Advanced Process and Chemical Complex Analysis Systems

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Abstract:

The Advanced Process Analysis System is used to perform economic and environmental evaluations of a plant. The main components of this system are a flowsheeting program, an on-line optimization program, a chemical reactor analysis program, a heat exchanger network design program, and a pollution assessment module. A Windows interface has been used to integrate these programs into one user-friendly application. An accurate description of the process is obtained from process flowsheeting and on-line optimization. Then an evaluation of the best types of chemical reactors is performed to modify and improve the process, and pinch analysis is used to determine the best configuration for the heat exchanger network and determine the minimum utilities needed for the process. The pollution index evaluation is used to identify and minimize emissions. A tutorial has two plant simulations and two actual plants.

The Chemical Complex Analysis System incorporates economic, environmental and sustainable costs and solves a MINLP for the best configuration of plants in a chemical production complex. The system incorporates a flowsheeting component where the simulations of the plants in the complex are entered through windows and stored in the database to be shared with the other components of the system. Also, entered are prices and economic, environmental and sustainable costs. Then the optimum configuration of plants in the complex is determined, and the results are presented to the user on the flowsheet and in tables from the GAMS solution of the MINLP . The tutorial has a complex simulation and an actual agricultural chemical complex.

These programs and users manual with tutorials can be obtained from the LSU Minerals Processing Research Institute's web site, www.mpri.lsu.edu at no charge.

ADVANCED PROCESS ANALYSIS SYSTEM

This advanced process analysis methodology is based on the framework shown in Figure 1 and structure shown in Figure 2. On-line optimization and data from the plant's distributed control system ensure these analyses match the performance of the actual plant and provide set-points for the distributed control system for the optimal operating conditions for the plant. Then the System is used for evaluating the best types and configuration of chemical reactors and separation units using the chemical reactor analysis, flowsheeting and pinch analysis programs. Also, processing options, i.e., changes in chemistry, chemical reactor configurations, solvents and associated optimal operating conditions for source reduction or recycling of identified pollutants, can be determined.

An interactive Windows program integrates the programs as outlined in Figure 2 to analyze source reduction, recycle and retrofit. It integrated process, economic and environmental data which are shared by chemical reactor analysis, process flowsheeting, pinch analysis and on-line optimization programs. The chemical reactor analysis program (Saleh, Hopper and Walker, 1995) determines the best chemical reactor type and operating conditions. The flowsheeting program, FlowSim, integrates the chemical reactor with the feed preparation and product purification facilities as illustrated in Figure 1. The pinch analysis program THEN (Knopf,

