

A prototype system for economic, environmental and sustainable optimization of a chemical complex

T.A. Hertwig, A. Xu, A.B. Nagy, R.W. Pike, J.R. Hopper, C.L. Yaws

Abstract 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 better of two sites 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. A second application of the prototype 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 the current configuration with the optimal one was made, and sensitivity to cost and prices was analyzed. The profit increased about 7.8% from the base case to the optimal solution. Also, environmental cost declined about 17%, and sustainability costs increased about 1.5%. These results illustrated the capability of the system to select an optimum configuration of plants in an agricultural chemical complex and to incorporate economic, environmental and sustainable costs. A brief sensitivity study gave predictable results and demonstrated additional capabilities of the system.

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 (economic and ecological). 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 are 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). This TCA 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

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T.A. Hertwig
Kaiser Aluminum and Chemical Company,
Baton Rouge, LA 70809, USA

A. Xu, R.W. Pike (✉)
Louisiana State University,
Baton Rouge, LA 70803, USA
E-mail: pike@lsu.edu
Fax: +1-225-5781476

A.B. Nagy
University of Veszprem,
Veszprem, Hungary

J.R. Hopper, C.L. Yaws
Lamar University, Beaumont,
TX 77710, USA

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 borne 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. 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. There have been many publications on sustainable development and environmental economics, which are described by Daly (1996), and in 1995 the President's Council on Sustainable Development issued a report giving 15 principles. These included calls to preserve the integrity of natural systems; to have economic growth, environmental protection and social equity be interdependent; to have a stable population consistent with the carrying capacity of the Earth; and to have all segments of society equitably share environmental costs. How these principles will be considered and ways to proceed involve complex political, trade, health, scientific and technical issues. Approaches have been and are being proposed by economists, government officials and business leaders. First, measures or metrics of sustainable development must be defined, tested and applied before sound policy decisions can be proposed and evaluated. An effort is underway to develop these metrics by an industry group through the Center for Waste Reduction of the American Institute of Chemical Engineers, and they have issued two interim reports (Adler 1999) and held a workshop (Beaver and Beloff 2000). Also, external or sustainable costs are the very difficult to quantify, and the TCA report gives some estimates for these costs from a study of environmental cost from pollutant discharge to air from electricity generation, e.g. U.S.\$0.22–2.38 per ton for CO, U.S.\$0–3.25 per ton for CO₂.

Prototype system for optimization of a chemical complex

A prototype system shown in Fig. 1 has been developed that combines components to determine the optimum configuration of plants in a chemical complex. Economic, environmental and sustainability costs are combined in the objective function to be optimized. The constraints include the material and energy balances, rate equations and equilibrium that describe the performance of the individual plants and how they are connected. Also included in the model of the complex are the equations that give the demand for product, availability of raw materials and capacity ranges for the plants. This formulation is a mixed integer nonlinear programming problem (MINLP), and the GAMS and SYNPHONY solvers are used to determine the optimal configuration from the superstructure of plants developed from a base case of existing plants.

The system has been 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 from the AIChE/CWRT Total Cost Assessment Methodology (Constable et al. 2000).

The System is designed for use by corporate engineering groups who 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 greenhouse 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.

As shown in Fig. 1, the Chemical Complex Analysis 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 Fig. 2. For each process, material and energy balances, rate equations, equilibrium relations and thermodynamic and transport properties are entered through windows and stored in an Access database to be shared with the other components of the system. Also, the objective function is entered as an equation associated with each process with related information for prices and economic, environmental and sustainable costs that are used in the evaluation of the TCA for the complex. The TCA 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 MINLP problem for 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. Referring to the left side of Fig. 1, 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. 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 program and users manual are available for downloading from the LSU Minerals Processing Research Institute's web site, <http://www.mpri.lsu.edu>.

