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# A Prototype System for Economic, Environmental and Sustainable Optimization of a Chemical Complex

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A prototype of a chemical complex analysis system has been developed and used to demonstrate optimization of a chemical complex. The system incorporates economic, environmental and sustainable costs, and solves a MINLP for the best configuration of plants. It 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. The system selected the best site for required new phosphoric and sulfuric acids production capacities and selected, sited, and sized the optional heat-recovery and power-generation facilities. System capability was demonstrated by duplicating and expanding the industrial case study.

## 1. Introduction

The business focus of chemical companies has moved from a regional to a global basis, and this has redefined how these companies organize and view their activities. As described by H. J. Kohlbrand of Dow Chemical Company (Kohlbrand, 1998), the chemical industry has gone from end-of-pipe treatment to source reduction, recycling and reuse. Pollution prevention was an environmental issue and is now a critical business opportunity. Companies are undergoing difficult institutional transformations, and emphasis on pollution prevention has broadened to include tools such as Total (full) Cost Assessment (accounting) (TCA), Life Cycle Assessment (LCA), sustainable development and eco-efficiency (*eco*nomic and *eco*logical). At this point in time there is no integrated set of tools, methodologies or programs to perform a consistent and accurate evaluation of new plants and existing processes. Some of these tools are available individually, e.g. TCA and LCA, and some are being developed, e.g. metrics for sustainability. An integrated analysis incorporating TCA, LCA and sustainability is required for proper identification of real, long-term benefits and costs that will result in the best list of prospects to compete for capital investment.

Chemical companies and petroleum refiners have applied total cost accounting and found that the cost of environmental compliance was three to five times higher than the original estimates (Constable, et. al., 2000). Total or full cost accounting identifies the real costs associated with a product or process. It organizes different levels of costs and includes direct, indirect, associated and societal. Direct and indirect costs include those associated with manufacturing. Associated costs include those associated with compliance, fines, penalties and future liabilities. Societal costs are difficult to evaluate since there is no standard, agreed-upon methods to estimate them, and they can include consumer response and employee relations, among others (Kohlbrand, 1998).

The Center for Waste Reduction Technology (CWRT) of the American Institute of Chemical Engineers (AIChE) recently completed a detailed report with an Excel spreadsheet on Total Cost Assessment Methodology (Constable, et. al., 2000). The report was the outgrowth of industry representatives working to develop the best methodology for use by the chemical industry. The AIChE/CWRT TCA program uses five types of costs. Type 1 costs are direct costs for the manufacturing site. Type 2 costs are potentially hidden corporate and manufacturing site overhead costs. Type 3 costs are future and contingent liability costs. Type 4 costs are internal intangible costs, and Type 5 costs are external costs that the company does not pay directly including those born by society and from deterioration of the environment by pollution within compliance regulations. This report states that environmental costs made up at least 22% of the nonfeedstock operating costs of the Amoco's Yorktown oil refinery. Also, for one DuPont pesticide, environmental costs were 19% of the total manufacturing costs; and for one Novartis additive these costs were a minimum of 19% of manufacturing costs, excluding raw materials. Also, external costs are the very difficult to quantify, and this report gives some estimates for these costs from a study of environmental cost from pollutant discharge to air from electricity generation. In addition, this TCA methodology was said to have the capability to evaluate the full life cycle and consider environmental and health implications from raw material extraction to end-of-life of the process or product.

Sustainable development is the concept that development should meet the needs of the present without sacrificing the ability of the future to meet its needs. An effort is underway to develop these metrics by an industry group through the Center for Waste Reduction Technology of the American Institute of Chemical Engineers, and they have issued two interim reports (Adler, 1999) and held a workshop (Beaver and Beloff, 2000).

## 2. Prototype System for Optimization of a Chemical Complex

Combining economic, environmental and sustainability costs with new methodology for the best configuration of plants is now feasible. The analyses and components exist. This paper describes the prototype system shown in Figure 1 that combines these components into an integrated system for use by plant and design engineers. They have to convert their company's goals and capital into viable projects that are profitable and meet environmental and sustainability requirements and have to perform evaluations for impacts associated with green house gases, finite resources, etc. This program can be used with these projects and evaluations and also can help demonstrate that plants are delivering environmental, social and business benefits that will help ameliorate command and control regulations.