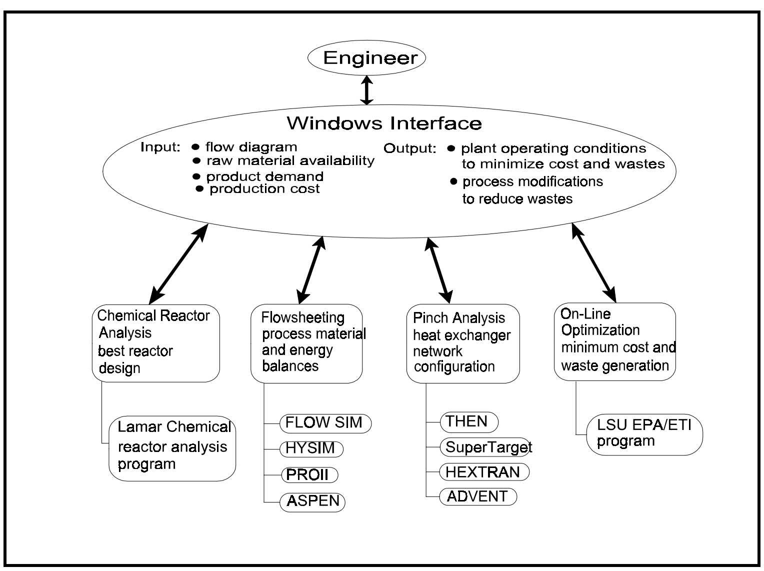

Figure 1 Advanced Process Analysis System Framework

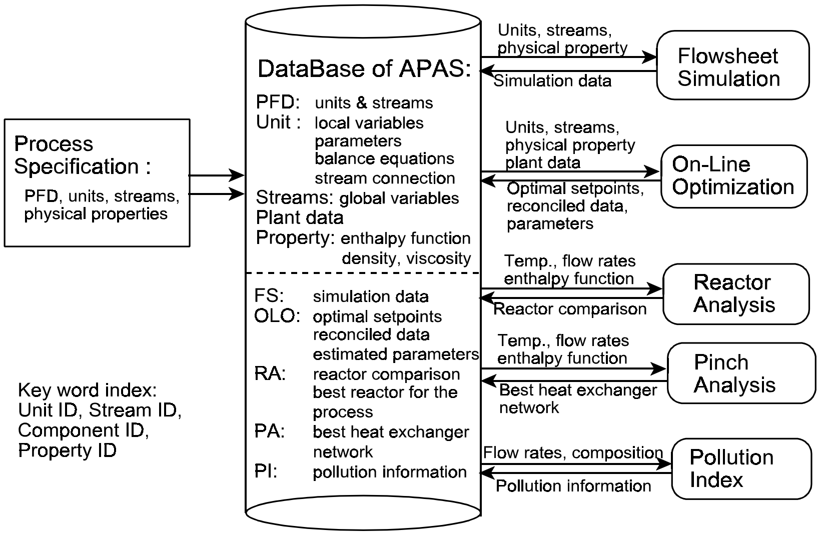

Fig. 2 Database Structure of Advanced Process Analysis System

1993), integrate the networks of heat exchangers, boilers, condensers and furnaces for best energy utilization. The on-line optimization program (Chen, et al. 1998) provides accurate plant data to validate the plant descriptions by the chemical reactor analysis, flowsheeting and pinch analysis programs. Also, the pollution index program is used to minimizes waste generation based on pollution balances and pollution indices.

The System has been applied to actual plants including the alkylation plant at the Motiva refinery in Convent, Louisiana and sulfuric acid contact plant at IMC Agrico's agricultural chemicals complex in Uncle Sam, Louisiana. Detailed plant descriptions of the refinery alkylation process and the contact sulfuric acid process were used with the System in collaboration with the process engineers from these companies. This ensured that the programs work on actual plants and meet the needs and requirements of the process and design engineers.

On-Line Optimization: On-line optimization is the use of an automated system which adjusts the operation of a plant based on product scheduling and production control to maximize profit and minimize emissions by providing set points to the distributed control system. The plant model has to describe the current performance of the plant, and plant data are sampled from the distributed control system for this purpose. This data is used to update and adjust parameters in the plant model to eliminate any plant and model mismatch. Before this can be done, the sampled data has to be processed through gross error detection procedures to eliminate erroneous information that could come from sources such as a broken instrument. Then it is processed through data reconciliation procedures to adjust it for consistency with material and energy balances. This reconciled data is precise and consistent data which is used to update the plant model parameters to ensure the plant model accurately predicts the performance of the plant. The parameters of the economics model are updated also, and these include sales prices and demand for products and costs and availability of raw materials. Typically, the optimization cycle is repeated every three to twelve hours, and this interval depends on the settling time of the plant.

Chemical Reactor Analysis: A comprehensive, interactive computer simulation for three-phase catalatic gas-liquid reactors and subsets of these reactors which has a wide range of applications such as oxidation, hydrogenation, hydrodesulfurization, hydrocracking and Fischer-Tropsch synthesis (Saleh, Hopper and Walker, 1995). The program interactively guides the engineer to select the best reactor design for the reacting system based on the characteristics of ten different types of industrial catalytic gas-liquid reactors which includes catalyst particle diameter and loading, diffusivities, flow regimes, gas-liquid and liquid-solid mass transfer rates, gas and liquid dispersions, heat transfer, holdup, among others. The program solves the conservation equations, and it has checks for the validity of the design, e.g. not allowing a complete catalyst wetting factor if the liquid flow rate is not sufficient.

Pinch Analysis: Pinch technology determines the minimum utilities for heat exchanger networks. It employs three concepts: the composite curves, the grid diagram of process streams and the pinch point; and these are applied to minimize energy use in the process. The composite curves are plots of temperature as a function of enthalpy from the material and energy balances for the streams that need to be heated, called cold streams, and those that need to be cooled, called hot streams. From the composite curves of the hot and cold streams, the potential for energy exchange between the hot and cold streams can be determined, as well as the process requirements for external heating and cooling from utilities such as steam and cooling water. At one or more points the curves for the hot and cold streams may come very close, the process pinch, and this means there is no surplus heat for use at lower temperatures. The grid diagram has vertical lines to represent the hot and cold streams with lengths corresponding to the temperature range with the hot streams going from top left and the cold streams from bottom right. With this arrangement the heat recovery network for the process design can be determined. A grand composite, temperature-enthalpy curve can be assembled from the composite curves and the grid diagram to help select utilities and appropriately place boilers, turbines, distillation columns, evaporators and furnaces. Also, the heat transfer surface area can be determined with the corresponding capital cost for both energy and cost minimization.

Pollution Assessment: The pollution assessment module is based on the Waste Reduction Algorithm and the Environmental Impact Theory (Cabezas et. al., 1997). The WAR algorithm is based on the generic pollution balance of a process flow diagram.

Pollution Accumulation = Pollution Inputs + Pollution Generation - Pollution Output (1)

It defines a quantity called as the 'Pollution Index' to measure the waste generation in the process. This pollution index is defined as:

$$I = \text{wastes/products} = -(\Sigma \text{Out} + \Sigma \text{Fugitive}) / \Sigma P_n \quad (2)$$

This index is used to identify streams and parts of processes to be modified. Also, it allows comparison of pollution production of different processes. The WAR algorithm can be used to minimize waste in the design of new processes as well as modification of existing processes. Also, the Environmental Impact Theory (Cabezas et. al., 1997) is a generalization of the WAR algorithm. It describes the methodology for evaluating potential environmental impacts, and it can be used in the design and modification of chemical processes. The environmental impacts of a chemical process are generally caused by the energy and material that the process takes from and emits to the environment. The potential environmental impact is a conceptual quantity that cannot be measured, but it can be calculated from related measurable quantities.

