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An Advanced Process Analysis System for Improving Chemical and Refinery Processes

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Abstract

An advanced process analysis system has been developed to perform comprehensive evaluations on chemical plants and refineries for process improvements. The system integrates programs for on-line optimization, chemical reactor analysis, flowsheeting, pinch analysis and pollution indices. These programs are used interactively and share plant data through a database. Results from applying the system to a Monsanto/IMC Agrico contact process for sulfuric acid include an increased profit, reduced emissions and improvements in the chemical reactors and heat exchanger network which demonstrates the applicability of the system for pollution prevention.

Keywords: on-line optimization, chemical reactor analysis, pinch analysis, pollution index

Introduction

An advanced process analysis system has been developed which is to be used by process and plant engineers to develop innovative and economically viable ways to optimize and modify processes significantly beyond their current capabilities. With this system, process engineers interactively and simultaneously use programs for on-line optimization, chemical reactor analysis, flowsheeting, pinch analysis and pollution indices. The results can be process modifications and controls that reduce wastes and energy consumption, in addition to increased profit and improved efficiency of operations.

An overview diagram of the advanced process analysis system is given in Fig. 1, and referring to this figure, the chemical reactor analysis program (Saleh, Hopper and Walker, 1995) evaluates modifications to have the best chemical reactor type and operating conditions. The flowsheeting program and the EPA pollution index methodology (Cabezas, et al,1997) identifies pollutants and determines modifications to have the best configuration for separations equipment. The pinch analysis program, THEN, (Knopf, 1993) evaluates modifications to integrate the network of heat exchangers, boilers, condensers and furnaces for best energy utilization. The on-line optimization program (Chen, 1998) provides accurate plant data to validate the plant descriptions used by the chemical reactor analysis, flowsheeting and pinch analysis programs. Also, it provides the set-points for the distributed control system for the optimal operating conditions for the plant to minimizes costs, energy use and waste generation.

The system has an interactive, Windows interface developed using Visual Basic 5.0, and it incorporates a database that maintains process, economic and environmental data which are shared by each program. The database structure is shown in Fig.2.

The program has been developed with industrial and academic collaboration using the Monsanto designed, IMC-Agrico sulfuric acid contact plant. Support has been provided by EPA, and the program will be available through the EPA Technical Assistance Tools program. In the following paragraphs, a brief description will be given of the programs used in the system, and results of applying the program to the IMC Agrico plant will demonstrate the system's capabilities.

Flowsheeting

Process flowsheet development is through an interactive Windows interface. A detailed description is provided in the users manual (Telang, 1998). As the process flow diagram is

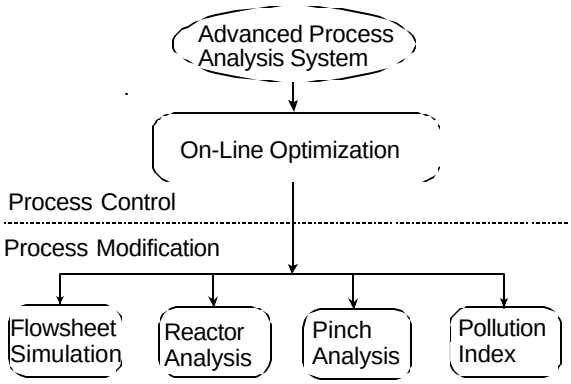


Fig. 1 Overview of Advanced Process Analysis System

prepared, equations for the process units and variables for the streams connecting the process units are entered and stored in the database using interactive data forms. This includes

