableness and saturation are included as a part of the data validation.

The plant input passes through a low-pass filter before the optimizer routine uses this plant input. This low-pass filter serves an important goal. It was concluded earlier that on-line optimization should only be applied to adjust for typically slow changes in the environment of the plant (Koninckx and Mc Avoy, [1986]). The optimizer preferably works at a significantly higher rate than the higher frequency of these environment changes, yet slower than the plant dynamics. An on-line optimized system can actually perform poorer with on-line optimizer than without for dynamic reasons only, if the frequency of the optimization routine is below the frequencies of the disturbances for which it attempts to compensate.

The on-line optimizer concept as it is presented above, complies with the discussion on on-line energy optimization presented by Poje and Smart [1986]. Poje and Smart stress process data validation. The three tests indicated by these authors are included in the presented scheme : comparison with low and high limits (check for reasonableness and saturation), rate of change check (steady state detection), mass and energy balance requirement (gross error identification).

An on-line optimizer as it is conceived here corresponds to a supervisory level of control (Poje and Smart, [1986]) and can be situated between process loop control and production scheduling. Figure 2 (Coombes *et al.*

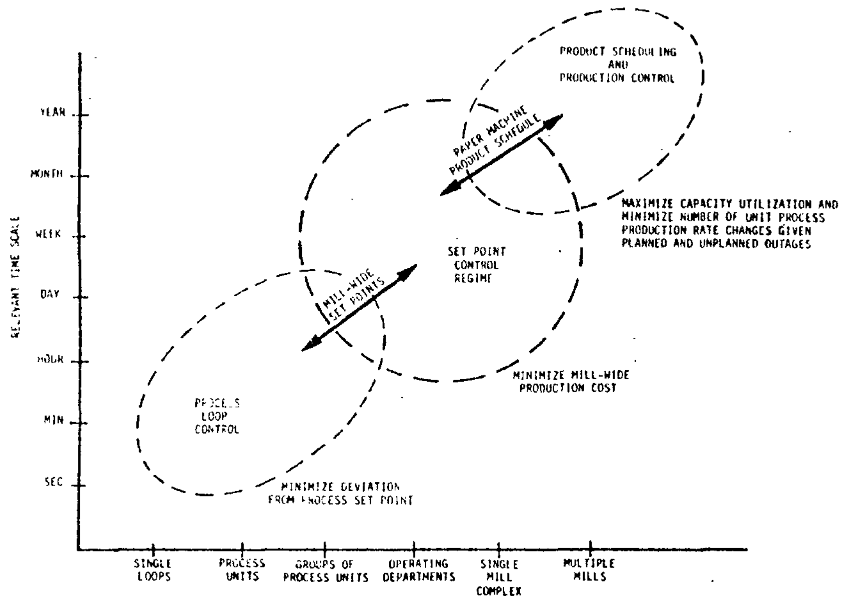

Fig.2 - *Scope of On-line Optimizer from Coombes et al.[1983]*

[1983]) illustrates the relation of on-line optimization to process loop control and production scheduling.

Coombes *et al.* [1983] report on the application of an on-line optimization scheme in a paper mill. They demonstrate the operating cost savings potential for an on-line optimized plant. A data validation step is not reported. The paper mill plant model and the optimization problem are linear. Similar applications in paper mills have been reported, possibly with nonlinear models and some with dynamic approaches (e.g. Wen, [1983]; Blevins *et al.* [1980]). Applications wich include reactors are rather rare. Näsi *et al.* [1985] report on the use of on-line optimisation in the advanced control of acetylene hydrogenation reactors. In this case the scope of the objective is restricted to an operational objective : acetylene removal from the de-ethanizer overhead, and minimization of the ethylene losses. There is no on-line model updating. The objective does not immediately correspond to plant economics and profit. This example is closer to advanced unit control using optimization as a technique for multi-variable decision taking as to a supervisory control technique. The application Sourander *et al.* [1984] report on, concerns on-line optimisation in the control of olefin-cracking heaters. This application is advanced, and is inspired by plant economics. The overall production objective is the maximization of the gross margin subject to market demand, feed availability and plant constraints. The highest control level module is a closed loop plant optimiser, which at scheduled intervals (four hours) converts the economic data together with the plant variables to new controller setpoints. The results are implemented on-line (no operator intervention) via the pyrolysis heater controls. A data validation is present, and checks are built in to prevent implementation of dynamically disadvantageous or erroneous results. A very interesting aspect is the possibility for the operator to choose one of two objective functions. One maximizes ethylene production, and the second maximizes the profit. Conforming with the scheme presented above, the model updating is independent from and asynchronous with the control and optimization implementation frequency. Succesive linear programming (SLP) is used in the optimization.

Other important fields of application are in distillation and in boiler load allocation. Both distillation and steam production are very widespread processes using large amounts of energy. Examples in distillation are reported by e.g. Sourander and Gros [1986], Martin *et al.* [1981]. Examples in steam production are reported by e.g. Lipták [1987], Cho [1978], Ko [1987], Green and Al ai-Shaikh [1980]. Two examples will be used as illustrations throughout this paper. One example concerns distillation, a second concerns boiler load allocation.

The first example is based upon the results presented by Martin *et al.* [1981], who discuss the on-line optimization of a propane propylene splitter that is part of an ethylene producing plant. Table 1 lists the operating conditions and specifications of this column.

Eduljee's equation (appendix A) fits these specifications for an average relative volatility of 1.105 [Edgar and Himmelblau,1988]. The operating conditions listed by Martin *et al.* [1981] were used in this example as

Symbol	Description	Value (dim)
c_1	reboiler heat cost	$3.165 \cdot 10^{-3}$ \$/J
c_2	condensor cooler cost	0 \$/J
N_{true}	number of trays	125
η	average tray efficiency	0.75
N	number of ideal trays	94
U	heavy key diff. value	−0.175\$/kg
W	light key diff. value	0.219\$/kg
λ	average latent heat	300768J/kg
α	relative volatility	1.105
F	feed mass flow	$550 \cdot 10^3$kg/day
x_F	propylene weight fract. in feed	0.7
$x_{D,m}$	required top purity	0.95
R	reflux ratio	17.2
R_m	mimimum reflux ratio	11.3
B	bottoms massflow	$151 \cdot 10^3$kg/day
x_B	bottoms propylene weigthfract.	0.044
D	top massflow	$396 \cdot 10^3$kg/day
x_D	top purity	0.95

TABLE 1 : Propane/Propylene Splitter Nominal Operation and Parameters

the nominal state. The optimization variables are the reflux ratio and the top composition. The objective is the minimization of the variable operational cost (see appendix A). The top composition is constrained by a minimum value of 95 weight percent propylene. This constraint appeared to be active in the entire range of operation that was considered here. The column has a high reflux ratio, and a low average relative volatility which are characteristic of a column interesting as an on-line optimization application. The model used by the on-line optimizer is based on Eduljee's equation (appendix A). A model updating routine adjusts the parameters of the Eduljee equation (relative volatility α, number of ideal trays N). Data validation is realized through data reconciliation with gross error identification and outlier detection. All simulations in this example are steady state. Funk *et al.* [1984] warn against partial optimization of ethylene plants. Indeed, the recycled bottom product can influence the global economics of the system. However, if the values of the intermediate products are correct at the optimum operation, then the partial optimization of the single unit is correct. The intermediate product values replace the connectivity equations in that case. Apart from that, the merit of this case is mainly as a simple example.

The second example concerns the optimal load allocation between three boilers. The objective of the optimization is the maximization of the global boiler network efficiency. As suggested by e.g. Cho [1978], Ko [1987] and Green and Al ai-Shaikh [1980], the steady state model used by the on-line optimizer is simply a second order relation between load and efficiency, and a linear relation between fuel and the product of load and efficiency. A detailed lumped parameter dynamic model [Bertrand,1986] is used as the plant. The 15 model parameters are updated periodically. A reduced gross error identification is applied to data that are collected and recognised as steady state.

In the following sections, these two examples will be used to illustrate different aspects of on-line optimizer applications. First, data reconciliation will be discussed.

3. DATA RECONCILIATION

Good data are of high importance to the operation of the on-line optimizer. Data from a chemical plant are often of unreliable quality. Therefore it is useful to check data for reasonableness, saturation and consistency before applying them. Checks for reasonableness and saturation can be done on a one by one measurement basis by comparing the measurements to preset values. Consistent data will meet certain simple relations such as mass and energy balances. Therefore data can be reconciled by using these equations, and significant deviations can be identified as gross errors. Several techniques for data reconciliation and gross error detection exist. The data reconciliation technique applied in the distillation example is presented by Serth *et al.* [1986] as the Modified Iterative Measurement Test (MIMT). Serth *et al.* [1986] characterize this reconciliation method as effective and reliable, and computationally less expensive than other methods (such as the screened combinatorial test). A measurement test method allows gross errors to be directly identified without a separate identification procedure (Iordache *et al.* [1985]).

