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An Advanced System for Optimizing the Design of a Chemical-Production Complex

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Le prototype d'un système avancé d'optimisation de complexes de production chimique a été exposé fournissant des configurations optimum pour deux stades d'expansion dans un complexe simulé de produits chimiques agricoles. Le système augmente au maximum le retour sur investissements car il faut choisir le meilleur site pour des capacités nécessaires de production nouvelle d'acide phosphorique et d'acide sulfurique et les dimensions des installations optionnelles de récupération de chaleur et de génération d'énergie. Le système sera disponible gratuitement par Internet.

Abstract

A prototype of an Advanced System for optimizing the design of chemical-production complexes has been demonstrated, giving optimum configurations for two stages of expansion in a simulated agricultural-chemical complex. The System maximizes return on investment as it selects the best site for required new phosphoric and sulfuric acids production capacities and the sizes for the optional heat-recovery and power-generation facilities. The System will be available free of charge via the Internet.

Introduction

Synthesis and improvement of multi-plant chemical complexes can be very challenging and requires a balance of safety, reliability, economics, quality, and an acceptable impact on the environment and society. Modeling plays a key role in defining many parts of that balance – selection of products, plant types, and plant's unit operations. Optimization quantitatively incorporates environmental effects (life cycle, sustainability, contingent cost analysis) as well as the more-traditional economic effects (costs, yield, long-term cost of ownership).

A significant driving force for a broader assessment of current and future manufacturing in the chemical industry is the anticipated next round of Federal regulations associated with global warming, ISO 14000, "the polluter pays" principle, and sustainable development. Companies will want to move from struggling to comply with environmental regulations to proactive pollution prevention. This means shifting company thinking, making institutional changes, and educating environmental critics about business decisions (1). End-of-pipe treatments forced by Federal regulations have reduced pollution significantly, but further reductions will be increasingly difficult to make. Further reductions will require a broader assessment of entire chemical complexes.

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At this time, there is no integrated set of tools, methodologies or programs to perform a consistent and accurate evaluation of new and existing complexes. Only recently can we consider the best configuration for processes based solely on raw materials available and desired products, a combinatorial problem of immense proportions. Combining an economic, environmental and sustainability measure of effectiveness with the new methodology for the best configuration of plants is now feasible. The analyses and components exist. This paper describes a prototype that combines components into an integrated system for use by plant and design engineers who have to convert their company's goals and capital into viable projects that are profitable and meet environmental and sustainability requirements.

A methodology has been developed by Friedler and Fan (2) to obtain the optimal configuration of chemical complexes with multiple plants using Process Graph theory. This has been incorporated in the computer program Synphony, and it is now feasible to determine the best configuration of a chemical complex containing a large number of plants. For example, with a chemical complex containing 35 different process units, there are 34 billion combinations of process structures, of which only a minute fraction is feasible to generate the required products from the available raw materials. This program determines the feasible plant configurations and then selects the one process configuration that is the best combination of process units that minimizes costs, wastes, and emissions, and that provides the best energy utilization. A superstructure for the complex is specified with feed and product components and flow rates defined. The optimal complex configuration is determined by the program based on an economic model along with intermediate flows.

Optimizer Development

Synphony looked like logical software to test for design optimization of the many interconnections in a chemical-production complex. Synphony works well for what it does, but it cannot optimize variable or operating relationships like fuel-to-air ratio. When this limitation was recognized, Synphony's developers were asked if a work-around could be developed. Meanwhile, the test demonstration was modified to the case studies presented below.

Alternate Optimizers to Consider

GAM (General Algebraic Modeling System) was developed at the World Bank for very large economic models. It can be used to determine the optimal configuration of chemical complexes by solving a mixed integer nonlinear programming problem using the DICOPT++ solver. There is no guarantee of finding a global optimum with GAMS/DICOPT++, only a local optimum. Results for plant optimal configuration are reported by Kocis and Grossmann (3).

Optimizer as a Component of the Advanced System for Chemical Complex Optimization

Another consideration in selecting optimizers is software cost, since one requirement of the system is that it can be distributed free of charge. A limited version of GAMS meets this requirement. Though the commercial version of Synphony is not free, this demonstration should be of mutual benefit and may impact pricing of a custom version for the system.

Synphony's Limitations

Synphony is based on graph theory, and it can find the global optimum but is limited in its ability to include material and energy balances (linear and nonlinear constraints). For a given piece of process equipment, the only process conditions Synphony can change are the flows. All flows are scaled up and down together to make material balances "balance". There is currently no provision to make flow relationships like "fuel-to-air ratio" to change with process conditions. The user can offer Synphony another set of conditions only by adding a parallel copy of the equipment that is run at the new conditions. The user must then specify in Synphony that only one of the two copies of the equipment be used.

