Integrated approach to unit optimisation

Using the flowsheeting, online optimisation and pinch analysis of an advanced process analysis system, increases in profit and energy saving were projected for an alkylation unit through reduced steam usage in the distillation columns

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The alkylation process is one of the most important refinery processes for producing conventional gasoline. Alkylation offers several key advantages to refiners, including the highest average quality of all components available to the gasoline pool, increased amounts of gasoline per volume of crude oil and high heats of combustion. The overall process is a composite of complex reactions, and consequently rigorous control is required of operating conditions and of catalyst to assure predictable results.

Commercial alkylation plants use either sulphuric acid (H_2SO_4) or hydrofluoric acid (HF) as catalysts. About 20 years ago, almost three times as much alkylate was produced using the H_2SO_4 catalyst as compared to processes using HF. Since then, the relative importance of processes using HF has increased substantially and currently these processes produce in the USA about 47% of the alkylate. There is a also significant HF-based alkylation capacity in other major refining regions, such as in the Middle East and Europe.

However, in the last five years, more H_2SO_4 than HF-type units have been built due to environmental and safety concerns. Recent information clarifying the dangers of HF is causing refineries that use HF to reconsider the catalyst, or improve the safety of equipment and procedures [Albright L F, Modern alkylate–1: Alkylation will be key process in reformulated gasoline era; *Oil and Gas Journal*, 88, 1990. Cupit C R et al, Catalytic alkylation; *Petro/Chem Engineer*, 33, 1961].

An advanced process analysis system was successfully applied to the 15 000bpd alkylation plant at the Motiva Enterprises refinery at Convent, in Louisiana, USA.

The system was developed for use by process and plant engineers to perform comprehensive evaluations of projects in-depth significantly beyond their current capabilities. The strategy has the advanced process analysis methodology identifying sources of excess energy use and of pollutant generation. This program has built on results from research on source reduction through technology modification in reactions and separations, energy conservation (pinch analysis) and online optimisation (process control).