If data reconciliation is applied to data that are used for model parameter estimation, then the equations used for the reconciliation step cannot be allowed to introduce linear relationships between the model responses. A parameter estimation criterion presented by Box and Draper [1965] is used. In this criterion the determinant of the matrix V given below is minimized.

$$v_{ij} = \sum_{k=1}^{N_k} \left((y_{ik} - \hat{y}_{ik})(y_{jk} - \hat{y}_{jk}) \right)$$

with N_k the number of data points or responses y_{ik}. This criterion allows for correlated errors and errors with unequal variances in the model responses, and eliminates the problem of setting weights between the model responses. However, if linear relationships exists between the responses, then the matrix V becomes singular and the criterion is not valid. Independence of the different responses is required. Usually, it is not difficult to achieve this independence since the equations used for parameter estimations often describe intra-unit phenomena whereas the equations that are used for reconciliation often are based on inter-unit balances. Nevertheless, attention has to be paid to a possible coincidence, certainly for large systems.

The usefulness of data reconciliation and gross error detection in an on-line optimization scheme is illustrated in three examples. In the first example, only random noise is added to correct data. In the second example, the feed flow measurement is systematically wrong. Finally, in the third example a failing sensor is simulated. The following mass balances are used by the MIMT data reconciler in this case study :

$$F = D + B$$

$$Fx_F = Dx_D + Bx_B$$

Example 1: Random Noise Only. Random noise with a standard deviation of five percent of the nominal value (see table 1) for the streams (F, B and D) and the bottom propylene fraction (x_B) and five percent of the top and feed (x_F, x_D) propane fraction (1. - propylene fraction) is added to one hundred data points, with inputs randomly ($\sigma_f^2 = 4.866 \cdot 10^9$, $\sigma_{x_F}^2 = 8.08 \cdot 10^{-4}$, $\sigma_{x_D}^2 = 7.86 \cdot 10^{-4}$, $\sigma_R^2 = 1.255$) chosen around the nominal steady state, and with corresponding plant outputs simulated using the Eduljee and Fenske equations, using $\alpha_{true} = 1.105$, $N_{true} = 94$. The parameter estimation finds :

$$\begin{cases} 1.1058 \leq \alpha \leq 1.1064 & \text{(center:1.1061)} \\ 99.0 \leq N \leq 107.4 & \text{(center:103.0)} \end{cases}$$

If data reconciliation is applied, and all datasets for which the reconciler determined a gross error are discarded, then the result of the parameter estimation becomes :

$$\begin{cases} 1.1141 \leq \alpha \leq 1.1144 & \text{(center:1.1143)} \\ 79.7 \leq N \leq 91.1 & \text{(center:85.0)} \end{cases}$$

Both results are very comparable. The residuals of both estimations show this. The number of discarded data points is 9. The confidence limit used was 95% which is rather small for detecting unreliable conditions. A 5% change exists that a correct condition is recognized as wrong (type 1 hypothesis test error). One can also use a 99% confidence. The probability for a type 1 testing error is then only 1%. In most practical situations the increase in probability of recognizing incorrect conditions as correct (type 2 hypothesis testing error) by using a 99% confidence instead of a 95% confidence, is not expected to be very large. The determination of the confidence level is a trade-off between both type hypothesis errors. For consistency 95% was used in the next two examples also.

Example 2: A Systematic Error. This example shows that it is possible that data reconciliation is responsible for a loss in quality of the parameter estimates. The parameter estimation only uses the three compositions of the feed stream, the top or product stream and the bottom stream. Data reconciliation checks these composition data. It therefore uses flow measurements. The total set of data is then reformed to the most probable one with respect to the raw data and the consistency with the data reconciliation equations. This technique is intended to reduce errors, but it can also cause the introduction of errors. If for instance the flow measurements have some error that is not always detected, then this will result in errors in the reconciled composition data, and hence in the parameter estimates. In this example the same set of raw data is used. However in approximately half of the datasets (randomly chosen) a 20% error (positive or negative) was added to the feed flow data. Of course the estimation result that uses the raw (unreconciled) data is the same with or without the added error in the redundant flow data. The estimation does not use the flow data. The results from unreconciled data are :

$$\begin{cases} 1.1058 \leq \alpha \leq 1.1064 & \text{(center:1.1061)} \\ 99.0 \leq N \leq 107.4 & \text{(center:103.0)} \end{cases}$$

If the data reconciliation technique is used, then the errors in F that slip through the reconciliation are spread over the composition data, reducing its quality. The result is definitely poorer than the result based upon the raw data. Especially the deviation in the α parameter has to be considered. Small changes in α cause important differences in the simulation results. The results are less sensitive to N. Sixty datasets remained after the reconciliation. The results are :

$$\begin{cases} 1.109 \leq \alpha \leq 1.111 & \text{(center:1.110)} \\ 81.0 \leq N \leq 96.4 & \text{(center:88.0)} \end{cases}$$

if datasets with at most one reconstructed data point are allowed, then 89 datasets from the original 100 are accepted. The results improved only slightly. This example shows that data reconciliation is not without any risk. Although the conditions here are somewhat exceptional (good composition data and one poor flow measurement), they are not impossible. The decrease in quality of the estimates is not dramatic.

Example 3: A Failing Sensor. This example shows the potential advantage of data reconciliation.In this case a failing sensor is simulated. Occasionally ($\frac{1}{4}$ of the cases, randomly chosen) the bottom composition sensor fails and produces a clearly erroneous value that is nevertheless not too obvious (no saturation). Otherwise it performs normal (noise variance = 2.5$\cdot$ the variance in the previous examples). If no data reconciliation is applied, the estimation becomes instable. The on-line optimizer would have to be stopped, unless it remains in operation with the old parameter values. If data reconciliation is applied, the data points with false bottom composition values can easily be recognized and rejected or reconstructed. Accepting up to one reconstruction per data set, and based upon reconciled data, the results are (86 datasets are accepted) :

$$\begin{cases} 1.1141 \leq \alpha \leq 1.1144 & \text{(center:1.1142)} \\ 78.3 \leq N \leq 90.3 & \text{(center:84.5)} \end{cases}$$

The results are not quite as good as the ones in example 1 (with a good sensor) because of the larger variance overall in the bottom composition measurements, and because some of the false values were not detected. Still the result is very useful, and that is not the case if data reconciliation would not have been used.

The previous three examples have shown that data reconciliation can be used effectively against systematic errors in data by checking consistency with the reconciliation equations. However, improvement in the result is not guaranteed. More specifically, if the data are accurate, except for a reasonable level of noise, then it seems that data reconciliation does not offer much improvement capacity in this case study. Under special conditions it is even possible that data reconciliation corrupts the estimation results by spreading errors over the different measurements. However, if an error as drastic as a broken sensor (gross error) occurs, then data reconciliation proves to be a potentially powerful data analysis tool. Reconstructed data can be applied or rejected. Using reconstructed data means full use of data redundancy, but it is difficult and the reliability of the reconstructed data may be unknown. If reconstructed data are not used, then data reconciliation can be considered as an error detection system with some plant knowledge.

A very important problem with data reconciliation is the fact that it is computationally expensive, and that the computational effort increases rapidly with the size of the problem. The MIMT method inverts a matrix of order equal to the number of reconciliation equations. This makes the application of data reconciliation on large systems very difficult. Assuming that Q, the measurement error covariance matrix, is constant, one could detect *single* gross errors using an off-line determined (and also constant) $V = QA^T(AQA^T)^{-1}AQ$. (A is the matrix of (linearized) reconciliation equation coefficients.)

The examples shown indicate that data reconciliation with gross error identification is not very useful if no gross errors are present and if the noise levels are not high. Therefore, one could instead only check for gross errors, without reconciling. This does not reduce the amount of work significantly. To limit the rapid growth of necessary computational effort with problem size, one could split up the problem in overlapping subproblems that are searched for gross errors individually. This technique is definitely inferior to checking the complete network at once, but is faster. For instance, in the boiler example, every boiler and the header are checked for gross errors separately. In that way, certain "problem nodes" will still be identified even if the exact identification of the gross error may be less probable than if all boilers and the header are checked together. The gross error identification scheme that is used to identify gross errors in every part of the boiler network is proposed by Narasimhan and Mah [1987] and is based upon the generalized likelyhood ratio test.

4. MODEL IDENTIFICATION

It was indicated in the introduction that the plant model identification is a very important step towards an effective on-line optimization. The choice of the model (steady state and in general nonlinear) is crucial. A trade-off has to be made between complexity and lack of fit. A complex, detailed model will have the advantage of a better fit and hence a better prediction capacity. However, more detailed models often contain more parameters, and result in more development costs during the preparation and more computing costs during the execution. In the distillation example, a short-cut model is used. Eduljee's equation is an excellent trade-off, providing a good fit together with relatively simple equations. The parameters in Eduljee's model (relative volatility and number of ideal trays) have a clear physical meaning, which often makes the interpretation of the estimation results easier. A strong correlation between both parameter estimates characterizes the parameter estimation. Eduljee's equation is also very nonlinear in the parameters. The combination of nonlinearity and strong correlation causes convergence problems for the Marquardt Levenspiel routine (CMLIB) that is applied here. The estimation criterion $\sum_{i=1}^{N}(x_{B,i} - \hat{x}_{B,i})^2$ is minimized with respect to α (relative volatility) and N (the number of ideal trays). A transformation to the $\ln\alpha, \frac{1}{N}$ plane improves the nonlinearity as well as the convergence. It is necessary to check convergence of the parameter estimation, since it is one of the basic assumptions and it is difficult to check on-line.