CHEMICAL COMPLEX (MULTI-PLANT) ANALYSIS SYSTEM

New methodology has been developed that determines the best configuration of plants in a chemical complex based on economic, energy, environmental and sustainable costs. The system structure is shown in Figure 3. This integrated system incorporates a flowsheeting component as shown in Figure 3 where simulations of the plants in the complex are entered. Each simulation includes the process or block flow diagram with material and energy balances, rates equations, equilibrium relations and thermodynamic and transports properties for the process units and heat exchanger networks. These equations are entered through windows and stored in the database to

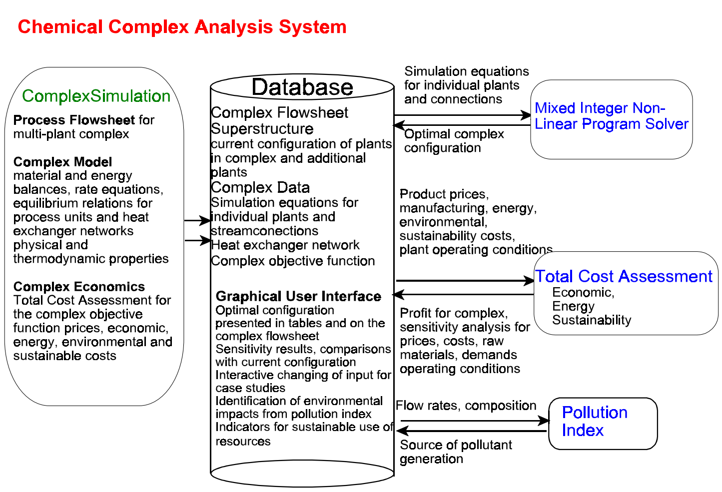

Figure 3 Program Structure for the Chemical Complex Analysis System

be shared with the other components of the system.

The objective function is entered as an equation associated with each process with related information for prices and economic, energy, environmental and sustainable costs that are used in the evaluation of the Total Cost Assessment (TCA) for the complex. The TCA includes the total profit for the complex that is a function of the economic, energy, environmental and sustainable costs and income from sales of products. Then the information is provided to the mixed integer nonlinear programming solver, GAMS, to determine the optimum configuration of plants in the complex. Also, sources of pollutant generation are located by the pollution index component of the system using the EPA pollution index methodology (Cabezas, et. al., 1997).

All interactions with the system are through the graphical user interface that is written in Visual Basic. As the process flow diagram for the complex is 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 as shown on the left side in Figure 3. Material and energy balances, rate equations and equilibrium relations for the plants are entered as equality constraints using the format of the GAMS programming language that is similar to Fortran. Process unit capacities, availability of raw materials and demand for product are entered as inequality constraints. 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. A detailed description is provided in a user's manual.

The system has the TCA component prepare the assessment model for use with determination of the optimum complex configuration. Economic costs are estimated by standard methods. Environmental costs are estimated from the data provided by Amoco, DuPont and Novartis in the AIChE/CWRT TCA report (Constable, et al., 1999). Sustainable costs are estimated from the air pollution data in the AIChE/CWRT TCA report. Improving the estimates is an on-going effort.

Industry Collaboration: The system is being developed in collaboration with engineering groups at Monsanto Enviro Chem, Motiva Enterprises, IMC Agrico and Kaiser Aluminum and Chemicals to ensure it meets the needs of the chemical and petroleum refining industries. The System incorporates TCA methodology in a program from the AIChE/CWRT Total Cost Assessment Methodology (Constable, 1999) which provides the criteria for the best economic-environmental design.

Validation - Application to Two Chemical Complexes: The system has been validated by application to two chemical complexes. In the first one, the system was applied to expanding production of sulfuric and phosphoric acid capacities and to evaluating heat recovery options at a major chemical company, and the results were compared to the company's case study. A second application of the system was based on an agricultural chemical complex with ten multiple plant production units as found in the Baton Rouge- New Orleans Mississippi river corridor. The optimal configuration of units was determined based on economic, environmental and sustainable costs. A comparison of current configuration with the optimal one was made, and sensitivity to cost and prices was analyzed.

References

Chen, X, T. A. Hertwig R. W. Pike and J. R. Hopper, 1998 "Optimal Implementation of On-Line Optimization," *Computers and Chemical Engineering*, Vol. 22, p. S435-S442.

Constable, D. et al., 1999, Total Cost Assessment Methodology; Internal Managerial

Decision Making Tool, AIChE/CWRT, AIChE, 3 Park Avenue, New York, NY, February 10, 2000.

Knopf, F. C. 1993, *THEN User's Manual*, Louisiana State University, Baton Rouge, LA 70803.

Saleh, J. M., J. R. Hopper and R. E. Walker, 1995, "Three-Phase, Catalytic Gas-Liquid Reactors: An Interactive Simulator," Paper No. 73d, 1995 Spring National Meeting, American Institute of Chemical Engineers, Houston, Texas.