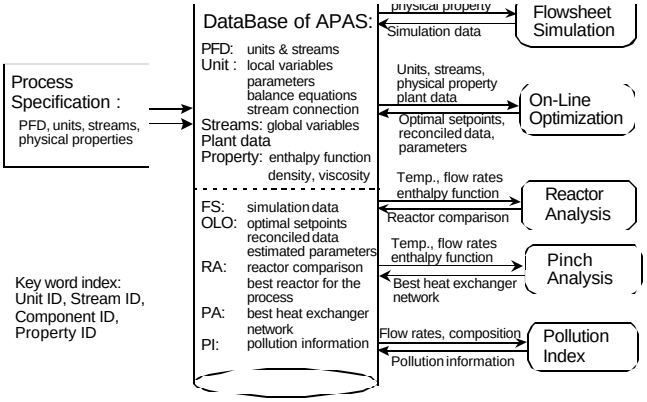


Fig. 2 Database Structure of Advanced Process Analysis System

material and energy balances, rate equations and equilibrium relations for the plant that are entered as equality constraints using the format of the GAMS programming language which is similar to Fortran. Process unit capacities, availability of raw materials and demand for product are entered as inequality constraints. Checking is conducted for redundancy and observability.

The flowsheet for the Monsanto/IMC Agrico contact process is shown in Fig. 3. Gas and steam can be on separate flowsheets, and the program provides the capability of having multiple flowsheets for a process. Features for developing flowsheets include adding, changing and deleting the equations that describe units and streams and their properties. Usual windows features include cut, copy, paste delete, print, zoom, reload, update and grid, among others.

On-Line Optimization

On-line optimization provides a means for maintaining a plant near its optimum operating conditions by providing set points to the plant distributed control system. This requires the solution of three nonlinear programming problems (NLPs): for combined gross error detection and data reconciliation, for parameter estimation and for process optimization. The plant model is a set of constraint equations in the NLPs obtained from the flowsheeting part of the system. The model has to match the current performance of the plant, and this is accomplished by having the parameters in the plant model updated using data sampled from the distributed control system that has been processed through gross error detection and data reconciliation procedures. The execution frequency for set point updating is based on the settling time of the process, i.e. the time required for the process to move from one set of steady-state operating condition to another, typically four to twelve hours.

The three nonlinear programs have a similar mathematical statement.

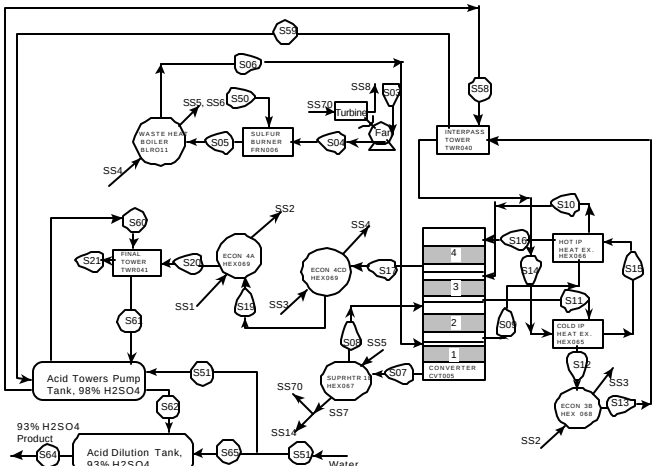
Optimize: Objective function (1)
Subject to: Constraints from plant model

The objective function is a joint distribution function for data reconciliation and parameter estimation and a profit function (economic model) for plant economic optimization. The constraint equations include material and energy balances, chemical reaction rates, thermodynamic equilibrium relations, among others. The optimal procedure for on-line optimization is based on the results of Chen (1998). Simultaneous gross error detection and data reconciliation is conducted to detect and rectify gross errors in plant data sampled from distributed control system using the Tjoa-Biegler method (the contaminated Gaussian distribution) for gross errors in the range of 3σ-30σ or the robust method (Lorentzian distribution) for larger gross errors. This step generates a set of measurements containing only random errors for parameter estimation. Then, this set of measurements is used for simultaneous parameter estimation and data reconciliation using the least squares method. This step provides the updated parameter values in the plant model for economic optimization. Optimal set points are generated for the distributed control system from the economic optimization using the updated plant and economic models.

The interactive on-line optimization part of the system uses the plant model from flowsheeting and has an interactive Windows interface for entering additional information needed to conduct on-line optimization. The program uses this information to write and run the three GAMS optimization programs, and it generates the optimal set points for the distributed control system. Also, summary and detailed reports are prepared. Options include using least squares, the Tjao-Biegler and Lorentzian methods. The process engineer does not need to know the details of the methodology for on-line optimization or the GAMS programming language. Application to the contact process is given in the results section.