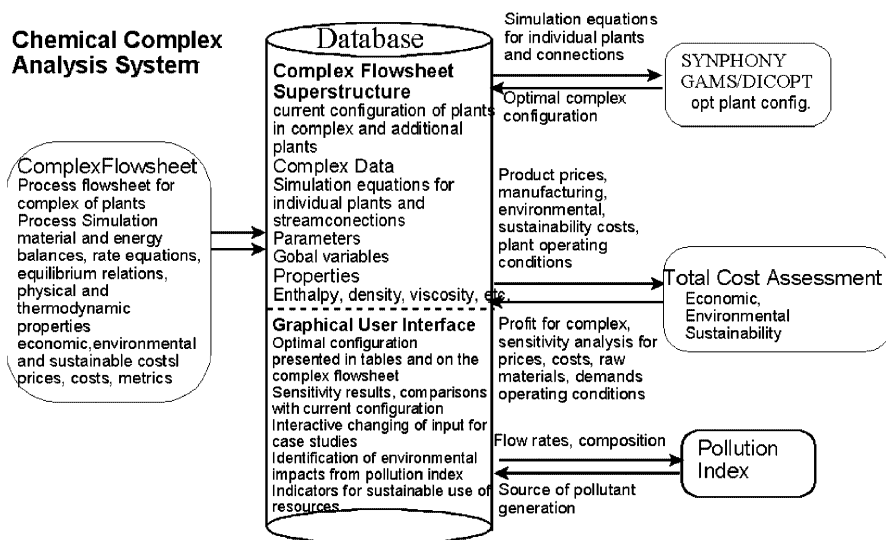


Fig. 1. Program structure for the chemical complex analysis system

As described above, the TCA report includes an Excel spreadsheet with an extensive listing of five types of costs. The prototype 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 Fig. 1, the system will provide an option to select one of two optimization methods. GAMS/DICOPT and SYMPHONY. 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). SYMPHONY uses process graph methodology based on the work of Friedler and Fan (Friedler et al. 1995) to solve the MINLP problem.

After determining the optimal complex configuration, the pollution index part of the system is called 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. These results are presented to the user for evaluation and stored in the database for subsequent retrieval. The EPA pollution index and potential environmental impact methodology (Cabezas et al. 1997) provides a quantitative way to identify pollutants and their potential impacts from the complex. There are 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.

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 plants located 10 miles (16 km) apart. This two-site, multiple-process expansion was used with the prototype system, and the results compared to the case study for validation of the system. In this complex, phosphate fertilizers are produced by reacting ammonia and phosphoric acid as illustrated in Fig. 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. Sulfuric acid can be shipped for miles and steam cannot; phosphoric acid 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. As long as the two-site sulfuric production capacity is adequate, there is some flexibility in how closely the sulfuric versus 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 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. In addition, the expansion was to be made in two stages, and 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