The transformation introduced also guaranteed a better spread of weights in the fits. In the following two examples, Underwood's equations [King, 1979] were used to model the distillation column, and hence serve as the "plant". Equal molal overflow was assumed and the relative volatility was assumed to be constant along the rectifier section and along the stripper section. Using simulation results created from a grid of 90 data points around the nominal operating conditions, Eduljee's equation was fitted to Underwood's results. Underwood's model serves here as the "plant", while Eduljee's equation serves as the short-cut model used by the on-line optimizer.Figure 3 compares the bottom compositions as a function of the reflux for both estimation techniques and the "plant". Figure 4 compares the derivative of the variable operation cost (appendix A) as a function of reflux. All other operating conditions are constant.

It is clear from figure 4 that the estimation in the $\ln\alpha$, $\frac{1}{N}$ plane predicts the optimal operating cost significantly better than the estimation in the α, N plane. Note that in both cases a certain offset exists. A model is never exact in practice, and even if the model predicts the optimal operating condition exactly, it does not mean it will allow to predict the optimum exactly. Apart from the response values also the values of the derivatives are very important.

In the load allocation example, a purely empirical model is used. The model is a second order polynomial relation between the boiler efficiency and the boiler load : $\eta = a + bl + cl^2$. Furthermore, a linear relationship is used between the fuel load and the product of boiler load and boiler efficiency. This model is not based on theory. It is used here because it is generally accepted. The shape of efficiency versus load curves can vary and is mainly function of the fuel type. Figure 5 shows the efficiency curves of the three biolers simulated using a

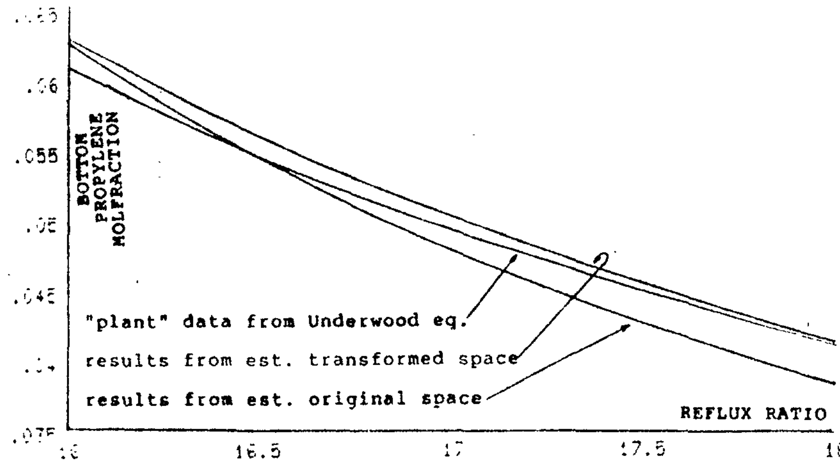

Fig.3 - ***Bottoms Propylene Fraction versus Reflux Ratio for Different Estimation Techniques***

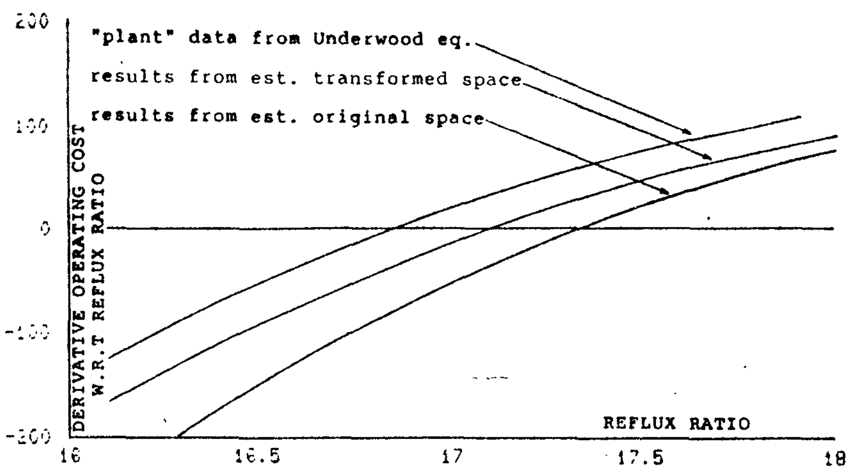

Fig.4 - ***Derivative of Variable Operating Cost with respect to the Reflux Ratio versus Reflux Ratio for Different Estimation Techniques***

detailed lumped parameter dynamic model [Bertrand, 1986]. Differences in efficiency are due to different heat transfer coefficients in various sections of the boilers, such as the superheater, etc. Figure 6 also gives the second order polynomial fitted to five points of the true efficiency curve, showing a rather poor fit to the original curve.

A poor fit can deter the performance of the on-line optimizer considerably. A following example shows the results of an on-line optimized boiler network. Figure 7 shows the global network load (stepwise going up) and the boiler loads. Figure 8 shows the true and the expected global ratio of enthalpy output (steam) to enthalpy input (fuel, air, feedwater, attemporator water). This ratio is the thermal efficiency at steady state and will be referred to as such from here on.

This simulation was free of noise, and the discrepance between expected and true network efficiency can only be due to dynamic effects (boiler and header dynamics, optimizer frequency (once per 20 min)). One boiler is a swing boiler, fuel controlled by pressure, the other boilers are controlled directly by the optimizer. Figure 9 gives the fuel loads. It is clear from figure 8 that the optimization routine under certain conditions expects an improvement which does not truly occur.

Due to the plant model mismatch it is possible that global efficiency actually decreases while expected network efficiency increases. Figure 10 again shows the true efficiency curve of one of the boilers. Two curves

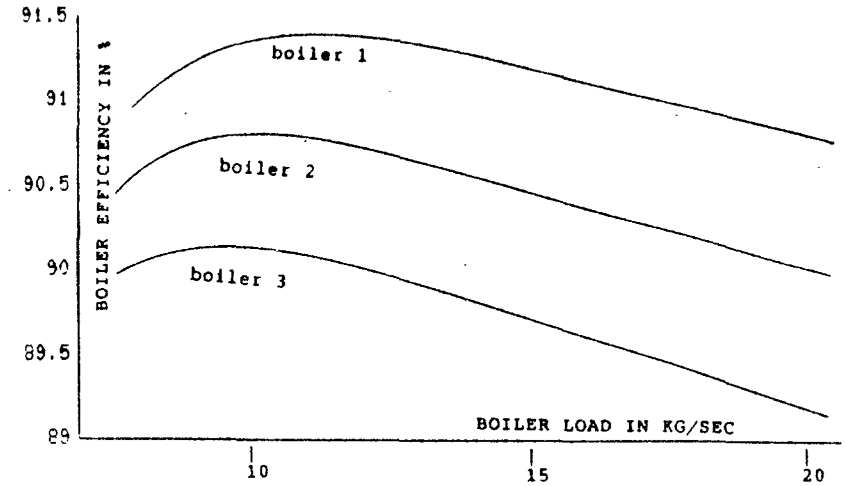

Fig.5 - ***Boiler Efficiencies for the Boilers Making up the Boiler Network***

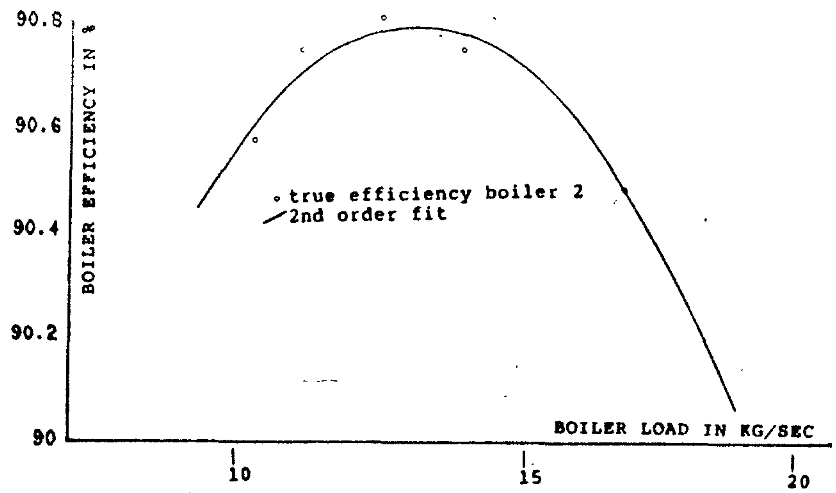

Fig.6 - ***Five True Boiler 2 Efficiencies and a Second Order Polynomial Fit***

show the fits used by the optimiser. The first model to data fit the on-line optimizer uses is the one presented in figure 6, but as soon as new steady state data come in fit '2' and later fit '3' are used. However, there is another reason for the plant/model mismatch. As the boiler network load increases, the individual boiler load increases also. Therefore the new steady state data coming in are steady states at higher loads. Although a certain spread of the data is guaranteed, fit '3' corresponds to data that at loads past the efficiency top. A narrow data field results in a better fit around that data field. However, a relatively large change in total boiler network load could result in a substantially erroneous optimization prediction. Not only the model mismatch but also the dynamic effects are illustrated by this plot 10. The "steady state" results used at low loads don't seem to be steady state results at all. Time constants of boilers increase significantly as load decreases (see e.g. Lipták,[1987]). This makes the criteria used for steady state detection invalid for low loads, and decreases the data quality. This illustrates the need for good steady state detection.

