K. S. Telang, R. W. Pike, F. C. Knopf, J. R. Hopper, J. Saleh, S. Waghchoure, S. C. Hedge and T. A. Hertwig,"An Advanced Process Analysis System for Improving Chemical and Refinery Processes," Computers and Chemical Engineering, Vol. 23, p. S727-730 (1999)

An Advanced Process Analysis System for Improving Chemical and Refinery Processes

K. S. Telang, X. Chen, R. W. Pike and F. C. Knopf
Louisiana State University, Baton Rouge, LA 70803
J. R. Hopper, J. Saleh, C. L. Yaws, S. Waghchoure and S. C. Hedge
Lamar University, Beaumont, TX 77710
T. A. Hertwig
IMC Agrico Company, Convent, LA 70821

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

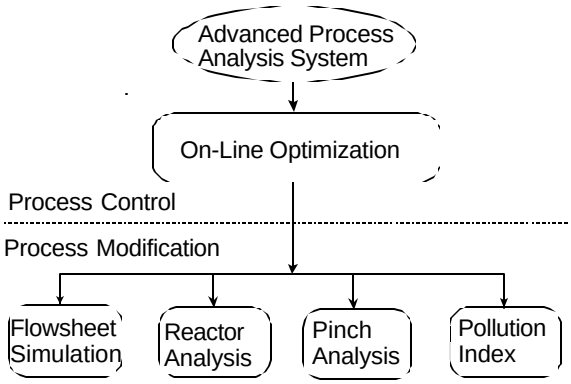
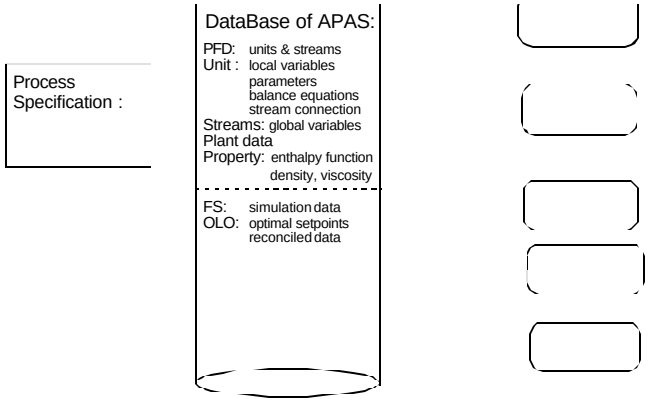


Fig. 1 Overview of Advanced Process Analysis System

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


Process
Specification :
DataBase of APAS:
PFD: units & streams
Unit : local variables
parameters
balance equations
stream connection
Streams: global variables
Plant data
Property: enthalpy function
density, viscosity
FS: simulation data
OLO: optimal setpoints
reconciled data

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 3EF. 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