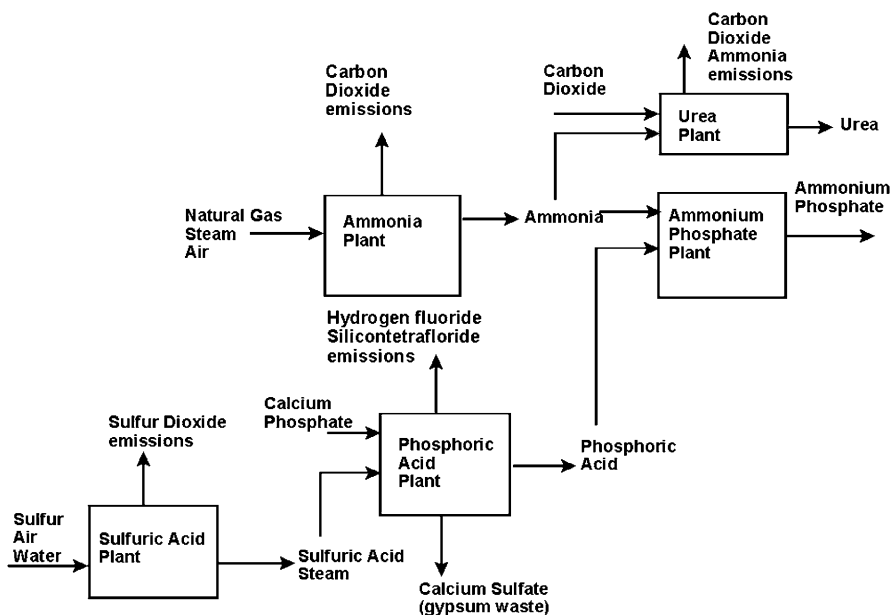


Fig. 2. Schematic diagram of agricultural chemicals complex with raw materials, products, emissions and wastes

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.

Based on the description above, a superstructure was developed that had 67 components [600 psig (4.24 MPa) steam, sulfuric acid, logic switches etc.] and 75 processing units. The detailed description process models and superstructure formulation was given by Hertwig et al. (2000). The superstructure was entered in the prototype, and SYNPHONY was used as the solver. Computing time for any one case was less than 15 s on a Pentium II PC. Results obtained with the system were consistent with the case studies done previously by the company. This served to validate that the system was giving consistent and accurate results. A summary of the evaluations includes 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. Also, 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 at stage two when the conversion cost was significantly less than the cost of a new plant.

Multi-plant, multi-product agricultural chemical complex evaluation

Blau and Kuenker of Dow AgroScience (Blau and Kuenker 1998) reported that delivering nutrients to the various crops rather than focusing on production of fertilizers would lead to the best overall economic, environmental and sustainable development solutions for agricultural chemicals. This statement provides direction for use of the prototype system. The system should help determine the

best way to make key nutrients of N, P and K available to crops where and when most needed.

An agricultural chemical complex based on plants in the Baton Rouge–New Orleans, Mississippi river corridor was developed with information provided by the cooperating companies and other published sources, as shown in Fig. 3. This complex is representative of the current operations and practices in the agricultural chemical industry and was used as the base case and starting point to develop a superstructure by adding plants. These additional plants gave alternative ways to produce intermediates that reduced and consumed wastes and greenhouse gases and conserved energy. These additional plants could provide combinations leading to a complex with lower environmental impacts and greater sustainability. Then this superstructure was evaluated using the economic, environmental and sustainable criteria in the system, and the optimum configuration determined as described below.

As shown in Fig. 3 there are ten production units plus associated utilities for power, steam and cooling water and facilities for waste treatment. A production unit contains more than one plant; and, for example, the sulfuric acid production unit contains five plants owned by two companies. For this base case there were 188 equality constraint equations describing the material and energy balances and chemical conversions. Also, there were 29 inequality constraint equations describing the demand for product, availability of raw materials and range on the capacities of the individual plants in the complex. The complete model of the complex is available in the Chemical Complex Analysis System program and users manual available from the LSU Mineral Processing Research Institute's web site, <http://www.mpri.lsu.edu> (Xu et al. 2001).

The raw materials used in the agricultural chemical complex include air, water, natural gas, sulfur, phosphate rock and potassium chloride as shown on Fig. 3. The products are a typical solid blend of [18% N–18% P_2O_5 –18% K_2O], a liquid blend of [9–9–9], ammonia and methanol. The flow rates shown on the diagram are in