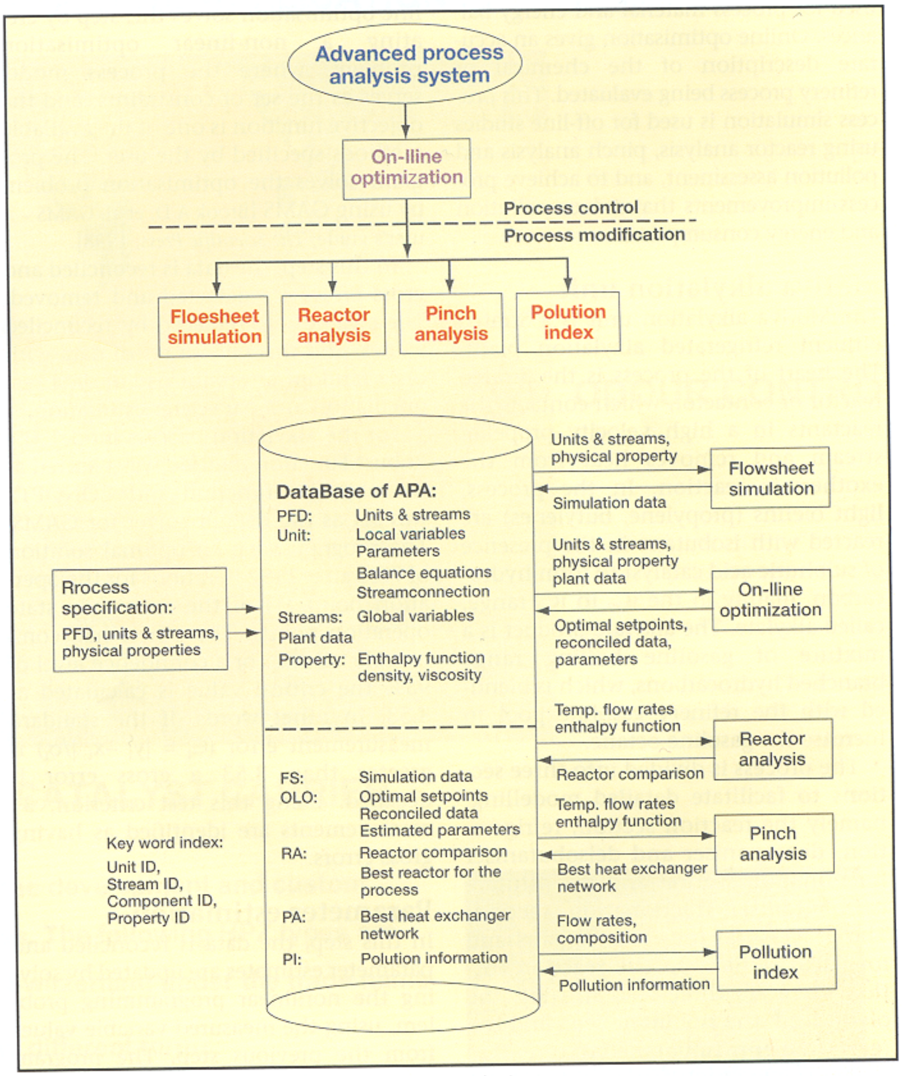

Figure 1 *Framework of advanced process analysis system*

The system uses a chemical reactor analysis program, online optimisation and pinch analysis programs, and the EPA pollution index methodology. Visual Basic was used to integrate the programs and develop an interactive Windows interface where information is shared through the Microsoft Access database.

The advanced process analysis methodology identifies sources of excess energy use and of pollutant generation and was based on the framework shown in Figure 1. The main components of this system are flowsheet simulation, on-line optimisation, reactor analysis, pinch analysis and pollution assessment.

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Summary of the alkylation process model

Feature	Quantity
Process units	76
Process streams	110
Equality constraints	1579
Inequality constraints	50
Measured variables	125
Unmeasured variables	1509
Parameters	64

Table 1

The flowsheet simulation program is used for process material and energy balances. Online optimisation gives an accurate description of the chemical or refinery process being evaluated. This process simulation is used for off-line studies using reactor analysis, pinch analysis and pollution assessment, and to achieve process improvements that reduce pollution and energy consumption.

Motiva alkylation unit

The Motiva alkylation unit is a Stratco effluent refrigerated alkylation plant. The heart of the process is the Stratco reactor or contactor, which contacts the reactants in a high velocity propeller stream and removes heat from the exothermic reaction. In the process, light olefins (propylene, butylenes) are reacted with isobutane in the presence of sulphuric acid catalyst to form hydrocarbon, mainly in the iC_7 to iC_8 range, called alkylate. The alkylate product is a mixture of gasoline boiling range branched hydrocarbons, which is blended with the refinery gasoline pool to increase the gasoline octane.

The process is divided into three sections to facilitate detailed modelling, namely the reaction section, refrigeration, depropaniser and deisobutaniser fractionation section and the saturate deisobutaniser fractionation section. The process has four reactor pairs and four acid settlers. In the reaction section there are three feed streams, the olefin feed, the isobutane feed and the recycled olefin/isobutane mixture.

The olefin feed contains the light olefins that are reacted with isobutane in the unit's stirred reactors. The isobutane stream is in excess to fully react with all of the olefins being charged to the unit.

Results

The alkylation process model developed using the flowsheet simulation program is summarised in Table 1. The degree of the freedom in the model is 55.

Online optimisation uses the plant model developed in flowsheet simulation to calculate optimal setpoints for the distributed control system. This involves rectifying gross errors of plant data sampled from the distributed control system using combined gross error detection and data reconciliation, estimating process parameters and reconciling plant data using simultaneous data reconciliation and parameter estimation, and optimising the operating setpoints using the updating process and economic models.

Gross error detection

Combined gross error detection and data reconciliation is the first step in conducting online optimisation. Online optimisation solves this step by creating a non-linear optimisation problem, where the process model serves as the set of constraints, and the objective function is one of the available methods specified by the user. The program solves the optimisation problem by using GAMS [Brook A D, et al, GAMS – A user's guide; *The Scientific Press*, 1998].

