Optimal Configuration of Chemical Complexes Based on Economic, Environmental and Sustainable Costs

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Introduction

Background and motivation

Describe the prototype of the system

Describe two applications

Conclusions

Background

Pollution prevention
- was an environmental issue
- now a critical business opportunity

Long term cost of ownership must be evaluated with short term cash flows

Companies undergoing difficult institutional transformations
emphasis on pollution prevention has broadened to include
- Total (full) cost accounting
- Life cycle assessment
- Sustainable development
- Eco-efficiency (*eco*nomic and *eco*logical)

Broader Assessment of Current and Future Manufacturing in the Chemical Industry

Driving forces
- ISO 14000,
- “the polluter pays principle”
- Anticipated next round of Federal regulations associated with global warming
- Sustainable development

Sustainable development
- Concept that development should meet the needs of the present without sacrificing the ability of the future to meet its needs

Sustainable development costs - external costs
- Costs that are not paid directly
- Those borne by society
- Includes deterioration of the environment by pollution within compliance regulations.

Koyoto Protocol - annual limits on greenhouse gases proposed beginning in 2008 - 7% below 1990 levels for U.S.

Cantor Fitzgerald Environmental Brokerage Services web site for greenhouse gas emissions trading www.cantor.com/ebs/

Status of TCA , LCA and Sustainability Metrics

Some of these tools exist and some are being developed

Standard methodologies and measurements have not developed as rapidly in the past twenty years as has the opportunity to apply them

Source:Kohlbrand, H. K., 1998, "From Waste Treatment to Pollution Prevention and Beyond - Opportunities for the Next 20 Years," *Proceedings of Foundations of Computer Aided Process Operations Conference*, Snowbird, Utah, July 5-10, 1998.

Total Cost Assessment

Identifies the real costs associated with a product or process

Includes direct, indirect, associated and societal costs

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.

AIChE Center for Waste Reduction Technology (CWRT) recently completed a detailed report with an Excel spreadsheet on Total Cost Assessment Methodology

Life Cycle Assessment

A “cradle to grave” approach.

AIChE/CWRT TCA methodology

- Capability to evaluate the full life cycle
- Considers environmental and health implications from raw material extraction to end-of-life of the process or product