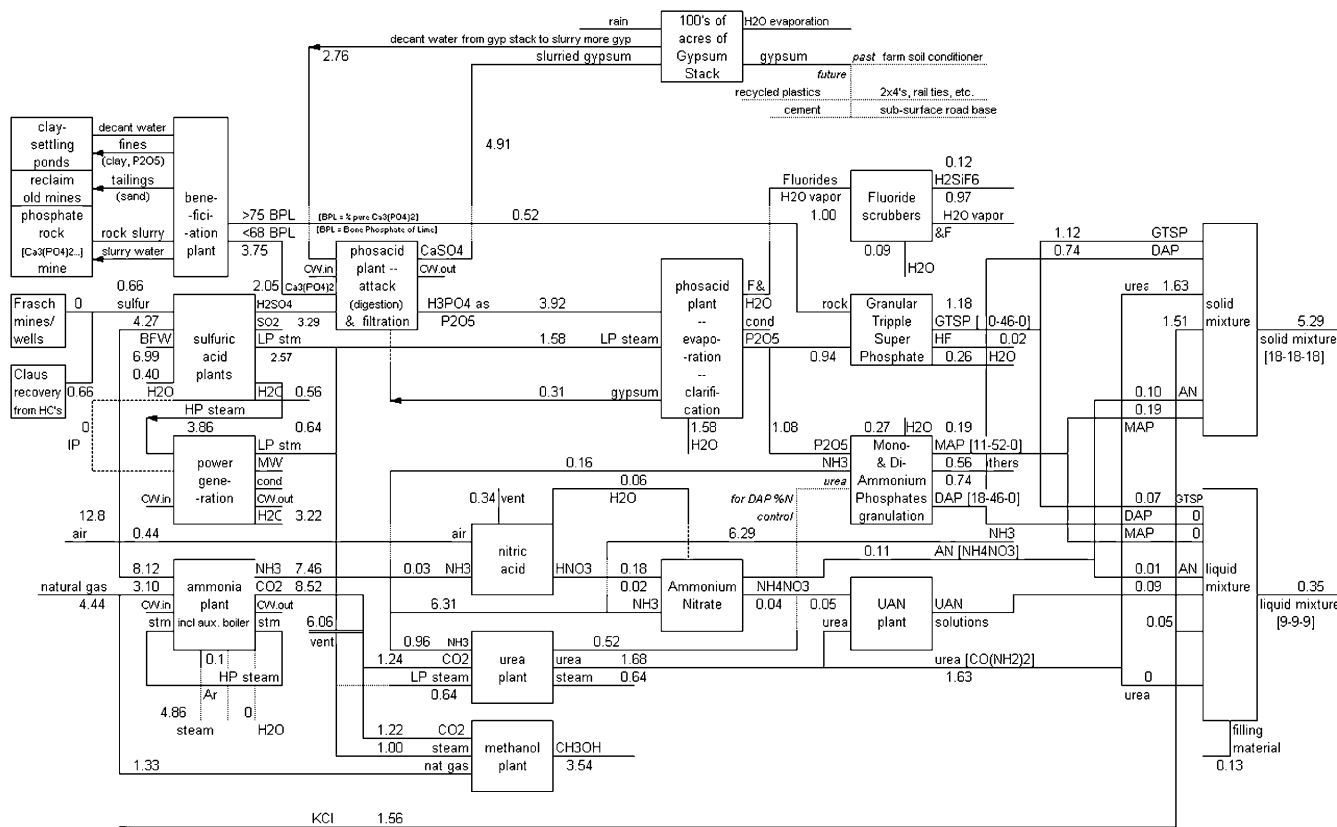


Fig. 3. Agricultural chemical complex based on plants in the Baton Rouge–New Orleans, Mississippi river corridor, base case flow rates million t/year

million tons per year. Intermediates are sulfuric acid, phosphoric acid, ammonia, nitric acid, urea and carbon dioxide. The intermediates are used to produce mono- and di-ammonium phosphate (MAP and DAP), granular triple super phosphate (GTSP), urea, ammonium nitrate, and urea ammonium nitrate solution (UAN). These compounds are used to make blends shown in Fig. 3. Their pre-blending compositions are: MAP [11–52–0], DAP [18–46–0], GTSP [0–46–0], urea (CO(NH₂)₂) [46–0–0], ammonium nitrate [34–0–0], and UAN [~30–0–0]. Also, potassium supplied as potassium chloride for blends is not produced on the Gulf coast but is imported from New Mexico and Utah, among other states. Ammonia is used in direct application to crops and other uses. Methanol is used to produce formaldehyde, methyl esters, amines and solvents, among others, and is included for its use of ammonia plant byproduct carbon dioxide. In actual practice several blends are produced, and they would just add blending constraints to the base case.