Chemical Reactor Analysis

The chemical reactor analysis part of the system uses interactive windows to enter information to describe multiple reaction systems with thirty reactions and thirty-six



components in the reaction mixture for the types of reactors listed in Table 1.

The reactors can be isothermal, adiabatic or nonisothermal, and Langmuir-Hinshelwood and power-law kinetics are included. Also, mass transfer resistance and intraparticle diffusion as catalyst effectiveness factors can be used.

Information required about the stoichiometry and kinetics of the reactions taking place in the reactor is entered through interactive windows, and error checking is incorporated to ensure consistent data is provided. Reactor feed rates and compositions are obtained from the advanced process analysis system's database for the process. Results are presented in graphs and tables of conversion, concentration, temperature and pressure. Application to the contact process is given in the results section.

Table 1 Chemical Reactors in the Simulation Program

Homogenous

Single Phase (Gas or Liquid): Plug Flow, CSTR, Batch

Heterogeneous

Catalytic (Gas or Liquid): Fixed Bed, Fluidized Bed

Two-Phase (Gas-Liquid): Trickle Bed, Fixed Bubble Bed, CSTR Slurry, Bubble Slurry

Three-Phase: Fluidized Bed

Pinch Analysis

The pinch analysis part of the system uses THEN, (Knopf, 1993) to evaluate modifications and integrate the network of heat exchangers, boilers, condensers and furnaces for best energy utilization. An interactive interface presents the user with the process variables from the database. This includes stream flow rates, compositions, heat capacities and the enthalpy data. Then the user selects hot and cold streams from the complete list of process streams and specifies the approach temperature. Hot streams are streams that need to be cooled, and cold streams are streams that need to be heated. The program then retrieves other necessary data for these streams from the database and then uses the pinch analysis algorithm to determine the existence of a pinch point, and the minimum hot and cold utilities. The program draws the grand composite curve showing the heat flows in the system. Also, it uses the pinch design algorithm to synthesize a heat exchanger network that meets the minimum utility requirement. This network is displayed as a grid diagram, showing the placement of the heat exchangers, heaters and coolers.

For an existing process, this network can be compared with the existing one. If the amount of utilities being used is greater than the minimum, excess utilities are being used; and modification to the existing configuration is necessary. The configuration should be made as close as possible to the optimum one obtained by the program. Application to the contact process is given in the results section.

Pollution Balances and Indices

The EPA pollution index methodology (Cabezas, et al.,1997) provides a quantitative way to identify pollutants and their potential impacts. The Waste Reduction Algorithm (WAR) performs a pollution balance on a plant using a pollution index (mass pollutant/mass product). The pollution index is used to identify streams and parts of processes to be modified.

This methodology has been extended to the conservation of potential environmental impact in a process(Cabezas et al.,1997). There are nine different categories of impacts. These can be subdivided into four physical potential impacts (acidification, greenhouse enhancement, ozone depletion and photochemical oxidant formation), three human toxicity effects (air, water and soil) and two ecotoxicity effects (aquatic and terrestrial). The pollution impact of a process is useful in determining the ability of the process to produce desired products while inflicting a minimum impact on the environment.

The pollution index part of the system is called by the system to perform a pollution prevention analysis. It reads all the necessary stream information from the database. Additional data such as specific environmental impact potentials and weighting factors are supplied. The program then calculates the various types of pollution indices for the process which are useful in identification of streams with higher pollutant content. These results are presented to the user for evaluation and stored in database for subsequent retrieval. Application to the contact process is given in the results section.

Application to the Contact Process

In this section a description of the results is given for applying the advanced process analysis system to the contact process. This process is a mature technology and only small increments of improvements are obtained, but the important result is demonstrating the capability of the system on an actual process.