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 prototype incorporates TCA methodology in a program from the AIChE/CWRT Total Cost Assessment Methodology (Constable, 1999) which provides the criteria for the best economic-

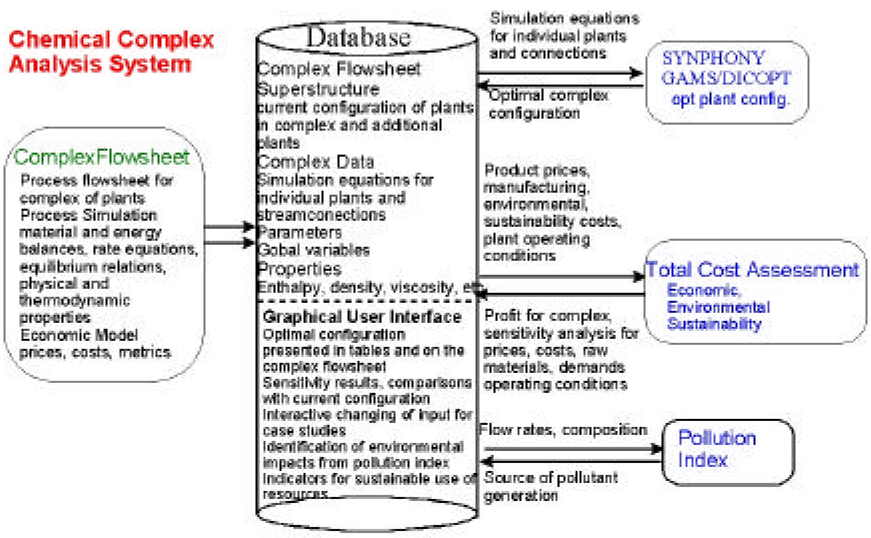

*Figure 1 Program Structure for the Chemical Complex Analysis System*

environmental design. Also, the programs SYNPHONY and GAMS/DICOPT are used for optimal plant configuration of the chemical complex. It includes the sustainability metrics developed by the AIChE/CWRT Sustainability Metrics Working Group (Adler, 1999) and the BRIDGES extensions (Beaver and Beloff, 2000).

The structure of the Chemical Complex Analysis System is shown in Figure 1. The system incorporates a flowsheeting component where the simulations of the plants in the complex are entered. Individual processes can be drawn on the flowsheet using a graphics program. The plants are connected in the flowsheet as shown in Figure 2. For each process material and energy balances, rate equations, equilibrium relations and thermodynamic and transport properties are entered through windows and stored in the database to be shared with the other components of the system. Also, the economic model is entered as an equation associated with each process with related information for prices, costs, and sustainablity metrics that are used in the evaluation of the Total Cost Assessment for the complex. The TCA component includes the total profit for the complex that is a function of the economic, environmental and sustainable costs and income from sales of products. Then the information is provided to either GAMS/DICOPT or SYNPHONY for solving the Mixed Integer Nonlinear Programming (MINLP) problem for the optimum configuration of plants in the complex. Also, the sources of pollutant generation are located by the pollution index component of the system using the EPA pollution index methodology (Cabezas, et. al., 1997).

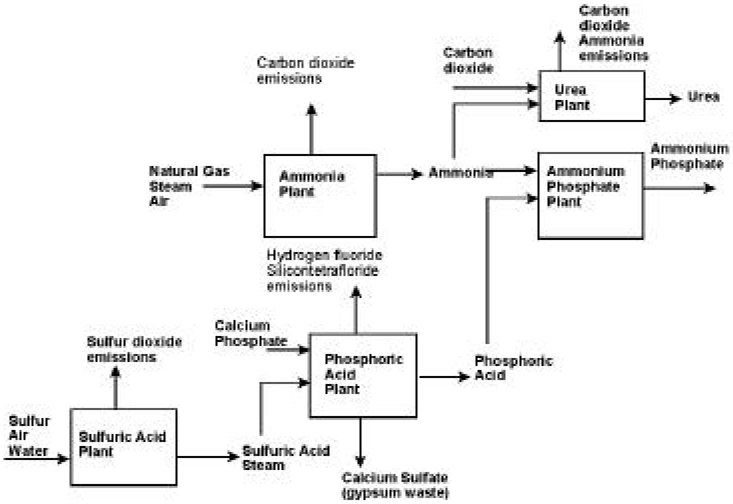

*Figure 2 Schematic of Agricultural Chemicals Complex with Raw Materials, Products, Emissions and Wastes.*