Emissions from an agricultural chemical complex include sulfur dioxide, nitrogen oxides, ammonia, methanol, silicon tetrafluoride, hydrogen fluoride and gypsum. According to EPA 1996 TRI (Anon 1998) Louisiana’s four chemicals for on- and off-site releases are phosphoric acid, ammonia, methanol and nitrate compounds in Louisiana. The total on- and off-site releases in the state were 29.7 (13.5), 27.7 (12.6), 25.2 (11.4) and 14.5 (6.6) million pounds (Gg) in 1996. Phosphoric acid plants had 28.3 million pounds (12.8 Gg) of surface water discharges from gypsum waste. Ammonia plants had 21.6 million pounds (9.8 Gg)

of air emissions. Methanol plants had 17.1 million pounds (7.8 Gg) of air emissions and 7.1 million pounds (3.2 Gg) of underground injection. Plants producing nitrate compounds had 8.4 (3.8) and 6.0 (2.7) million pounds (Gg) of surface water and underground injection, respectively.

The agricultural chemical complex shown in Fig. 3 was expanded into a superstructure, and several approaches were incorporated in this expanded complex with alternative ways to produce intermediates that reduce wastes and energy and consume greenhouse gases. There were two alternative plants added to produce phosphoric acid. One was the electric furnace process, which has high energy costs but produces calcium oxide. The other reacts calcium phosphate ore with HCl to produce phosphoric acid with dissolved calcium chloride that is dispersed with the product versus gypsum (calcium sulfate) waste that accumulates adjacent to the phosphoric acid plant. Also, phosphoric acid and sulfuric acid can be purchased from other sources such as smelters. Potassium chloride can be purchased directly from plants using the Trona, IMCC and sylvinitic ore processes and can be purchased from suppliers or dealers. An ammonium sulfate plant was included to provide an additional blending component. An acetic acid plant was included that would use a new/experimental technology for the catalytic reaction of carbon dioxide and methane, consuming two greenhouse gases. Carbon dioxide, beyond amounts required in the methanol plant, was used to produce acetic acid, a new product for the complex. In summary, the superstructure included four options for producing/buying each of phosphoric acid and

Table 1. Raw material and product prices (U.S.\$/t). Source Green Market Sheet (10 July 2000), Internet and AIChE/CWTR TCA Report

Raw materials	Cost (U.S.\$/t)	Raw materials	Cost (U.S.\$/t)	Raw materials	Cost (U.S.\$/t)
Natural gas	40	Market cost for short term purchase		Ammonia	190
Phosphate rock wetprocess	27			Methanol	96
electrofurnace	24	KCl	101	Acetic acid	45
HCl process	25	H ₃ PO ₄	176	Solid blend	160
HCl	50	H ₂ SO ₄	86	Liquid blend	60
Sulfur				HP steam	10
Frasch	42	Sustainability credits and costs (U.S.\$/t)		IP steam	64
Claus	38	Credit for CO ₂ consumption			6.50
Brine KCl ore	2				
Searles Lake KCl ore	15	Debit for CO ₂ production			3.25
Sylvinite KCl ore	45				

potassium chloride, two options for sulfuric acid, and new plants to produce ammonium sulfate and acetic acid. The block flow diagram and associated equations for the superstructure are given by Xu et al. (2001) in the program and users manual. The superstructure had 265 continuous variables, 10 integer variables, 232 equality constraint equations for material and energy balances and 37 inequality constraints for availability of raw materials, demand for product and capacities of the plants in the complex.