Process Description The IMC Agrico contact plant in Convent, Louisiana was designed by the Enviro-Chem System Division of Monsanto and began operation in March, 1992. It produces 3200 TPD 93%(wt) sulfuric acid and process steam as a by-product, and it has a Bailey INFI 90 distributed control system. This process incorporates packed bed catalytic reactors, absorption towers and heat exchanger networks, among others. It represents the state-of-art contact sulfuric acid technology. A detailed description of the process is given by Telang (1988).

Process Model An open form model was developed from the process flow diagram and process design data. The packed bed catalytic reactor was simulated with a kinetic model given by Chen (1998). The process model has 43 measured variables, 732 unmeasured variables, 11 parameters and 761 linear and nonlinear equality constraints. The model equations were entered in the flowsheeting program, and a comparison of results from the process model with the plant design data was made to assess the validity and accuracy of the simulation. The simulation matched the plant design data within the accuracy of the data. Also, a comparison was made with process data taken from the plant operating five years after start-up, and the simulation with parameters updated with reconciled plant data agreed within the accuracy of the data, e.g. outlet temperatures from the packed bed reactors agreeing within 3°F. Details of these comparisons are given by Chen (1998).

On-Line Optimization Two sets of plant data from DCS were used to evaluate on-line optimization of the contact process, and the details of these optimal solutions are reported by Chen (1998). Six measurements of the total of 43 were

detected as containing gross errors using the contaminated Gaussian function option. These were four temperatures, a flow rate and composition, and they were caused by incorrectly calibrated instruments. These values were replaced by reconciled data, and the simultaneous data reconciliation and parameter estimation program was executed. Then the updated parameters were used in the plant model for economic optimization to obtain the optimal set points. Economic optimization gave an increased profit of 3.0% (or $350,000/ year) and a 10% reduction in sulfur dioxide emissions over current operating condition. This is consistent with other reported applications of on-line optimization and could lead to a typical return on investment of one year.

Chemical Reactor Analysis The process has four packed bed catalytic reactors that use two different types of vanadium pentoxide catalyst to convert sulfur dioxide to sulfur trioxide. This reaction is exothermic and equilibrium is approached exiting each bed. Heat is removed to shift the equilibrium, and this heat is used to produce steam. Also, the equilibrium conversion is increased the fourth catalyst bed by removing SO_3 in the inter-pass absorption tower. A detailed description of the kinetic model is give by Chen (1998), and it includes an intrinsic reaction rate, pore diffusion temperature gradient between the gas and pellet, and reversible reaction using the equilibrium constant. The kinetic model was entered in the chemical reactor analysis, and an evaluation of the effect of reactor pressure on conversion was made. This showed that the conversion could be increased by 19% in the first reactor and the volume could be decreased by 87% by using a reactor pressure of 10.3 atms. rather than the current operations at 1.3 atms.

Pinch Analysis The heat exchanger network program was used to apply pinch analysis to the contact process This process is a highly exothermic, and heat released from combustion of sulfur and conversion of sulfur dioxide to sulfur trioxide is used to produce steam which is a valuable product. The process was determined to be below the pinch, and no hot utility was required. The minimum amount of cold utility was 3.703×10^8 KJ /hr. A proposed heat exchanger network has thirteen heat exchangers with a total area of 25% less than the current one. The results showed that the existing process is not using any excess utilities, and the energy efficiency can not be improved. However, the network solution provided by the program has less area than the existing network. This shows that the program can be used to check the optimality of existing networks and develop better designs.

Pollution Indices The pollution index part of the system was used to demonstrate the pollution prevention analysis with the contact process. The pollution indices were calculated for the process, and the results indicated that the stack gas was the primary pollution impact from the process. The sulfur furnace and the converter were identified as the candidates for process modification. Thus, the pollution index program can be used to evaluate the environmental efficiency of a plant and assist in making decisions regarding process improvement

Conclusions

An advanced process analysis system has been developed to perform comprehensive evaluations on chemical and refinery processes for waste minimization. With this system, process engineers can use programs interactively and simultaneously for on-line optimization, chemical reactor analysis, flowsheeting, pinch analysis and pollution indices. Results from applying the system to a Monsanto/IMC Agrico contact process for sulfuric acid demonstrate the applicability of the system for process improvement and pollution prevention.

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