5. OPTIMIZATION AND SENSITIVITY ANALYSIS

It was indicated earlier that the actual optimization run is conceptually the most important task in the on-line optimisation scheme. Much attention has to be devoted to the formulation of objective and constraints.

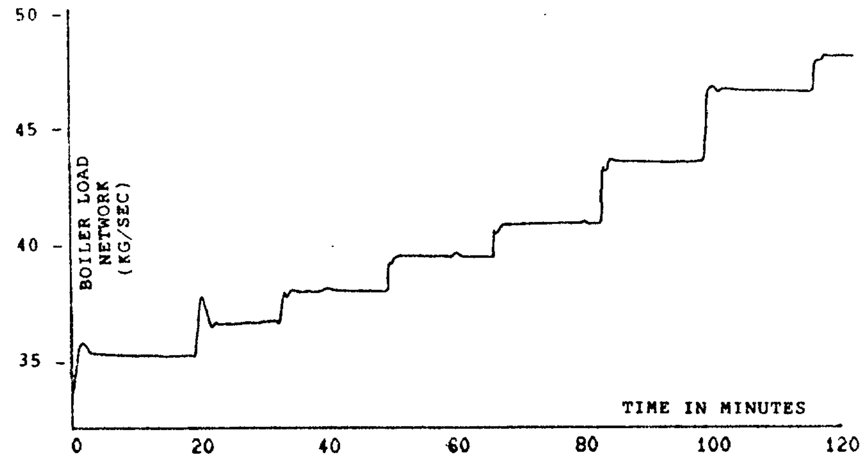

Fig.7a - *Total Boiler Network Load Increase with Time*

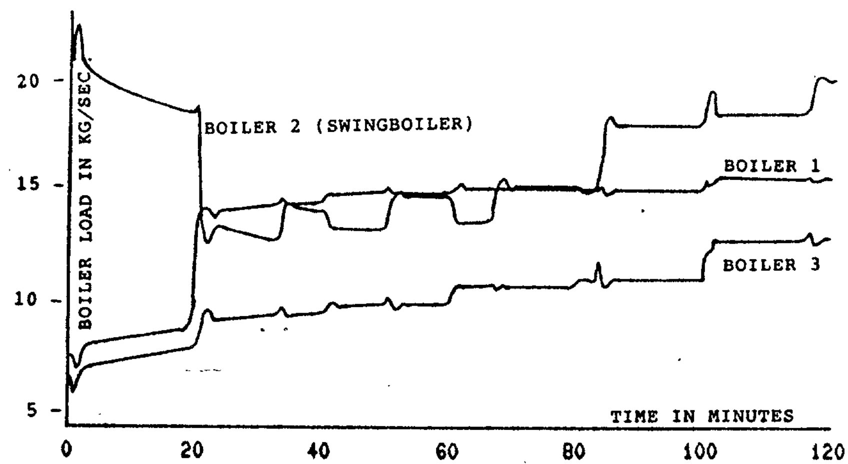

Fig.7b - *Individual Boiler Load as a Function of Time*

The problem formulation has to correspond to a feasible optimization problem for all possible plant inputs. Nonlinearity has to be avoided where possible. Plant profit or operating costs are the generic objectives that are to be maximized and minimized respectively. In the distillation tower example, the part of the operating cost that was function of the optimization variables was used by the optimizer. In the boiler network example, the minimal operational cost objective is reduced to a maximization of the global network (thermal) efficiency. Nath *et al.* [1986] discuss objective, constraint and optimization variables in the joint optimization of process units and utility systems. A primary constraint for the process units is to meet the market requirements (quantity and specification). For the utility units, the primary constraint is to satisfy the utility needs of the process units. It is interesting to point out the discrepancy between Poje and Smart [1986] and Nath *et al.* [1986] on including on/off status of equipment in the list of optimization variable. Nath *et al.* consider on/off status of equipment as possible on-line optimization variables, but Poje and Smart are more careful and consider these as off-line decisions with necessary intervention of an operator.

Linear and nonlinear programming have been subject of extensive research and are still being studied, resulting in many optimization algorithms. The optimization problem that has to be solved by an on-line optimizer can be large, but for linear as well as nonlinear programs, robust and powerful optimization routines are available. In most applications, no interest is found in obtaining feasible intermediate results. Therefore,

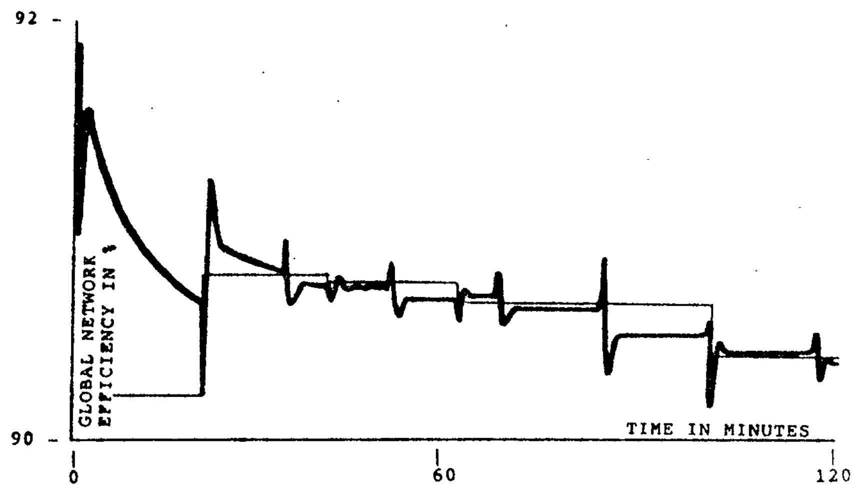

Fig.8 - *True (thick line) and Expected (thin line) Global Network Efficiency as a Function of Time The Expected Network Efficiency is Updated Every On-line Optimizer Run (in this Case Every 20 Minutes).*

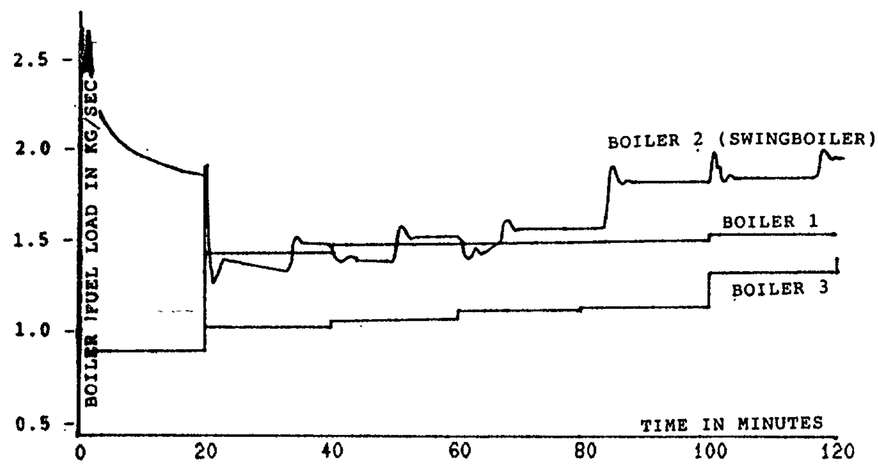

Fig.9 - *Individual Boiler Fuel Load as a Function of Time*

nonfeasible path algorithms should be applied, since in general they are more efficient. In the distillation example the optimization was extremely simple, and a Rosenbrock Hillclimb routine with relatively short code was applied [Kuester and Mize, 1973]. In the boiler network example, a successive quadratic programming (SQP) package was used. The requirements that the nonlinear programming algorithm must meet are : ability to solve problems with nonlinear constraints, ability to solve problems with a sparse Jacobian, and, as indicated above, nonfeasible path algorithm. Renfro [1986] analyzed nonlinear programming algorithms and concluded that SQP is a very good choice to meet these requirements. An additional advantage of the SQP-algorithm is that a number of variables such as the Hessian of the objective at the optimum are approximated and are available for use in sensitivity calculations. The additional effort to obtain sensitivity results remains relatively small. Sensitivity calculations quantify the sensitivity (1st order derivative and for some results 2nd order) of the objective and the optimization variables for various parameters (e.g. model parameters). A sensitivity analysis of an optimization problem characterizes the status of this solution. Without sensitivity information, it is unlikely that optimization will ever be used in large scale multivariable problems.