Sustainability Metrics

Ratios

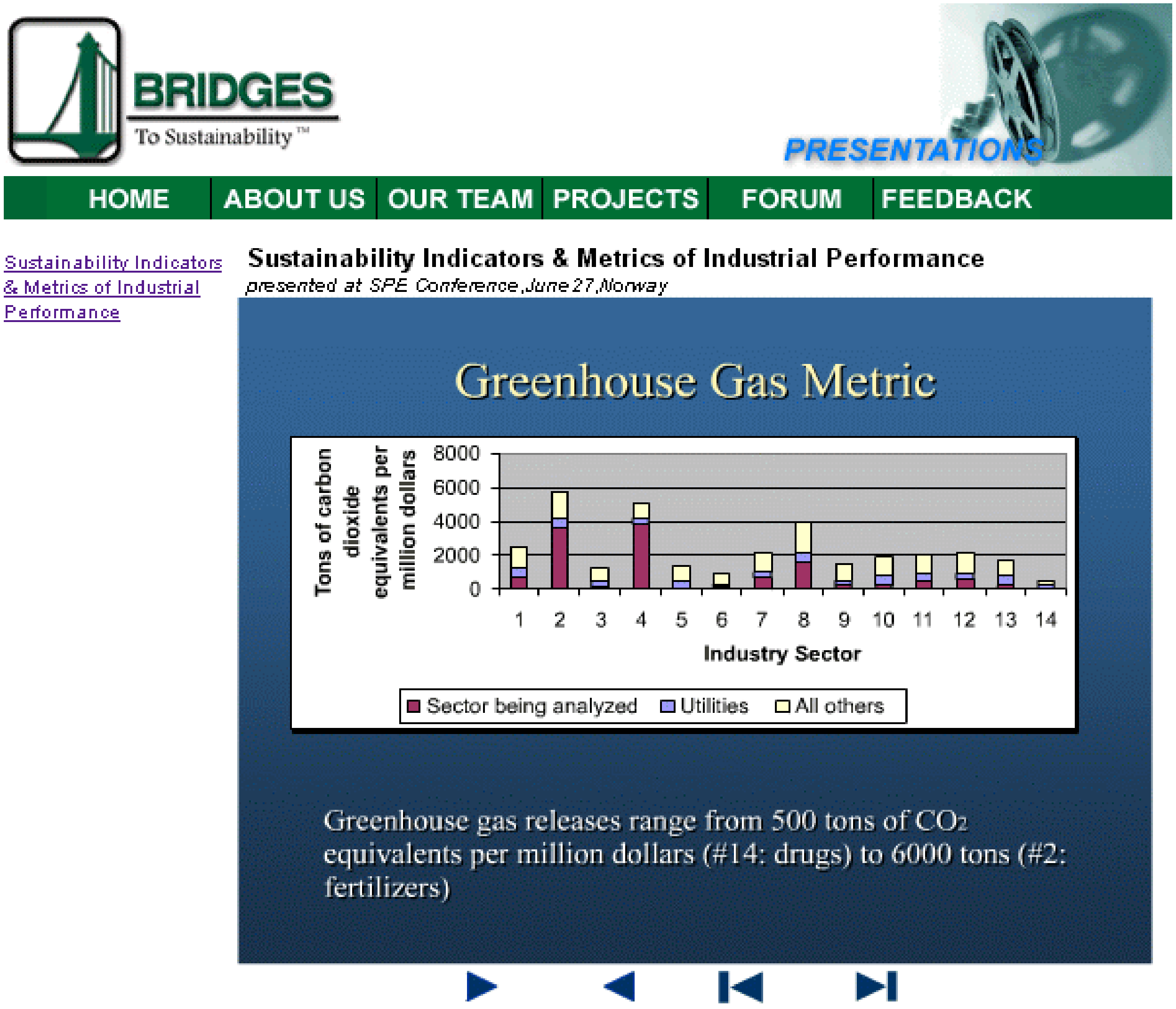
- Numerators are materials, energy, pollution dispersion and toxics dispersion
- Denominators are revinue, mass and value added for a product

Sustainable Metrics Project of the CWTR/AIChE

- Representatives from twelve major chemical companies
- Issued two interim reports
- Held a workshop

AIChE/CRWRT TCA Report includes sustainable costs estimated from a study of power generation

BRIDGES to Sustainability www.bridgestos.org



Sustainability Indicators & Metrics of Industrial Performance

Sustainability Indicators & Metrics of Industrial Performance

presented at SPE Conference,June 27,Norway

Greenhouse Gas Metric

Greenhouse gas releases range from 500 tons of CO_2 equivalents per million dollars (#14: drugs) to 6000 tons (#2: fertilizers)

Prototype System for Optimization of a Chemical Complex

Integrated system
- Economic, environmental and sustainability costs
- Best configuration of plants

Use by plant and design engineers
- Meet environmental and sustainability requirements
- Evaluations for impacts associated with green house gases, finite resources, etc.

Collaboration with engineering groups
- Monsanto Enviro Chem
- Motiva Enterprises
- IMC Agrico
- Kaiser Aluminum and Chemicals
- Meets the needs of industry