All interactions with the system are through the graphical user interface of the system 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 1. 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. The AIChE/CWRT TCA program (Constable, D. et. al., 2000) is an Excel spreadsheet that has the cost in five types, as describe above. This Excel spreadsheet is an extensive listing of all possible costs. The TCA component combines these five categories of costs into three costs: economic, environmental and sustainable. Types 1 and 2 are included in economic costs, Types 3 and 4 are included in environmental costs, and Type 5 is sustainable costs. Economic costs are estimated by standard methods (Garrett, 1989). Environmental costs are estimated from the data provided by Amoco, DuPont and Novartis in the AIChE/CWRT report. Sustainable costs are estimated by the study of power generation in this report. It is an on-going effort to refine and update better estimates for these costs.

As shown in Figure 1, the system will provide an option to select one of two optimization methods. Determining the optimal configuration of plants in a chemical complex is a mixed integer nonlinear programming problem where the equality and inequality constraints include material and energy balances, process unit capacities and others as described above. There are two methodologies to solve this type of optimization problem, GAMS/DCOPT and SYNPHONY. GAMS (General Algebraic Modeling System) was developed at the World Bank for very large economic models, and it can be used to determine the optimal configuration of a chemical complex by solving a MINLP programming problem using the DICOPT solver (Kocis and Grossmann, 1989). SYNPHONY uses process graph methodology based on the work of Friedler and Fan (Friedler, Varga and Fan, 1995) to solve the MINLP problem.

## 3. Agricultural Chemical Complex Expansion Evaluation

A major agricultural chemical company had performed a case study for expanding production of sulfuric and phosphoric acid along with heat recovery options at two locations that ten miles apart. This multiple site, multiple-plant expansion was used with the prototype system, and the results compared to the case study for validation of the prototype. In this complex, phosphate fertilizers are produced by reacting ammonia and phosphoric acid as illustrated in Figure 2. Phosphoric acid is made by digesting phosphate rock with sulfuric acid. Sulfur, air, and water are used to make sulfuric acid, and in that process, waste heat is recovered as steam to drive turbines for power generation, and to evaporate water from phosphoric acid.

With excess ammoniation capacity available, the objective of the case study was to expand phosphoric acid production capacity by 28%. This requires additional sulfuric acid and steam. Since sulfuric acid can be shipped for miles and steam cannot, phosphoric acid

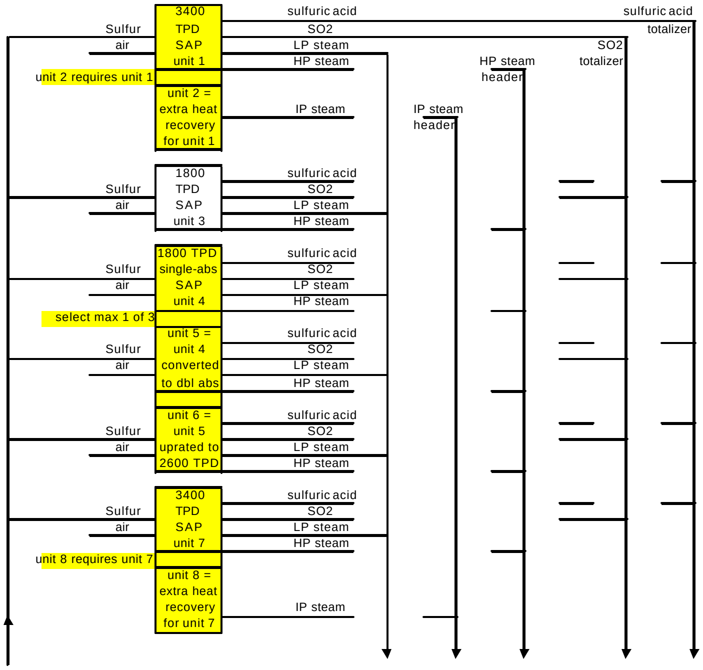

*Figure 3. Sulfuric Acid Plant Options at One of Two Plant Sites*
*Part of Superstructure for SYNPHONY*

