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# OPTIMAL CONFIGURATION OF CHEMICAL COMPLEXES BASED ON ECONOMIC, ENVIRONMENTAL AND SUSTAINABLE COSTS

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## Abstract

A prototype of a chemical complex analysis system has been developed and used to demonstrate optimization of a chemical complex incorporating economic, environmental and sustainable costs and solving a MINLP for the optimal configuration of plants. It was applied to an agricultural chemical complex in the Baton Rouge- New Orleans Mississippi river corridor with ten multiple plant production units. A comparison of current configuration with the optimal one was made, and sensitivity to cost and prices was analyzed. Profit declined about 10% when environmental and sustainability costs were included, and carbon dioxide consumption credit was not sufficient to outweigh these costs. These results illustrated the capability of the system to select an optimum configuration of plants and incorporate economic, environmental and sustainable costs.

## 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), pollution prevention was an environmental issue and is now a critical business opportunity. 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). 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 TCA and found that the cost of environmental compliance was three to five times higher than the original estimates (Constable, et. al., 2000). TCA 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 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 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. 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 sustainability metrics by an industry group through the AIChE/CWRT, 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 air pollution from electricity generation, e.g. \$0.22-2.38 per ton for CO, 0-\$3.25 per ton for $CO_2$.

## 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, societal and business benefits that will help ameliorate command and control regulations.

The system is being developed in collaboration with engineering groups at several companies 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-environmental design. Also, the programs SYNPHONY (Friedler, Varga and Fan, 1995) and GAMS/DICOPT (Kocis and Grossmann, 1989) 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).

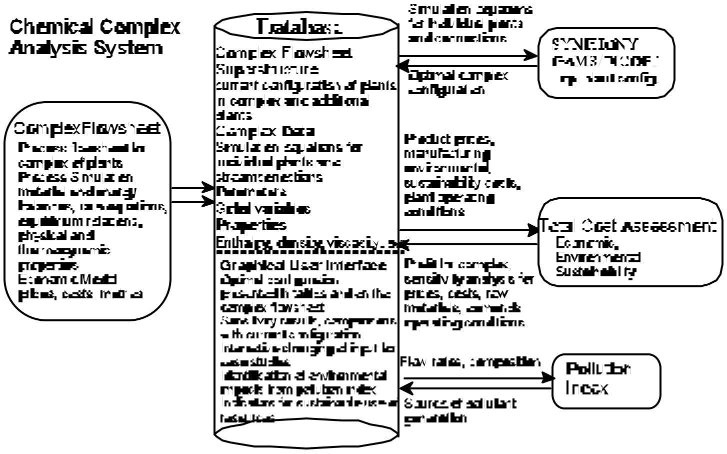

*Figure 1 Program Structure for the Chemical Complex Analysis System*

The Chemical Complex Analysis System incorporates a flowsheeting component where simulations of the plants in the complex are entered. Each simulation includes material and energy balances, rate equations, equilibrium relations and thermodynamic and transport properties These equations 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 plant with information for prices, costs, and sustainablity metrics that are used in the evaluation of the TCA 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 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 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. 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 TCA report. Sustainable costs are estimated from the air pollution data in the AIChE/CWRT TCA report. Improving the estimates is an on-going effort.

## 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 will 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 was assembled from production units with one or more plants in the Baton Rouge - New Orleans, Mississippi river corridor with information provided by the cooperating companies and other published sources, as shown in Figure 2. This complex is representative of the current operations and practices in the agricultural chemical industry. It was used as the base case and starting point to develop a superstructure using additional plants to give alternate 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. 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 Figure 2 there are 10 production units in the agricultural chemical complex plus associated utilities for power, steam and cooling water in the base case. Flow rates shown on the diagram are in million tons per year. 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. 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.

The raw materials include air, water, natural gas, sulfur, phosphate rock and potassium chloride. 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 Figure 2. Their pre-blending compositions are: MAP [11-52-0], DAP [18-46-

0], GTSP [0-46-0], urea ($CO(NH_2)_2$) [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 and is imported from New Mexico and Utah, among other states.