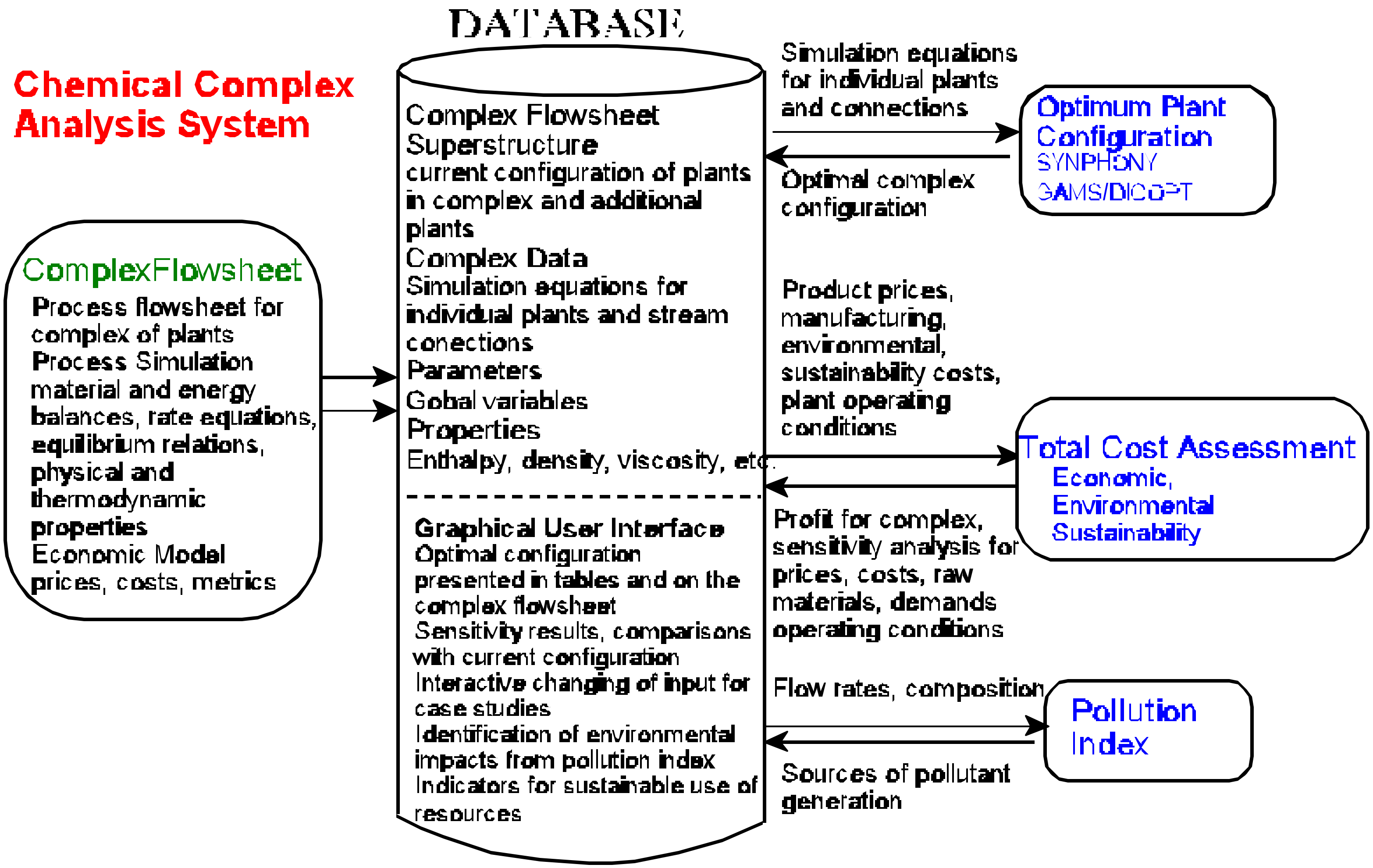


Figure 1 Program Structure for the Chemical Complex Analysis System

Chemical Complex Analysis System

Flowsheet
- Processes can be drawn using a graphics program.
- Equations, parameters and properties entered through windows for each plant.