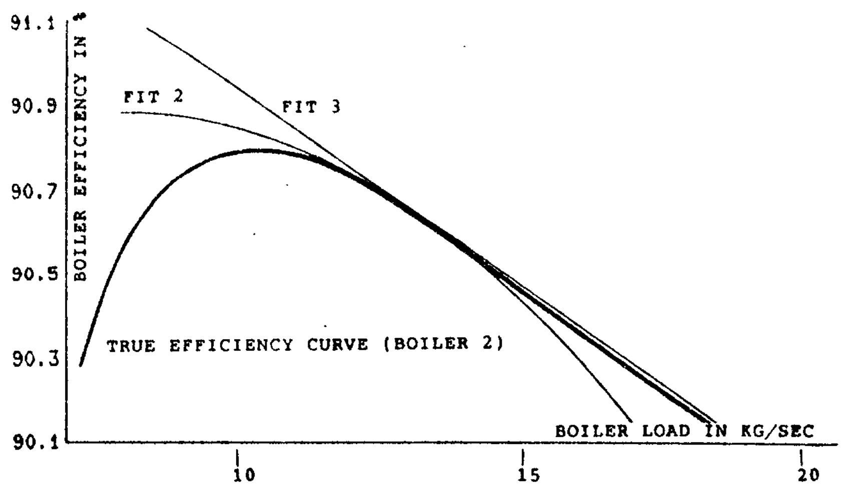

Fig.10 - *True Boiler 2 Efficiencies and a Two Second Order Polynomial Fits Used by the On-line Optimizer as New Steady State Results Become Available*

The following formula are used to calculate the sensitivity results. Main assumptions are :

- **the exact optimum is known,**
- **the exact optimum is a Kuhn-Tucker point,**
- **strict complementary slackness applies,**
- **appropriate stability and continuity conditions are met.**

From Fiacco [1983] :

$$\nabla_\varepsilon f_1^\star = \nabla_\varepsilon L$$

$$= \nabla_\varepsilon f_1|_\star - \sum_{i=1}^{m} u_i(\varepsilon)\nabla_\varepsilon g_i|_\star + \sum_{j=1}^{p} w_j(\varepsilon)\nabla_\varepsilon h_j|_\star$$

and :

$$\nabla_\varepsilon^2 f_1^\star = \nabla_\varepsilon(\nabla_\varepsilon^T L)$$

$$= \nabla_{x\varepsilon}^2 L \nabla_\varepsilon x - \sum_{i=1}^{m} \nabla_\varepsilon g_i^T \nabla_\varepsilon u_i(\varepsilon) + \sum_{j=1}^{p} \nabla_\varepsilon h_j^T \nabla_\varepsilon w_j(\varepsilon) + \nabla_\varepsilon^2 L$$

For the derivatives of the Kuhn Tucker triple :

$$\nabla_\varepsilon\{[x \quad u \quad w]^T\} = M^{-1}N$$

with :

$$M = \begin{pmatrix} \nabla_\varepsilon^2 L & -\nabla_\varepsilon g_1^T & \cdots & -\nabla_\varepsilon g_m^T & -\nabla_\varepsilon h_1^T & \cdots & -\nabla_\varepsilon h_p^T \\ u_1\nabla_\varepsilon g_1 & g_1 & & 0 & & & \\ \vdots & & \ddots & & & 0 & \\ u_m\nabla_\varepsilon g_m & 0 & & g_m & & & \\ \nabla_\varepsilon h_1 & & & & & & \\ \vdots & & 0 & & & 0 & \\ \nabla_\varepsilon h_p & & & & & & \end{pmatrix}$$

$$N = \left(- \nabla_{\varepsilon x}^2 L^T, -u_1\nabla_\varepsilon g_1^T, \cdots, -u_m\nabla_\varepsilon g_m^T, -\nabla_\varepsilon h_1^T, \cdots, \nabla_\varepsilon h_p^T\right)^T.$$

In these formula :

$f_1 =$ optimization objective

$\varepsilon =$ variables in the sensitivity study
$x =$ optimization variables
$u =$ Kuhn-Tucker multipliers for the inequality constraints
$w =$ Kuhn-Tucker multipliers for the equality constraints
$L =$ Lagrangian
$h =$ equality constraints
$g =$ inequality constraints

The most time consuming part of the calculation is probably the calculation of various derivatives. Using sensitivity results :

$$\varepsilon_{\text{nominal}} = \varepsilon_o$$

$$\tilde{\varepsilon} = \varepsilon - \varepsilon_o$$

$$f_1^*(\varepsilon) \simeq f_1^*(\varepsilon_o) + \left(\nabla_\varepsilon f_1^*\right)_o^T \tilde{\varepsilon}\left(+ \frac{1}{2}\tilde{\varepsilon}^T \left(\nabla_\varepsilon^2 f_1^*(\varepsilon)\right)_o \tilde{\varepsilon}\right)$$

At this point it should be emphasized that the objective function as it was developed before (appendix A), is not the operating cost but only that part of the operating cost that depends upon the reflux ratio and the top composition. The remaining part is still function of ε, and the corresponding derivatives have to be calculated separately and have to be added to the parts calculated using sensitivity theory. Results for the nominal case are listed in table 2.

Symbol	Sensitivity
c_1	$216.8 \cdot 10^{10}$J/day
c_2	$216.8 \cdot 10^{10}$J/day
N_{true}	-91.746\$/day
U	19800kg/day
W	6698kg/day
λ	$109700 \frac{\$ \cdot J}{kg \cdot day}$
α	$-0.133 \cdot 10^6$\$/day
$x_{D,min}$	$0.124 \cdot 10^6$\$/day
F	-14016.113\$/lb
x_F	3.46\$/day

TABLE 2.: Sensitivity of the Optimal Value Function
for Various Variables Determining the Column Operation
(A Legend for the Symbols can be Found in Table 1.)

The results for the sensitivity of $-(f - f_1)$, the part of the operating cost that does not depend upon the optimization variables, was obtained by differentiating :

$$c_D x_F F + c'_B(1 - x_F)F - c_F x_F F - c' F(1 - x_F)F$$

using the nominal values and the definitions for the light and heavy differential values :

$$W = c_D - c_B$$

$$U = c'_B - c'_D$$

and their derivatives.

Sensitivities are hard to compare. They may have different dimensions. It is easier to look at small equally likely changes of the operating conditions, and compare the consequences for the optimal value function. For instance, an increase in the reboiler heating cost of 10 cents per million BTU (or $9.5 \cdot 10^{-9}$c/J) (on 3 \$ per million BTU) makes the optimal operating cost increase about 200 $\frac{\$}{day}$ (205.56). A loss of 2% of the tray efficiency, resulting in a decreasing number of ideal trays, would be expected to increase the operating cost of the column with about 250 $\frac{\$}{day}$ (247.71). It has to be stressed that these sensitivities are derivatives of the *optimal* cost at the nominal operating conditions, and not of the objective function. The possible influence of the variables grouped in ε on the solution of the optimization problems (the values of the optimization variables at the optimum) is of interest also. In this case only the influence on the reflux ratio is important. The top purity sensitivity is zero for all variables, since the top purity constraint is stably constant.

The following table 3 lists the sensitivity of the optimal reflux ratio for various variables. Here again, it is easier to compare sensitivities by investigating the results of small changes in the variables on the optimal reflux ratio. For instance, an increase of 10 cents per million BTUs in the heating cost would have almost no influence on the optimal reflux ratio ($+10^{-18}$), and a decrease of 2 % tray efficiency would increase the optimal reflux ratio with 0.05, also relatively small. The feed mass flow rate has a stronger influence on R, but the strongest influence probably comes from the required top purity.

Symbol	Sensitivity
c_1	$-1.141 \cdot 10^{-8}$J/\$
c_2	$-1.141 \cdot 10^{-8}$J/\$
N_{true}	$-0.17129 \cdot 10^{-1}$
U	$-7.833 \cdot 10^{-10}$kg/\$
W	$1.458 \cdot 10^{-8}$kg/\$
λ	$-5.655 \cdot 10^{-3}$kg/J
α	$-0.16326 \cdot 10^{3}$
$x_{D,min}$	$0.11679 \cdot 10^{4}$
F	$1.884 \cdot 10^{-2}$day/kg
x_F	$-0.35906 \cdot 10^{2}$

TABLE 3 : Sensitivity of the Optimal Reflux Ratio
for Various Variables Determining the Column Operation
(A Legend for the Symbols can be Found in Table1.)

6. SENSITIVITY AND STATISTICAL INFORMATION COMBINED

The optimization routine uses information about the plant steady state behavior from the model identification routine. The model identification estimates parameters and provides statistical information concerning the parameter estimates (parameter estimates covariance matrix). Sensitivity of the optimization results for the parameter estimates is combined with these parameter estimate covariances to obtain the accuracy with which the expected optimal objective value can be calculated. In preliminary studies this accuracy of the expected optimal objective value has to be sufficiently small, compared to the range over which the objective can vary during common changes in operation. As an on-line result, the expected optimal objective value is an indication for precision of the on-line optimizer. If the confidence intervals for the expected optimal objective value suddenly increase, the result becomes unreliable and should not be applied to the plant. In other words, the optimizer loop should then be broken. Off-line as well as on-line use will be illustrated with an example.