In this step, the data is reconciled and gross errors are detected and removed. Their values are replaced by reconciled values, and this gives a set of data with only random errors for use in data reconciliation and parameter estimation.

For the alkylation process model, the Robust Function method was selected as the objective function and CONOPT2 was set as the default solver for GAMS. The program gave an optimal solution of 78.8 after 1192 iterations for the operation point (1) of the six steady state operation points. The others had comparable values. For a confidence level of 95% the critical value is calculated as 3.53. In other words, if the standard measurement error ($\in_i = |y_i - x_i|/\sigma_i$) is greater than 3.53 a gross error is declared. Using this test criterion, 31 measurements are identified as having gross errors.

Parameter estimation

In this step, the data is reconciled and parameter estimates are updated by solving the nonlinear programming problem, using the measured variable values from the previous step. The program gave an optimal solution of 113.8 after 1490 iterations for the operation point (1) of the six steady states.

The performance for the other five steady state operation points was similar. The values of 36 of the 64 parameters remained the same whereas the adjustments for the rest during parameter estimation are minimal. These values along with the error-free, reconciled measured variables, represent the current specifications of the process plant, which can be used to calculate the optimal operating setpoints.

Economic optimisation

Maximising profit was used as the objective of economic optimisation of the alkylation process model.

The economic model was developed as shown by the following equations:

Profit = Sales – Cost – Utilities

Sales = Alkylate (C_3, C_4 and C_4 raffinate) produced * Price of alkylate

Cost = ∑ Input * Cost

Utilities = ∑ Input * Utility Cost.

In these equations, the input for cost includes olefins (propylene and butylene), C_4s from the reformer (feed to the saturate deisobutaniser column), isobutane and sulphuric acid, and the input for the utilities includes steam, water and electricity.

This economic model was used with operation point (1) and the program gave an optimal solution after 63 iterations. The profit for the process was calculated to be $29.11/min, which is an increase of 144% over the operating condition (1). The profit from the current operating condition was evaluated using the reconciled data prior to economic optimisation. This improvement in the profit is caused by 8.5% reduction in costs and 2.2% increase in sales.

The economically optimum solution had 5.5% more olefin charge, almost 100% reduction in isobutane purchase cost (by increasing the separation in the saturate deisobutaniser column rather than using isobutene from the raw material storage tank), 7.2% reduction in saturate feed to the saturate deisobutaniser column and 2.2% increase in the alkylate. The alkylate quality did not change at the economically optimal operation.

The results for all of the six cases show an increase in profit from 25% to 216%. This wide range of increase in the optimal profit for six different operation points is observed because of even wider ranges existing in the plant data. The flow measurements differ as much as 300% and mass fraction measurements as much as 4000%, between operation points.

Collectively, these results show that by applying online optimisation to the alkylation process with reconciled data and estimated parameters, the profit of the plant can be improved significantly.

Heat exchanger optimisation

The alkylation process is very energy intensive. The alkylation reactions occurring in the contactors are exothermic, and the heat generated is removed by effluent refrigeration. The process requires proper control of temperature, which is done by feed-effluent heat exchanging and also by external utilities. Also, energy is required in the separation