AIChE/CWRT Total Cost Assessment Methodology
- Criteria for the best economic-environmental design
- Prices, costs, sustainablity metrics

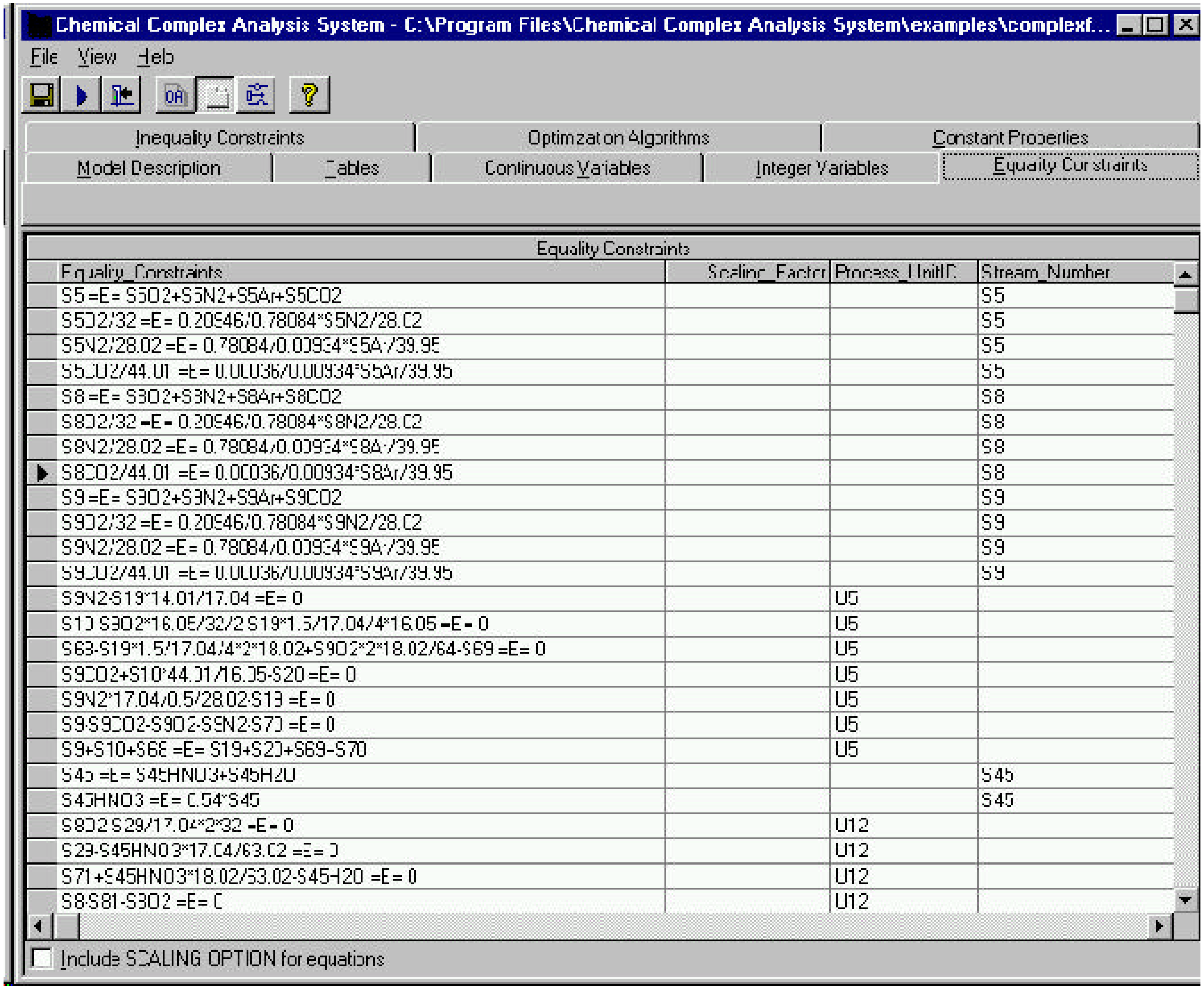
Optimal plant configuration
- Mixed integer nonlinear programming problem
- SYNPHONY and GAMS/DICOPT or SBB

Database

Material and energy balances, rate equations, equilibrium relations and thermodynamic and transport properties shared components of the system.