At every step through the process, Synphony calculates forward, requiring sufficient feeds. Optimization minimizes excesses, but excesses are not otherwise prohibited. With these "forward calculations", the user must design artificial feedback streams to get Synphony to respond to lower limits on feeds or upper limits on products. Also, excesses are not flagged without special effort by the user.

Synphony normally displays just one optimum, even when there are several equivalent optima. When there are several equivalent optima, the optimum displayed may be different on different runs. Display of equivalent and secondary choices is possible and probably needs to be made available to the user.

Synphony divides capital costs by a user-specified payback period to combine capital and operating costs. Though Synphony's financial analysis is simple and is useful for selecting best paths, a formal analysis of the best few options is still needed before committing capital.

These limitations are presented only to display the challenges inherent in software development. This paper is more the story of an ongoing development than the description of a commercial product.

Description of Fertilizer Complex to be Modeled

The objective chosen for this first Synphony demonstration was to select the best way for hypothetical XYZ Phosphate Fertilizer Company to expand production. Phosphate fertilizers are produced by ammoniating phosphoric acid. 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, including for power generation, and to evaporate water from phosphoric acid.

Assuming excess ammoniation capacity is available, the objective is 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 evaporators require some steam capacity from a 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.

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 barge all the acid to the other site to make phosphoric acid.

To add more options to challenge Synphony, the expansion is 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 expansion with an option for over-sizing the first to serve as the second. A second sulfuric expansion does not have to be sited away from the first expansion.
- An option for adding heat recovery equipment to one old and any new sulfuric plants.
- An option for adding one turbo-generator per site per stage.

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

Synphony Model Description

In Figure 1 a schematic is shown of how multiple sulfuric acid units were made available for selection by Synphony. The Synphony model for this demonstration had 67 different species (600# steam, sulfuric acid, logic switches, etc.) and 75 processing units. A sulfuric plant was one unit using 8-10 species. Figure 2 shows how a new turbo-generator took 7 units and 10 species to model. Two of those species were fabricated to properly couple the 7 units to work as one. Figure 3 shows sample Synphony input and output tables. Computing time for any one case was less than 15 seconds on a Pentium II PC.