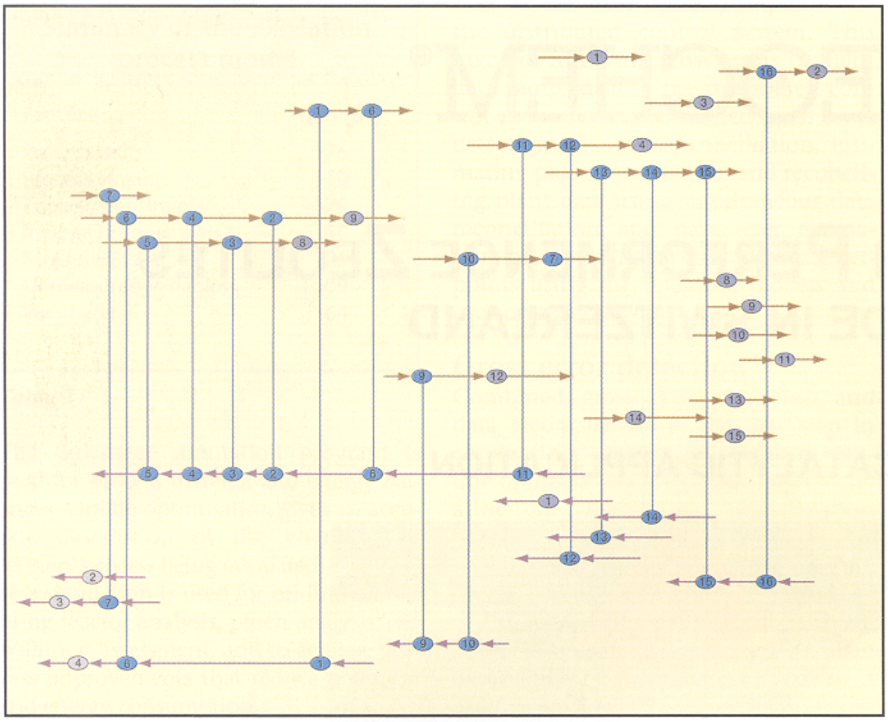

Figure 2 Network grid diagram for alkylation process

units of the process. The alkylation process model has 28 heat exchangers, plus four pair of contactors. The heat exchange within the contactors using the cold refrigerant condensate through the tube bundle is not included in the pinch analysis since any new arrangement for the contactors will be impractical.

According to the pinch analysis, the alkylation process requires a minimum of 1742 MJ/min external heat and 4043 MJ/min of external cooling. From the data validation results, the current external utility requirements are 1907 MJ/min of heat and 4300 MJ/min of cooling. The economic optimisation decreases the heating requirement by 1% to 1888 MJ/min whereas the initial pinch analysis reduces it another 7.7%.

The cooling requirement can be reduced as much as 7.4% by using pinch analysis from 4367 MJ/min after economic optimisation. This is because the economic optimisation results in a 1.6% higher cooling requirement than the current value of 4300 MJ/min.

The pinch analysis program also has the ability to design a maximum energy recovery (MER) network for the process under consideration. The network grid diagram that makes use of the external utilities calculated in the grand composite curve (GCC) can be seen in Figure 2.

The network found by pinch analysis consists of 16 heat exchangers, four heaters and 15 coolers, whereas the process has only six heat exchangers, four heaters and 12 coolers. This suggests that the improvement in the energy requirements is achieved by these additional heat exchangers. Heat integration above the pinch involves streams such as the flow to the saturate deisobutaniser reboiler, the charge to the depropaniser column and the sidestream to the inter-reboiler of the deisobutaniser column, which are heated up by streams such as deisobutaniser bottoms, depropaniser bottoms and the side stream from deisobutaniser.

This integration eliminates some of the heat exchangers existing in the current plant configuration. However, the configuration from the analysis may result in operational difficulties because of a more intense interaction between input and output streams of the three distillation columns. Moreover, these three distillation columns are placed across the pinch, which is not an appropriate placement of distillation columns for energy integration.

To integrate the columns with the remainder of the process, one can remove the columns from the process analysis and then try to use as much energy as possible from the process for the energy requirements of the columns by pressure-shift [Douglas M J, *Conceptual Design of Chemical Processes*; McGraw-Hill Inc,1988].

A pressure shift applied to the saturate deisobutaniser column (a decrease in the operation temperature by 7K) can reduce the heating and cooling requirements by 550 MJ/min. Pressure shifts resulting in 25K and 9K decreases in operation temperature for the depropaniser and saturate deisobutaniser columns can reduce the separation energy requirements by 650 MJ/min. These changes should be considered if it is feasible with the other operating conditions in the plant.