- **off-line use | accuracy check** - Whether or not the application of an on-line optimizer is feasible from the plant economics point of view, depends upon many factors. Cost of the installation of the on-line optimizer depends upon the level of instrumentation already available in the plant. The operation of an on-line optimizer on a distillation column requires more instruments than the minimum required for feedback control of top and bottom compositions. The on-line optimization algorithm requires some computer time. For the models and estimation techniques used in this case study CPU time on the order of magnitude of a few seconds on a MicroVax II in MicroVMS is needed depending upon initial guess and operating conditions . This CPU time may be available at marginal cost on an existing plant computer, or a new machine may have to be purchased. Finally, the structure for the implementation of the optimization results has to be provided. This implementation usually corresponds to not more than a disk access or a computer communication. Operators have to be trained to work with the optimizer etc.

The potential profit of the on-line optimizer is difficult to estimate. A critical issue is the comparison of the expected accuracy of the on-line optimiser (how close will the estimated optimum be to the true optimum) to the range of operation. If the accuracy is small compared to the range, then on-line optimization is not likely to be attractive, and vice versa. A good outcome of this accuracy test is a neccesary condition for continuation of a project that considers the installation of an on-line optimizer, but it does not guarantee success. Therefore an initial feasibility study should be centered around an accuracy study. This study can be based upon relatively few data, and requires few calculations. An accuracy study will allow one to distinguish between processes that are definitely interesting candidates for on-line optimization, and processes that are definitely not. In between, some processes will be found for which an accuracy study seems indecisive and for which more data are needed. An accuracy test will detect processes that are clearly uninteresting subjects for on-line optimization in an early phase. The only information used in this rough accuracy estimate is :

* The steady state plant model used by the optimization algorithm as an equality constraint.
* The first order optimal function sensitivity results obtained for the nominal steady state (a base case).
* Expected accuracy for various data.

The following assumptions are made :

* Except for the estimated model parameters, inaccuracies in all data used are uncorrelated.
* The model is perfect.
* All errors are random and normal.
* Accuracies in data are a good indication of a 95% confidence interval.
* It is accurate to assume the models behave linearly within the range of inaccuracies around the nominal state.

Model inaccuracies, bias and dynamics will reduce the accuracy of the expected The total cost f is split into two parts. A first part f_1 grouped all the terms that depend upon the optimization variables. The other part, which from here on will be denoted f_2, is independent of the optimization variables and is therefore not included in the optimization problem. The optimal value function of f_1 is referred to as f_1^*. Then,

$$f^* = f_1^* + f_2,$$

with f^* the optimal total operating cost. f^*, f_1^* and f_2 can be considered statistics, and their values are samples of normal distributions. In this accuracy study, f_2 will not be considered. f_2 is not involved in the optimization, and therefore it does not influence the accuracy of the optimization. Variations in other variables than the optimization varaibles can influence the value of f_2. If this is considerable, then this can influence the range over which the operation cost can vary significantly. If on-line optimization seems accurate enough if only f_1^* is taken into account, then this will definitly be so if f_2 is also considered. Then :

$$\sigma^2_{f_1^*} = \sum_i \left([\frac{\partial f_1^*}{\partial v_i}]^2 \sigma^2_{v_i} \right) \qquad (\Delta),$$

if there is no correlation between the different v_i. In this equation v_i are factors that influence the optimization problem significantly. In this example these factors are the reboiler heat cost, the condensor cooling cost, the average latent heat, the feed mass flow rate, the feed purity and the model parameters (α and N). The light and heavy key differential values are considered constant. The terms $\frac{\partial f_1^*}{\partial v_i}$ are the first order optimal function sensitivities that were calculated and listed before (table 2). Covariance terms can be added to the last expression if necessary.

First we look at the accuracy of the parameter estimation and how this influences the accuracy of the optimization. The parameter estimates are strongly correlated, and therefore a covariance factor has to be included. Because it is difficult to determine the covariance between both parameter estimates in an analytical way, the covariance will be obtained numerically. Using data generated with Eduljee's model, with one hundred randomly perturbed inputs around the nominal input and adding 5% noise to the feed mass flow, bottom propylene fraction, bottom and top flow, and 5% noise to the propane fraction in feed and top, parameters are estimated in the $\ln\alpha$, N^{-1} space. Data reconciliation and outlier detection are applied. The following results are obtained :

$$\sigma^2_{\ln\alpha} = 0.3311 \cdot 10^{-8}$$
$$\sigma^2_{N^{-1}} = 0.1022 \cdot 10^{-6}$$
$$\sigma^2_{\ln\alpha, N^{-1}} = -0.1829 \cdot 10^{-7}$$

Applying $(\triangle)$:

$$\sigma^2_{f_1^*} = \Big(\frac{\partial f_1}{\partial\alpha}\cdot\alpha\Big)^2\sigma^2_{\ln\alpha} + \Big(\frac{\partial f_1}{\partial N}\cdot N^2\Big)^2\sigma^2_{N^{-1}} + 2\cdot\Big(-\frac{\partial f_1}{\partial N}\cdot N^2\Big)\Big(\frac{\partial f_1}{\partial\alpha}\cdot\alpha\Big)\sigma^2_{\ln\alpha,N^{-1}}$$

and (from table 2)

$$\frac{\partial f_1}{\partial\alpha} = -0.132\cdot 10^6 \frac{\$}{day}$$
$$\frac{\partial f_1}{\partial N} = 83.7\frac{\$}{day}$$

then :

$$\sigma^2_{f_1^*} \simeq 52\cdot 10^3\Big(\frac{\$}{day}\Big)^2$$

The inaccuracy of the on-line optimization operations could be expressed as a confidence interval. Then the 95% confidence interval of f_1^* is about 450 $\frac{\$}{day}$. That is about 8.5% of the variable cost of the tower listed by Martin *et al.* [1981]. It is about half of the profit listed by the same author. However, in the example of Martin *et al.* [1981], the range of operation that is considered is rather narrow. Even if this range would correspond to the actual operating range, then still a 97.5% change would exist that the profit is larger than approximately 390 $\frac{\$}{day}$ ($+140,000\frac{\$}{year}$) and a 50% change that the profit is over 840 $\frac{\$}{day}$. These expectations still interesting. The calculation presented above assumed that all other factors, such as reboiler heat cost, average latent heat etc. were all known and exact. The considered range is quite narrow,as mentioned above. Considering a larger range of operating conditions would improve the situation.

The results obtained indicate that there may be a potential gain in on-line optimization of the column in this case study. The ratios of accuracy to range are not very large, but seem large enough to indicate a possible profitable operation. As was mentioned initially in this section, this simple accuracy to range comparison does not touch upon all aspects of practical on-line optimization. First of all, the conclusion is limited by the assumptions made in the beginning. Many covariances between variables are neglected, which is often realistic. This accuracy study does not consider any dynamic effects.

- off-line use | marginal optimization gain - This section presents another necessary condition for an interesting on-line optimization application. Let $f(x,\varepsilon)$ be the optimization objective, x are the optimization variables, and ε are other parameters. Furthermore, let $x^*(\varepsilon)$ be the optimal set of x, or in other words, the solution to the optimisation variables. The on-line optimizer adjusts x to make up for changes in ε. Before applying on-line optimization, it is useful to check whether or not on-line optimization is profitable. Therefore, the difference between the performance of the on-line optimized system has to be compared to the not on-line optimized system. Assume that the nominal operation of the system under consideration corresponds to $\varepsilon = \varepsilon_0$. The nominal operation results in a performance corresponding to an objective value of $f(x^*(\varepsilon_0),\varepsilon_0) = f^*(\varepsilon_0)$. If the operating conditions change from ε_0 to ε_1, then the performance in the regularly optimized case will be $f(x^*(\varepsilon_1),\varepsilon_1) = f^*(\varepsilon_1)$. In the case where the optimization is not re-executed, the performance will correspond to $f(x^*(\varepsilon_0),\varepsilon_1)$. The sensitivity results that are presented in section 5 allow an expansion of the difference between $f^*(\varepsilon_1)$ and $f(x^*(\varepsilon_0),\varepsilon_1)$. That difference is referred to as the marginal optimization gain. In the special case in which no constraints are active, the first order term of this expansion is equal to zero. From Fiacco [1983], the result for the unconstrained optimization case is as follows :

$$\nabla^2_\varepsilon f^*\big|_0 - \nabla^2_\varepsilon f\big|_{*,0} = \big(\nabla^2_{x,\varepsilon} f\big|_{*,0}\big)\cdot\big(\nabla^2_x f\big|_{*,0}\big)^{-1}\cdot\big(\nabla^2_{x,\varepsilon} f\big|_{*,0}\big)^T$$

Consider the boiler load allocation example. The following discussion is restricted to this part of the range of operating conditions where none of the boilers meets its maximum or minimum steam production. In that case, the optimization problem to be solved by the on-line optimizer can be written as :

$$\max_{l_i, i=1,3} \left(\sum_{i=1}^{3} [a_i l_i + b_i l_i^2 + c_i l_i^3] / l_{tot} \right)$$

$$\text{subject to : } \sum_{i=1}^{3} l_i = l_t ot$$

. The objective is the global network steam production efficiency($\sum_{i=1}^{3} \eta_i l_i / l_{tot} = \sum_{i=1}^{3} [a_i l_i + b_i l_i^2 + c_i l_i^3] / l_{tot}$). The equality constraint specifies that all three boilers combined have to produce the required total boiler network load, and can be substituted in the objective. This results in an unconstrained optimization problem, the special case for which specific results were presented above. It allows for a comparison between an on-line optimized boiler network, and one in which the ratios between the loads of the individual boilers are kept constant. Considering a total network load of $36.5 kg/sec$, an optimal load allocation of $l_1 = 12.4 kg/sec$, $l_2 = 13.7 kg/sec$, $l_3 = 10.4 kg/sec$ is obtained for boiler efficiency coefficients as presented in table 4.