EPA pollution index methodology locates sources of pollutant generation

Chemical Complex Analysis System

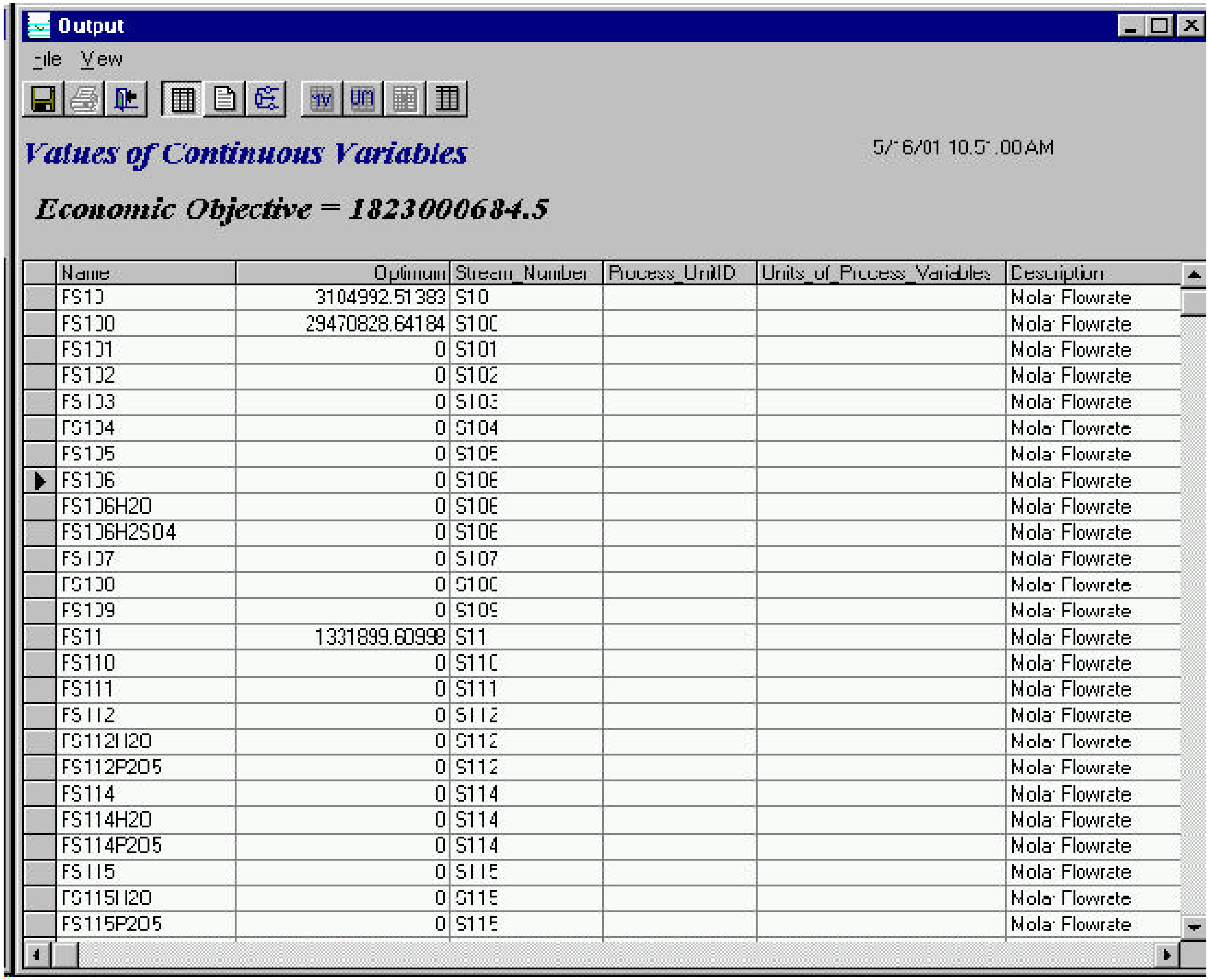


Equality Constraints

Equality_Constraints	Scaling_Factor	Process_UnitID	Stream_Number
S5 =E= S5O2+S5N2+S5Ar+S5CO2			S5
S5O2/32 =E= 0.20946/0.78084*S5N2/28.02			S5
S5N2/28.02 =E= 0.78084/0.00934*S5Ar/39.95			S5
S5CO2/44.01 =E= 0.00036/0.00934*S5Ar/39.95			S5
S8 =E= S8O2+S8N2+S8Ar+S8CO2			S8
S8O2/32 =E= 0.20946/0.78084*S8N2/28.02			S8
S8N2/28.02 =E= 0.78084/0.00934*S8Ar/39.95			S8
▶ S8CO2/44.01 =E= 0.00036/0.00934*S8Ar/39.95			S8
S9 =E= S9O2+S9N2+S9Ar+S9CO2			S9
S9O2/32 =E= 0.20946/0.78084*S9N2/28.02			S9
S9N2/28.02 =E= 0.78084/0.00934*S9Ar/39.95			S9
S9CO2/44.01 =E= 0.00036/0.00934*S9Ar/39.95			S9
S9N2-S19*14.01/17.04 =E= 0		U5	
S10 S9O2*16.05/32/2 S19*1.5/17.04/4*16.05 =E= 0		U5	
S63-S19*1.5/17.04/4*2*18.02+S9O2*2*18.02/64-S69 =E= 0		U5	
S9CO2+S10*44.01/16.05-S20 =E= 0		U5	
S9N2*17.04/0.5/28.02-S13 =E= 0		U5	
S9-S9CO2-S9O2-S9N2-S70 =E= 0		U5	
S9+S10+S68 =E= S19+S20+S69-S70		U5	
S45 =E= S45HNO3+S45H2O			S45
S45HNO3 =E= 0.54*S45			S45
S8O2 S29/17.04*2*32 =E= 0		U12	
S29-S45HNO3*17.04/63.02 =E= 0		U12	
S71+S45HNO3*18.02/63.02-S45H2O =E= 0		U12	