From the pinch analysis, three loops and one path in the heat exchanger network can be located. These provide additional degrees of freedom for further optimisation of the system by eliminating some of the exchangers within the loops or on the path.

In summary, pinch analysis provided an extensive insight for the optimisation of the energy consumption in the alkylation plant and showcased the benefits of heat integration for the process.

Pollution assessment

The alkylation process has 10 input and output streams relevant to the pollution assessment. The output streams are classified as product and non-product. For example, spent acid is a non-product whereas alkylate is a product stream. The components present in each of these streams are specified and the flow rates and compositions of streams are obtained from the results of the online optimisation program.

Pollution impact is calculated using specific environmental impact potentials (SEIP) of the components in the streams. Relative weighting factors for the nine categories of impact were all assumed to be one in the absence of actual values. Using the SEIP values and relative weighting factors, the program calculates pollution indices for each

Pollution assessment values for alkylation process

Before and after the economic optimisation

	Value		
Index type	*Before*	*After*	
Total rate of impact generation	–4.9120	–4.7966	impact/time
Specific impact generation	–3.2860	–3.4584	impact/product
Pollution generation per unit product	–0.9777	–0.9742	mass of pollutant/mass of product
Total rate of impact emission	1.0325	1.0337	impact/time
Specific impact emission	0.6897	0.7453	impact/product
Pollutant emission per unit product	0.1069	0.1154	mass of pollutant/mass of product

Table 2

input, product and non-product stream in the process, scaling the effect of the stream to the environment. These values are used to calculate the six pollution indices for the process, which are listed in Table 2, *Before* and *After*, the economic optimisation of the process. Negative values mean that the input streams are actually more harmful to the environment than the non-products if they are not processed through the alkylation process.

Pollution assessment results show that the economic improvement that is achieved by the economic optimisation does not come with a reduced environmental impact. The plant operating at the optimal set point emits more pollutants since the rate of impact generation is increased, although specific component's consumption might be less (sulphuric acid consumption is reduced by 2.2%).

Conclusion

Using the flowsheeting capability of the advanced process analysis system, a simulation of the alkylation process was developed that consist of 76 process units, 110 process streams, 1579 equality and 50 inequality constraints with 1634 variables. The simulation was validated using plant data and data reconciliation to show that the simulation predicted the performance of the plant within the accuracy of the data.

The analysis of the plant data resulted in detecting six steady state operation points. For each operation point gross errors were detected, data were reconciled, parameters were updated and economically optimum setpoints were determined for the distributed control system.

The economic optimisation of the process for six operation points resulted in 25.4% to 215.4% increase in the profit. As an example, the profit for the process was calculated to be $29.11/min, which is an increase of 144.6% over the operating condition (1). This improvement in the profit is caused by 8.5% reduction in costs and 2.2% increase in sales.

The economically optimum solution results in 5.5% more olefin charge, almost 100% reduction in isobutane purchase cost, 7.2% reduction in saturate feed to the saturate deisobutaniser column and 2.2% increase in the alkylate. The alkylate quality didn't change at the economically optimal operation. Another result obtained from the economic optimisation of the alkylation process is a 2.2% reduction in the sulphuric acid consumption.

According to the pinch analysis the alkylation process requires a minimum of 1742 MJ/min external heat and 4043 MJ/min of external cooling. From the data validation results, the current external utility requirements are 1907 MJ/min of heat and 4300 MJ/min of cooling. The economic optimisation decreases the heating requirement by 1% to 1888 MJ/min whereas the initial pinch analysis reduces it another 7.7%. The cooling requirement can be reduced as much as 7.4% by using pinch analysis. A further reduction in the energy requirements can be achieved by an appropriate pressure shift applied to distillation columns accounting a maximum reduction of 650 MJ/min.

Pollution assessment of the alkylation plant revealed the extent and location of the pollutant emissions of the process. It has also shown that the economically optimal solution can result in higher overall pollution levels even if the consumption of the sulphuric acid is reduced.

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