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) the largest on- and off-site releases were from the manufacture of phosphoric acid, ammonia, methanol and nitrate compounds in Louisiana. Phosphoric acid plants had 28.3 million pounds of surface water discharges from gypsum waste. Ammonia plants had 21.6 pounds of air emissions. Methanol plants had 17.1 million pounds of air emissions and 7.1 million pounds of underground injection. Plants producing nitrate compounds had 8.4 and 6.0 million pounds of surface water and underground injection, respectively. Also, some of these plants are major energy consumers, e.g., ammonia and phosphoric acid, and others produce energy, e.g., sulfuric acid.

The agricultural chemical complex shown in Figure 2 was expanded into a superstructure with alternate ways to produce intermediates that reduced and consumed wastes and greenhouse gases and conserved energy. Two alternate plants were included to produce phosphoric acid. One was the electric furnace process which which has high energy costs but produces calcium oxide. The other digested with HCl to produce calcium chloride that is dispersed with the product vs. gypsum (calcium sulfate) waste that accumulates adjacent to wet process phosphoric acid plants. Also, phosphoric acid and sulfuric acid could be purchased from other sources such as smelters. Potassium chloride could be purchased directly from plants using the Trona, IMCC and sylvinite ore processes and could 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 potassium chloride, two options for sulfuric acid, and new plants to produce ammonium sulfate and acetic acid.

Value added or profit margin was used as the economic model for the base case. Value added 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, 1999). 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

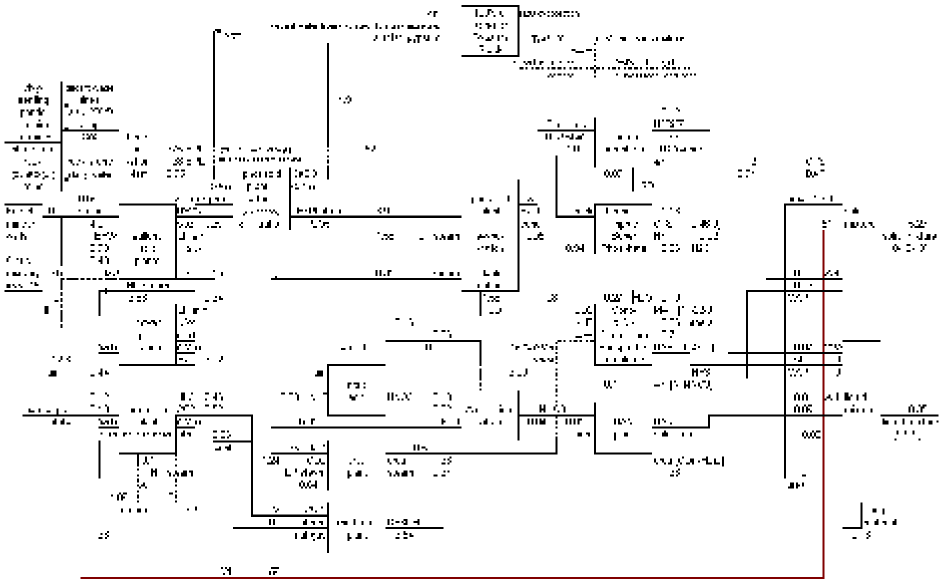

Figure 2 Agricultural Chemical Complex Based on Plants in the Baton Rouge- New Orleans Mississippi River Corridor, Base Case, Flow Rates are TPY

Table 1 Raw Material and Product Prices
Source Green Market Sheet (July 10, 2000), Internet and AIChE/CWTR TCA Report

| Raw Materials | Cost ( $/T) | Raw Materials | Cost ( $/T) | Products | Price($/T) |
|---|---|---|---|---|---|
| Natural Gas | 40 | Market cost | | Ammonia | 190 |
| Phosphate Rock | | for short term | | Methanol | 96 |
| wet process | 27 | purchase | | Acetic Acid | 45 |
| electrofurnace | 24 | KCl | 101 | Solid Blend | 160 |
| HCl process | 25 | H3PO4 | 176 | Liquid Blend | 60 |
| HCl | 50 | H2SO4 | 86 | HP Steam | 10 |
| Sulfur | | | | IP Steam | 6.4 |
| Frasch | 42 | | | | |
| Claus | 38 | Credit for $CO_2$ | | 6.50 | |
| Brine KCl ore | 2 | Consumption | | | |
| Searles Lake KCl ore | 15 | Debit for $CO_2$ | 3.25 | | |
| Sylvinite KCl ore | 45 | Production | | | |