Boiler #	a_i	b_i	c_i
1	$0.8819713 \cdot 10^2$	0.1001671	$-9.6453661 \cdot 10^{-4}$
2	$0.8742575 \cdot 10^2$	0.1413982	$-1.2469101 \cdot 10^{-3}$
3	$0.8878001 \cdot 10^2$	0.0581466	$-6.3949076 \cdot 10^{-4}$

TABLE 4 : Coefficients for Boiler Efficiency 2nd Order Polynomials
($\eta_i = a_i + b_i l_i + c_i l_i^2$)
l = Boiler Load in kg/sec, η = Boiler Efficiency in %

This results in $d^2 \Delta\eta^* / dl_{tot}^2 = 1.05 \cdot 10^{-3} \% \cdot (sec/kg)^2$. If $\Delta l_{tot} = 5 kg/sec$ then the marginal optimization gain is approximately 0.03%. Noise, plant model mismatch, dynamics etc. will probably even reduce this very small gain. From this result, on-line optimization of this boiler network does not seem to be very attractive.

This study is repeated on results published by Cho [1978]. Cho discusses on-line optimization of a network of four boilers. Boiler efficiencies are given in table5. For a load allocation of (conversion : 1lb=0.456kg) $l_1 = 51698.1 lb/h$, $l_2 = 21485.7 lb/h$, $l_3 = 75722.2 lb/h$ and $l_4 = 101094.0 lb/h$ ($l_{tot} = 250000.0 lb/sec$), $d^2 \Delta\eta^* / dl_{tot}^2 = 6.43 \cdot 10^{-11} \% \cdot (hr/lb)^2$. A load increase of $25000 lb/h$ (10% of the total load) results in a marginal optimization gain of (in the best case) 0.04%. This again compares an on-line optimized network to a network with a constant ratio of the individual boiler loads. Based on data given by Cho [1978], the optimization gain for a load increase of $25000 lb/h$ results in a profit approximately $2200\$/year$. On-line optimization of this steam network does not seem significantly more interesting than just keeping the ratios of the individual boiler loads at the optimal for the nominal load.

- on-line use - Consider the boiler load allocation example. Figure 8 showed expected and true global network efficiency for an on-line optimized boiler network for varying loads. In figure 11, confidence (95%) intervals are added to the figure.

These intervals are only based upon plant model mismatch. The confidence intervals are calculated from :

$$\sigma_{\eta^*}^2 = \sum_{i=1}^{3} \left(\sigma_{a_i}^2 \cdot \frac{\partial \eta^*}{\partial a_i} + \sigma_{b_i}^2 \cdot \frac{\partial \eta^*}{\partial b_i} + \sigma_{c_i}^2 \cdot \frac{\partial \eta^*}{\partial c_i} \right)$$

Boiler #	a_i	b_i	c_i
1	$0.86 \cdot 10^2$	$1.733 \cdot 10^{-5}$	$-3.618 \cdot 10^{-10}$
2	$0.85 \cdot 10^2$	$9.187 \cdot 10^{-6}$	$-3.656 \cdot 10^{-10}$
3	$0.85 \cdot 10^2$	$9.125 \cdot 10^{-5}$	$-8.14 \cdot 10^{-10}$
4	$0.84 \cdot 10^2$	$9.5 \cdot 10^{-5}$	$-6.0 \cdot 10^{-10}$

TABLE 5 : Coefficients for Boiler Efficiency 2nd Order Polynomials from Cho [1978]
($\eta_i = a_i + b_i l_i + c_i l_i^2$) (conversion $1lb = 0.456kg$)
$l =$ Boiler Load in lb/h, $\eta =$ Boiler Efficiency in %

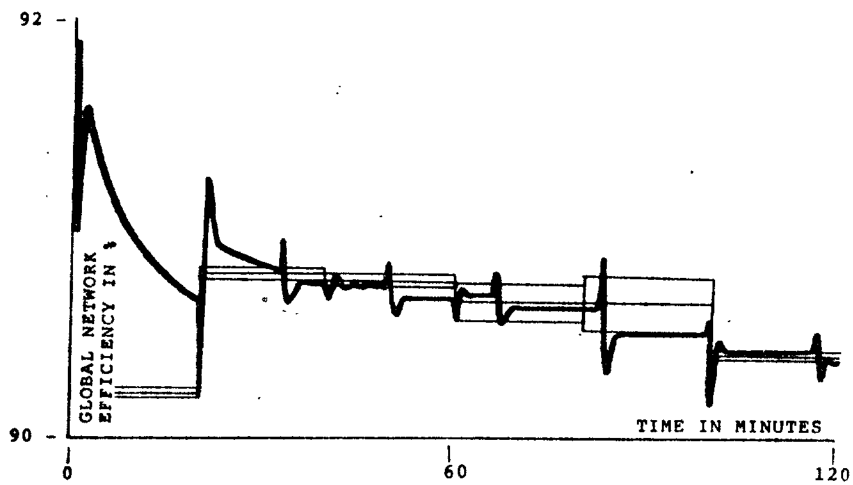

Fig.11 - ***True (thick line) and Expected (thin line) Global Network Efficiency with 95% Confidence Intervals as a Function of Time. The Expected Network Efficiency is Updated Every On-line Optimizer Run (in this Case Every 20 Minutes).***

with confidence intervals $= 1.96 \cdot \sqrt{\sigma^2_{\eta^*}}$. In this example, only the plant model mismatch can cause the gap between true and expected global efficiency. The true efficiency is indeed contained by the confidence envelope around the expected efficiency. If the confidence interval suddenly increases strongly or reaches a preset value, then the results of the on-line optimizer should not be implemented. The optimizer loop has to be broken at that point. Errors in almost any step of the procedure such as erroneous steady state detection, lack of convergence in the parameter estimation can cause faulty actions of the on-line optimizer. Many of these possible malfunctions can be acted upon by the accuracy check which interrupts the optimizer result implementation.

7. CONCLUSIONS AND FUTURE WORK

The concept, the structure and some characteristics of an on-line optimizer using steady state models

have been presented. An increasing industrial interest in this supervisory control technique is demonstrated by various industrial applications. Many fundumental questions concerning this technique are still unanswered.

On-line optimization can be applied to well instrumented plants. The control of the plant has to work effectively (reaching setpoints in a reasonably short time), and has to be able to deal with constraints. On-line optimization indeed needs powerful and reliable optimization routines. Due to the extensive research in the numerical technique of optimization, the optimization routines are available. Data acquisition and data processing are more difficult and certainly of critical importance. Because the model is not perfect, model parameters have to be updated regularly, based upon a set of steady state data. Obtaining good steady state data, and processing these is critical for the good working of the on-line optimizer. The usefulness of gross error detection as data validation technique was shown. It was indicated that reconciliation in absense of gross errors is not often useful. Because the rapid increase of the computational effort with the size of the problem, it was suggested to check for gross errors in parts of the global network in an attempt to identify problem nodes.

The importance of good modeling techniques was stressed and illustrated. Poor modeling or poor parameter estimation can deter the optimizer performance. Extensive models may add significantly to the computational load. A trade-off has to be made.

It was shown how sensitivity results characterize the optimization results and can be used in their interpretation. Also the on-line and off-line use of the combination of sensitivity information and statistical characteristics of model parameters was shown to be applicable. Off-line this combination allows for the evaluation of the expected accuracy of the optimizer predictions, a neccesary condition for a good operation. On-line it provides the possibility to check the overall working of the on-line optimizer, and in that way, makes it possible to interrupt automatic implementation of the "optimal" setpoints in case problems occur. Sensitivity and statistical information characterize the status of the results of the two most important "units" in an on-line optimizer : the model updating routine and the optimizer. Without this status description, it is virtually impossible to evaluate the performance of the on-line optimizer. Therefore, it is not expected that on-line optimization will be applied on a widespread scale without these analysis tools.