evaporators require some steam capacity from an on-site sulfuric acid plant. When producing the sulfuric acid needed to produce phosphoric acid, the sulfuric plant produces more byproduct steam than is needed to evaporate the phosphoric acid. So, as long as the two-site sulfuric production capacity is adequate, there is some flexibility in how closely the sulfuric vs phosphoric acids production capacities have to match within each site. Also, spare power-generation capacity at a site will encourage the addition of extra heat recovery equipment to old and new plants at that site. Many U. S. fertilizer complexes have justified new power generation equipment. When a MWH sells for less than a bought MWH, the incentive drops when generated power displaces the last of the site's purchased power. When utility's "avoided costs" for new construction are high, many fertilizer complexes have justified excess generating capacity to sell power to their local utility. Site power differences could make it profitable to build a sulfuric plant at one site for the steam and ship all the sulfuric acid to the other site to make phosphoric acid.

More options were added to challenge the prototype, and the expansion was to be made in two stages where stage two should waste only a minimum of stage one. Stage one should still be a best choice in case stage two is never justified. Each of the two expansion stages will have one phosphoric acid expansion, and the second expansion will be at the "other" site; one sulfuric acid expansion with an option for over-sizing the first to serve as the second; and a second sulfuric acid expansion does not have to be sited away from the first expansion. Also, there are options for adding heat recovery equipment to one old and any new sulfuric plants and for adding one turbo-generator per site per stage.

Enough site differences were specified to make the study interesting. The question for the prototype to answer now was what size phosphoric acid, sulfuric, heat recovery, and power-generation expansions should be built at each site for each stage of expansion.

The file input-output version of SYNPHONY was used for the optimal configuration determination. The superstructure for this demonstration had 67 different species (600 psig steam, sulfuric acid, logic switches, etc.) and 75 processing units. In Figure 3, part of the superstructure for multiple sulfuric acid units is shown for one plant site. A sulfuric plant was one unit using 8-10 species. A new turbo-generator took 10 species and 7 units to model. Two of those species were fabricated to properly couple the 7 units to work as one. Computing time for any one case was less than 15 seconds on a Pentium II PC.

The results obtained with the system were consistent with the case studies done previously at the actual complexes that were modeled here, and this served to validate that the system was giving consistent and accurate results. The results of using the system gave the following evaluations. By raising the cost of shipping sulfuric acid between sites, the sites could be forced to be self-sufficient in sulfuric production capacity. This impacted steam- and power-generation capacities at each site. Similarly, the cost of extra storage tanks to handle more than a minimum of sulfuric shipping could be made to limit sulfuric shipping and bias the siting of sulfuric production capacity. This happened when the cost of extra tanks overcame the energy efficiencies of specific sites. Production rate for a higher-emissions, single absorption sulfuric acid plant was curtailed as expected by voluntarily limiting the two-site $SO_2$ emissions to pre-expansion levels. With this old plant curtailment, the new sulfuric plant was built with corresponding extra capacity. The curtailed, single-absorption sulfuric plant was converted to double-absorption for expansion stage two when the conversion cost was significantly less than the cost of a new plant and excess capacity was built in expansion stage one. However, few companies would build excess capacity in stage one without a power incentive or strong anticipation of stage two. Extra heat-recovery and power-generation equipment was justified only when longer payback periods were acceptable. Heat-recovery and power-generation equipment was installed or not installed based on installation cost and the value of the power. The value of power varied because incremental power displaced purchase at one site and added to sales at the other site. In conclusion, the prototype of a chemical complex analysis system has been demonstrated on an agricultural chemical complex expansion.

## 4. Conclusions

A prototype of a chemical complex analysis system has been described and its capability demonstrated by duplicating and expanding an industrial case study. The system selected the best site for required new phosphoric and sulfuric acids production capacities and selected, sited, and sized the optional heat-recovery and power-generation facilities.

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