in the AIChE/CWRT report where carbon dioxide emissions had a sustainability cost of $3.25 per ton of carbon dioxide. A cost of $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 $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 comparison of the base case and the optimal solution from the superstructure is summarized in Table 2. The base case profit only includes economic costs, and economic, environmental and sustainability costs were used with the superstructure to evaluated the optimal configuration of production units. The profit was about 10% for the optimal solution because the carbon dioxide consumption credit and the new acetic acid plant were not sufficient to outweigh environmental and sustainability costs. Also, sulfuric acid production rate increased, mostly for stream credits. 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. If the acetic acid plant was not included in the computation of the profit in the optimal solution, the profit was an additional 7.0% less than the base case. These results illustrate 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 cursory 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. First, the cost of brine to Trona process was increased by 90%, and the Trona process was replaced with IMCC process in the optimal solution. The Trona process consumes sulfuric acid, and the IMCC process does not. Consequently, sulfuric acid production rate was smaller than that of the original optimal structure, and the profit was about 6% less. Second, the cost of

| | | Base Case | Optimal Structure |
|---|---|---|---|
| Profit (million $/yr) | | 1,960 | 1,820 |
| | Capacity (tons/yr) | Capacity (tons/yr) | Capacity (tons/yr) |
| Plant Name | (upper-lower bounds) | | |
| Ammonia | 10,000-74,57100 | 7,457,100 | 7,457,100 |
| Nitric Acid | 100,000-1,067,000 | 100,000 | 100,000 |
| Ammonium Nitrate | 10,000-909,410 | 127,040 | 127,040 |
| Urea | 10,000-3,032,000 | 1,694,300 | 1,694,300 |
| Methanol | 10,000-3,546,200 | 3,546,200 | 3,546,200 |
| UAN | 10,000-2,061,300 | 90,633 | 90,633 |
| MAP | 10,000-189,300 | 189,300 | 189,300 |
| DAP | 10,000-737,790 | 737,790 | 737,790 |
| GTSP | 10,000-1,186,000 | 1,186,000 | 1,186,000 |
| Sulfuric Acid | 0-12,238 | 661,270 | 661,270 |
| Phosphate Rock (>75 BPL) | 0-4,518,000 | 2,547,500 | 2,547,500 |
| Phosphate Rock(<68 BPL) | 0-4,575,400 | 3,064,700 | 3,064,700 |
| Wet Process Phosphoric Acid | 0-4,012,400 | 918,980 | 918,980 |
| Phosphoric Acid (Electric Furnace) | 0-3,497,000 | na | 0 |
| Phosphoric Acid from HCl | 0-3,497,000 | na | 0 |
| Ammonium Sulfate | 0-2,839,000 | na | 0 |
| Acetic Acid | 0-90,000 | na | 90,000 |
| Trona KCl | 0-578,610,000 | na | 39,706,000 |
| IMCC KCl | 0-1,4251,000 | na | 0 |
| Sylvinite Ore KCl | 0-5,312,000 | na | 0 |
| Purchased H3PO4 | 0-127,640,000 | na | 0 |
| Purchased KCl | 0-5,600,000 | 1,556,500 | 0 |
| Purchased H2SO4 | 0-12,238,000 | na | 0 |
| Solid Product Blend | 50,000 lower bound | 5,288,600 | 5,288,600 |
| Liquid Product Blend | 50,000 lower bound | 349,310 | 349,310 |
| | | | |

Table 2 Comparison of Base Case and Optimal Structure

sylvinite was decreased by 52%, and the Trona process used in original optimal structure was replaced with Sylvinite process. The sulfuric acid production rate was smaller because the Sylvinite plant does not consume sulfuric acid, and the profit was essentially the same.. Third, 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 the original optimal structure. Fourth, the cost of phosphate rock (<68BPL) 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 applying the prototype to 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. Profit declined about 10% by including environmental and sustainability costs, and carbon dioxide consumption credit was not sufficient to outweigh these costs. 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 cursory sensitivity study gave predictable results and demonstrated additional capabilities of the system.

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