Future work will concentrate on the influence of noise of different types in the optimizer scheme, on the dynamics of the plant optimizer combination, and on steady state detection techniques. Also simple parameter estimation schemes will be compared to the more accurate least squares approach.

APPENDIX A

A simple model is used as the steady state model in the on-line optimizer. Short-cut models are necessary to keep on-line optimization of larger systems feasible. A good fit has to be traded off against model complexity and hence a greater computation effort. A poor fit will undoubtly falsify the results, and a too complex model may make the parameter estimation difficult, and it will make the optimization more complex. The on-line optimization concept is aimed at plant-wide application. This implies processing of numerous measurements, and estimating many parameters. A good engineering solution will often fall back on short-cut models. This case study illustrates the use of short-cut models.

The on-line optimizer makes use of the Eduljee correlation, which is based upon a fit of a graph by Gilliland [1940]. The Fenske equation [1932] is used as well. The use of these equations for short cut modeling of binary distillation towers has been described and illustrated by many authors, e.g. Mc Avoy [1983] and Edgar and Himmelblau [1988].

First, using x_D, x_F and the average relative volatility (α), calculate the minimum reflux at which the desired top composition can be obtained.

$$R_m = \frac{1}{\alpha - 1}\left(\frac{x_D}{x_F} - \frac{1 - x_D}{1 - x_F}\right)$$

The obtained value for the minimum reflux ratio R_m and the number of ideal trays are entered in the Eduljee correlation to find the minimum number of ideal trays N_m necessary to realize the split at total reflux.

$$\frac{N - N_m}{N + 1} = \frac{3}{4}\left(1 - \left(\frac{R - R_m}{R + 1}\right)^{0.5668}\right)$$

The equation of Fenske can be used to calculate the bottom composition :

$$N_m = \frac{\ln\left(\frac{x_D}{1-x_D} \cdot \frac{1-x_B}{x_B}\right)}{\ln(\alpha)}$$

Finally, solving the mass balances provides us with the top and bottom flow rates. Assuming equal molal overflow, the column liquid and vapor streams in the column become available.

$$F = D + B$$

$$Fx_F = Dx_D + Bx_B$$

$$L = RD$$

$$V = (R+1)D$$

As mentioned before, the objective function for the optimization is the daily operation profit. This profit is itemized as follows :

(propylene sales + propane sales - utility cost - raw material cost) (*)

If the following notation is used :

- ⋆ c_d : price of propylene in the distillate ($/kg)
- ⋆ c'_d : price of propane in the distillate ($/kg)
- ⋆ c_b : price of propylene in the bottom product ($/kg)
- ⋆ c'_b : price of propane in the bottom product ($/kg)
- ⋆ x_b : weight fraction of propylene in the bottom product
- ⋆ x_f : weight fraction of propylene in the feed flow
- ⋆ x_d : weight fraction of propylene in the distillate
- ⋆ B : bottom flow (kg/day)
- ⋆ F : feed flow (kg/day)
- ⋆ D : distillate flow (kg/day)
- ⋆ Q_r : reboiler heat load (J/day)
- ⋆ Q_c : condensor heat load (J/day)
- ⋆ c_1 : heating cost ($/J)
- ⋆ c_2 : cooling cost ($/J)

then the daily operating cost can be written as :

$$f = \{c_d x_d D + c_b x_b B\} + \{c'_d(1-x_d)D + c'_b(1-x_b)B\} -$$
$$\{c_1 Q_r + c_2 Q_c\} - \{c_f x_f F - c'_f(1-x_f)F\}$$

The terms in the braces correspond to the terms in words (equation *) in the initial itemization. By using $W = c_d - c_b$ (light key differential value) and $U = c'_b - c'_d$ (heavy key differential value), this equation can be rearranged to :

$$f = c_d x_f F + c_b(1-x_f)F - c_f x_f F - c_f(1-x_f)F - c_1 Q_r - c_2 Q_C - W x_b B - U(1-x_d)D$$

The feed composition and flowrate are given, and cannot be changed by adjusting the manipulated variables of the optimization : the reflux ratio and the top purity. Once x_f and F are given, the on-line optimizer will estimate an optimal reflux ratio and top composition subject to the objective, the constraints, and the plant input. Therefore the first four terms in this equation are constant, and are of no importance during the optimization. They can be omitted in the optimisation objective. The remaining terms will be called $-f_1$. Changing the sign makes the objective a cost that has to be minimized.

$$f_1 = c_1 Q_r + c_2 Q_c + W x_b B + U(1-x_d)D$$

One has to keep in mind however that f_1 is not the complete operating cost, but only the fraction of the operating cost that is variable with the reflux ratio and the top composition. Finally the following assumption is sufficiently accurate for the purposes of this case study as well as for modeling many others towers :

$$Q_r \simeq Q_c = \lambda V$$

In this equation λ equals the average latent heat per unit of mass, V the vapor boilup in mass [Edgar & Himmelblau,1988]. Then f_1 reduces to :

$$f_1 = (c_1 + c_2)\lambda V + W x_b B + U(1 - x_d)D$$

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REFERENCES

C.R. Bertrand; *A Study on Dynamic Simulation and Control of Steam Systems*, Master's Thesis, University of Maryland, Department of Chemical and Nuclear Engineering, 1986

T. Blevins, D. Roberts, L. Block, C. Andreasen; 'A Standardized Software Package for Energy Monitoring and Energy System Optimization in the Pulp and Paper Industry', ISA Conference, Houston 1980

G.E.P. Box; N.R. Draper; 'Bayesian Estimation of Common Parameters from Several Responses', Biometrika, **52**, 1965

C.H. Cho; 'Optimum Boiler Load Allocation'; Instrumentation Technology, Oct 1978

G. Coombes, K. Randall, J.V. Wiseman; 'Pulp Mill Set Point Control System'; ACC Conference 1983

T.F. Edgar, D.M. Himmelblau; 'Optimization of Chemical Processes', to be published, 1988

A.V. Fiacco;*Introduction to Sensitivity and Stability Analysis in Nonlinear Programming*, Academic press, Mathematics in Science and Engineering, Volume 165, New York, NY, 1983

M.R. Fenske; 'Fractionation of Straight-Run Pennsylvania Gasoline'; I& EC **24**, 1932

G.L. Funk, C.C. Kania, R.D. Terhune; 'Why Risk Partial Optimization ?'; Hydrocarbon Processes, Nov 1984

D. Green, Al ai-Shaikh; 'Evaluating and Improving Efficiency in a Boiler Complex Through Computer Control'; JACC 1980

E.R. Gilliland; 'Multicomponent Rectification'; I& EC,**32**, 1940

C. Iordache, R.S.H. Mah, A.C. Tamhane; 'Performance Studies of the Measurement Test for Detection of Gross Errors in Process Data', AIChE Journal, **31**, 7 (July 1985)

J. King; *Separation Processes*, 2nd edition, Mc Graw Hill, New York, NY, 1979

J. Koninckx, T.J. Mc Avoy; 'Steady State On-Line Optimization Of Chemical Plants'; First Annual SRC Conference, University of Maryland, College Park, 1986

J.L. Kuester, J.H. Mize; 'Optimization Techniques with Fortran', McGraw-Hill, New York 1973

B.G. Lipták; 'Improving Boiler Efficiency'; Chemical Engineering, May 1987

G.D. Martin, P.R. Latour, L.A. Richard; 'Closed-Loop Optimization of Distillation Energy'; CEP, Sept 1981

T.J. Mc Avoy; *Interaction Analysis*, ISA Monograph Series 6, Research Triangle, NC-27709, 1983

S. Narasimhan, R.S.H. Mah; 'Generalized Likelyhood Ratio Method for Gross Error Identification'; AIChE Journal, **33**, 9 (Sept 1987)

M. Näsi, D.J. Libby, H.J. Duhon; 'Advanced Control of Acetylene Hydrogenation Reactors'; Hydrocarbon Processing, June 1985

R. Nath, D.J. Libby, H.J. Duhon; 'Joint Optimization of process Units and Utility Systems'; CEP, May 1986

J.B. Poje, A.M. Smart; 'On-Line Energy optimization in a Chemical Complex', CEP, May 1986

J.G. Renfro;*Computational Studies in the Optimization of Systems Described by Differential/Algebraic Equations*; Ph.D. Thesis, University of Houston, Department of Chemical Engineering, 1986

R.W. Serth, W.A. Heenan; 'Gross Error Detection and Data Reconciliation in Steam Metering Systems'; AIChE Journal, **32**, 5 (May 1986)

M.L. Sourander, M. Kolari, J.C. Cugini, J.B. Poje, D.C. White; 'Control and Optimization of Olefin- Cracking Heaters', Hydrocarbon Processing, June 1984

M.L. Sourander, S. Gros; 'Controlling and Optimizing Integrated Fractionation Processes in a Petroleum Refinery'; from *Dynamics and Control of Chemical Reactors and Distillation Columns*; Preprints of an IFAC Symposium, Bournemouth, UK, 8-10 dec, 1986

J. Wen ; 'Mill-Wide Production Coordination Possible with Distributed Control'; Pulp & Paper July 1983