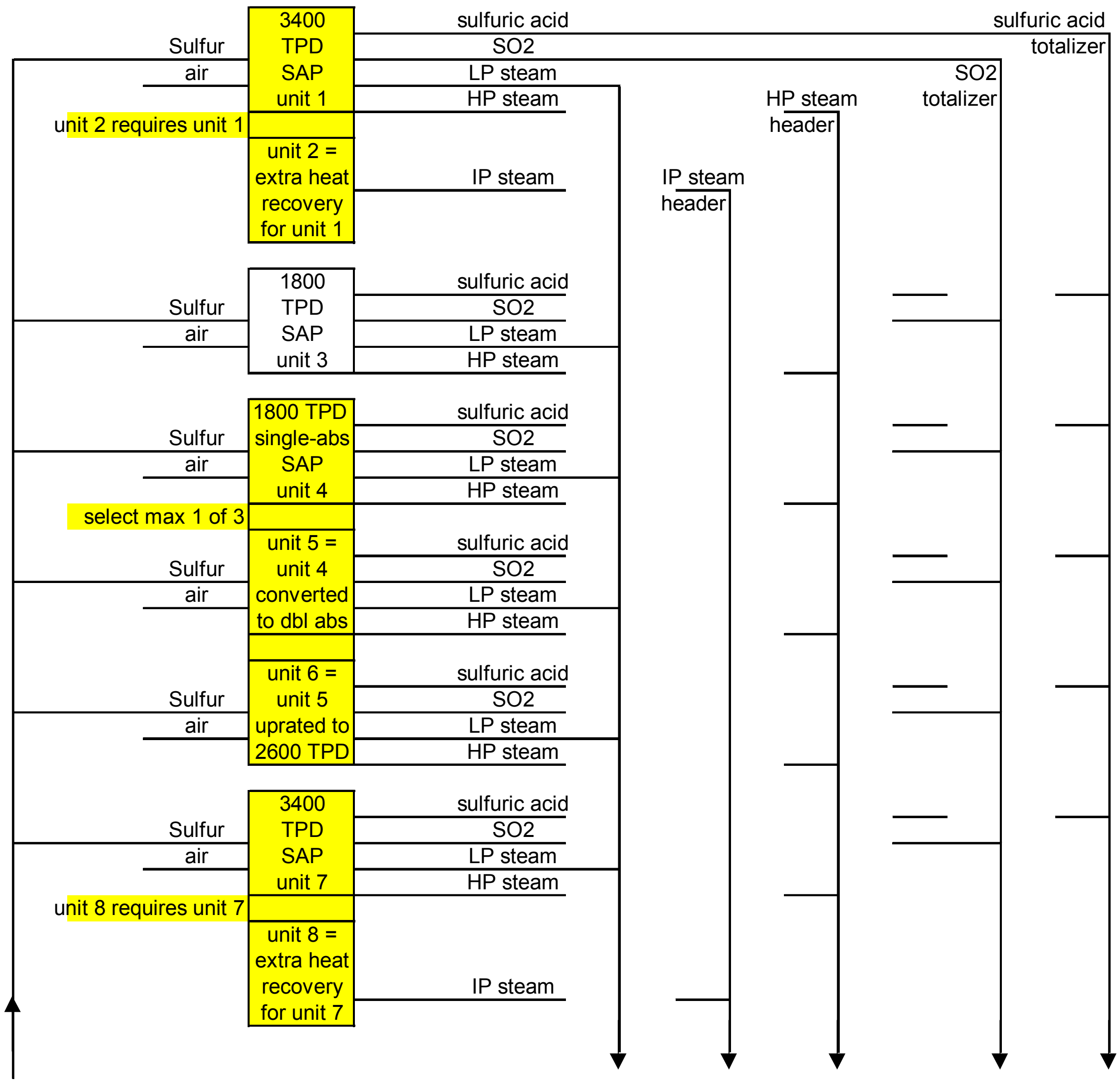
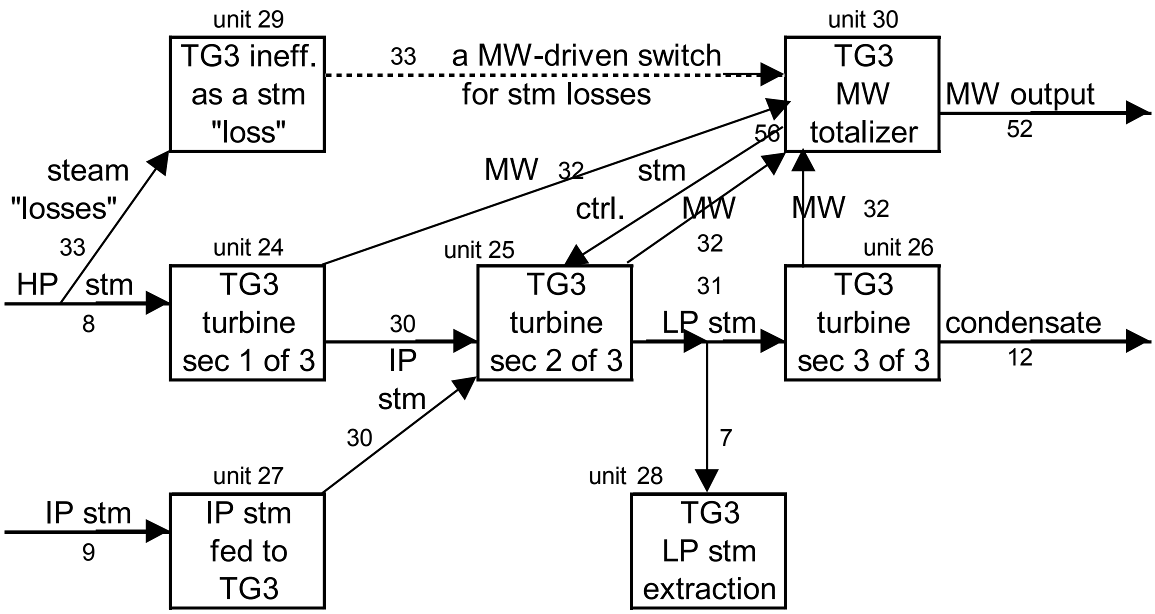


Figure 1. Schematic for the Synphony's Sulfuric Acid Plant options at 1 of 2 plant sites



The new Turbo-Generators were specified with dual-feed, single-extraction condensing turbines.
The TG uses 7 "units" represented here as squares.
The TG uses 10 "streams":

stream no.	
8	High Pressure steam supply to TG
33	a MW stitch to stop HP steam losses if no MW are being produced
9	Intermediate Pressure steam supply to TG
30	IP steam between TG's units
31	Low Pressure steam between TG's units
7	LP steam exported
12	condensate
32	MegaWatt subtotals to TG's totalizer
52	MW total for this TG
56	an IP steam flow controller to keep MW within the generator's capacity