A value added economic model was used for the base case, and it is the difference between sales and the cost of raw materials and assumes other manufacturing costs are constant. The sales prices for products and costs of raw materials are given in Table 1. For the superstructure, the economic model was expanded to account for environmental and sustainability costs. Environmental costs were estimated as 67% of the raw material costs, which is based on the data provided by Amoco, DuPont and Novartis in the AIChE/CRWRT report (Constable et al. 2000). This report lists environmental costs as approximately 20% of the total manufacturing costs and raw material costs as approximately 30% of total manufacturing costs. Sustainable costs were estimated from results given for power generation in the AIChE/CWTR report where carbon dioxide emissions had a sustainable cost of U.S.\$3.25 per ton of carbon dioxide. A cost of U.S.\$3.25 per ton was charged as a cost to plants that emit carbon dioxide, and plants that consume carbon dioxide were given a credit of twice this cost or U.S.\$6.50 per ton. This credit was included for steam produced from waste heat by the sulfuric acid plant displacing steam produced from a package boiler firing hydrocarbons and emitting carbon dioxide.

The prototype was used to obtain the optimum configuration of plants from the superstructure. The complete solution is given by Xu et al. (2001), and a comparison of the base case and the optimal solution from the superstructure is summarized in Table 2. A comparison of the base case and the optimal solution from the superstructure is summarized in Table 2. The profit increased about 7.8% from the base case to the optimal solution. Also, as shown in the table, environmental cost declined about 17%, and sustainable costs increased about 1.5%. Also, the sulfuric

acid production rate increased, providing power in place of electricity from package boilers. Production rates for the products in the optimal solution were constrained at their upper limit, which was set at the base case values. In addition, it was optimal to obtain KCl from the Trona process. The acetic acid plant was operating at the upper limit, but it was not optimal to operate the ammonium sulfate plant. The carbon dioxide consumption credits and the new acetic acid plant were sufficient to outweigh the environmental costs. If the acetic acid plant was not included in the computation of the profit in the optimal solution, the profit increased only 7.7% over the base case. These results illustrated the capability of the system to select an optimum configuration of plants in an agricultural chemical complex and incorporate economic, environmental and sustainable costs.

A brief sensitivity study was performed to test the capability of the system. Four cases involved changing the cost of raw materials and sales price of products as shown in Table 3 where Case 1 is the optimal structure shown in Table 2. For Case 2, the cost of brine to the Trona process was increased by 90%, and the Trona process was replaced by the IMCC process in the optimal solution. The Trona process consumes sulfuric acid, and the IMCC process does not. Consequently, Case 2 sulfuric acid production rate was smaller than that of Case 1, and the profit was about 6% less. For Case 3, the cost of sylvinite was decreased by 52%, and the Trona process used in Case 1 was replaced by the Sylvinite process. The sulfuric acid production rate in Case 3 was smaller than Case 1 because the Sylvinite plant does not consume sulfuric acid, and the profit was essentially the same as Case 1. In Case 4, the cost of phosphate rock was decreased by 50%, and the cost of HCl was decreased 80% for the plant using HCl to produce phosphorous acid. As expected with these unrealistic reductions, the HCl plant replaced the wet-process plant to produce phosphorous acid, and the sulfuric acid production rate was 98% less. However, the profit was essentially the same as Case 1. In Case 5 the cost of phosphate rock (<68 bone phosphate of lime, BPL) was increased by an unrealistic 360%, and there was a decrease in all related products. Also, the profit declined 21%. In summary, this sensitivity study gave predictable results and demonstrated additional capabilities of the system.

Conclusions

A prototype of a chemical complex analysis system has been described, and its capability was 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. A second application of the prototype was based on an agricultural chemical complex with ten multiple plant production units in the Baton Rouge–New Orleans, Mississippi river corridor. The optimal configuration of plants was determined based on economic, environmental and sustainable costs. A comparison of the current configuration of units with the optimal one was made and sensitivity to cost and prices was analyzed. The profit increased about 7.8% from the base case to the optimal solution. Also, environmental cost declined about 17%, and sustainability costs increased about 1.5%. These results illustrated the capability of the system to select an optimum configuration of plants in an agricultural chemical complex and incorporate economic, environmental and sustainable costs. A brief sensitivity study gave predictable results and demonstrated additional capabilities of the system.

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