Figure 2. Synphony representation of a Turbo-Generator

documentation	Synphony input	Synphony output	explanation
max no. of units presented	75	Input file: SynphIn.pns	
no. of materials presented	67	Size of the Maximal Structure:74	
no. years & days operated per yr	4 328 // payout, workday in one year	Number of Units: 75	
no. of products	8	The number of solved LP: 372	
	22(1598000) 26(0.1) 60(0.1) 61(0.1) 62(0.1)		
1-year prod'n req'ts; xs is allowed	63(0.1) 64(0.1) 65(0.1) 66(0.1) 67(0.1) // products		
		The optimum and the optimal	
no. of priced raw mat'ls	7	solution: z=929644.23287064	
	1(100,INF) 2(0,INF) 3(0.3,INF) 4(25,INF) 5(4,INF)		
raw mat'ls ($/unit, max units)	6(1,INF) 51(0,1) // raw materials		
site 1 SAP 1	1 UNIT**	1: 3.4,	site 1 SAP 1 @ full rate
MTPD min/max	3.4 3.4	3: 1.8,	site 1 SAP 2 @ full rate
$capital: intercept & slope	0 0	4: 1.05968,	site 1 SAP 3 @ 59% rate
$operating: i'cept/yr & slope/unit	0 2000	7: 0.9,	site 1 new SAP @ min rate
no. inputs	3	8: 2.3,	site 2 SAP 1 @ full rate
mat'l (flow)	1(327.86) 2(490.8) 3(47.7) 6(341.5)	9: 2.3,	site 2 SAP 2 @ full rate
no. outputs	5	10: 1.4530,	site 2 new SAP @ 1453 TPD
mat'l (flow)	10(1000) 11(2) 19(2) 7(54.95) 8(54.95) 48(1)	11: 1.4530,	add HRS to site 2 new SAP
SAP 1's extra heat recovery	2 UNIT**	14: 0.1343956993,	
IP steam Mlb/hr	0 10	15: 0.1343956993,	
	6000000 0	17: 15,	
	0 0	18: 14,	site 1 TG1 @ max MW
	1	19: 0.1847088167,	
	48(1)	20: 0.0941417278,	
	1	21: 0.09056708888,	
	9(44.12)	22: 15,	
site 1 SAP 2	3 UNIT**	23: 14,	site 1 TG2 @ max MW
MTPD min/max	1.8 1.8	38: 0.3176148864,	
	0 0	39: 0.3817232229,	
	0 2000	40: 0.3051544923,	
	4	41: 0.06410833645,	
	1(327.86) 2(490.8) 3(47.7) 6(341.5)	42: 0.07656873063,	
	4	43: 15,	
	10(1000.0) 11(2) 7(54.95) 8(54.95)	44: 33.42139436,	site 2 new TG @ 33 MW
site 1 SAP 3 as single-absorption	4 UNIT**	52: 1.32,	site 1 PAP 1 rate
MTPD min/max	0.9 1.8	53: 1.32,	site 1 PAP 2 rate
	0 0	56: 1.635,	site 2 PAP 1 rate
	0 2000	57: 0.5969512195,	site 2 PAP expansion
	6	59: 2.64,	
	1(333.36) 2(496.3) 3(47.7) 6(341.5) 51(0.55) 67(1)	60: 2.23195122,	
	4	61: 6.910200562E-006,	
	10(1000) 11(13) 7(54.95) 8(54.95)	62: 61.42139436,	
site 1 SAP 3 as double-absorption	5 UNIT**	67: 3.048780488E-007,	
MTPD min/max	1.8 1.8	68: 3.048780488E-007,	
	16000000 0	69: 3.048780488E-007,	
	0 2000	71: 3.048780488E-007,	
	5	72: 3.048780488E-007,	
	1(333.36) 2(496.3) 3(47.7) 6(341.5) 51(0.55)	74: 1.8,	
	4	75: 1.05968,	
	10(1000) 11(2) 7(54.95) 8(54.95)	Time: 10.110000	CPU time, seconds
etc.	etc.		

Figure 3: Sample Synphony input and output tables.

Optimizer Results

Without a precise, real-world base case, this study was run more to demonstrate sensitivities than to claim any one optimum. Specifications and costs were varied to demonstrate the following sensitivities:

- By raising the cost of barging 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 barging could be made to limit sulfuric barging 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 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.

- Sufficient changes to the capital or operating costs of new plants at the different sites did change the siting of each new plant – sulfuric or phosphoric acid. (This sensitivity was the basis for specifying that the two phosphoric acid expansions be at different sites. There is a big cost advantage in using up excess capacities available in other parts of each site needed to support phosacid production.) A site difference in incremental labor requirements to operate an incremental sulfuric plant could be made to tip the balance in siting when other factors were relatively balanced.

- 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. Installation costs varied because the one anticipated heat-recovery retrofit was cheaper than in a new plant and an unanticipated retrofit was more expensive than in a new plant. The value of power varied because incremental power displaced purchase at one site and added to sales at the other site. In Louisiana and until recently, power sales were worth “30%” less than displaced power purchase.

Conclusions

A prototype of an Advanced System for optimizing the design of chemical-production complexes has been demonstrated on a simulated fertilizer-production complex. The Synphony-based 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. The System will be available free of charge via the Internet.

Acknowledgement

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