S8-S81-S8O2 =E= 0		U12	

☐ Include SCALING OPTION for equations

Chemical Complex Analysis System



Values of Continuous Variables

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Economic Objective = 1823000684.5

Name	Optimum	Stream_Number	Process_UnitID	Units_of_Process_Variables	Description
FS10	3104992.51383	S10			Molar Flowrate
FS100	29470828.64184	S100			Molar Flowrate
FS101	0	S101			Molar Flowrate
FS102	0	S102			Molar Flowrate
FS103	0	S103			Molar Flowrate
FS104	0	S104			Molar Flowrate
FS105	0	S105			Molar Flowrate
FS106	0	S106			Molar Flowrate
FS106H2O	0	S106			Molar Flowrate
FS106H2SO4	0	S106			Molar Flowrate
FS107	0	S107			Molar Flowrate
FS108	0	S108			Molar Flowrate
FS109	0	S109			Molar Flowrate
FS11	1331899.60998	S11			Molar Flowrate
FS110	0	S110			Molar Flowrate
FS111	0	S111			Molar Flowrate
FS112	0	S112			Molar Flowrate
FS112H2O	0	S112			Molar Flowrate
FS112P2O5	0	S112			Molar Flowrate
FS114	0	S114			Molar Flowrate
FS114H2O	0	S114			Molar Flowrate
FS114P2O5	0	S114			Molar Flowrate
FS115	0	S115			Molar Flowrate
FS115H2O	0	S115			Molar Flowrate
FS115P2O5	0	S115			Molar Flowrate

Agricultural Chemical Complex Expansion Evaluation

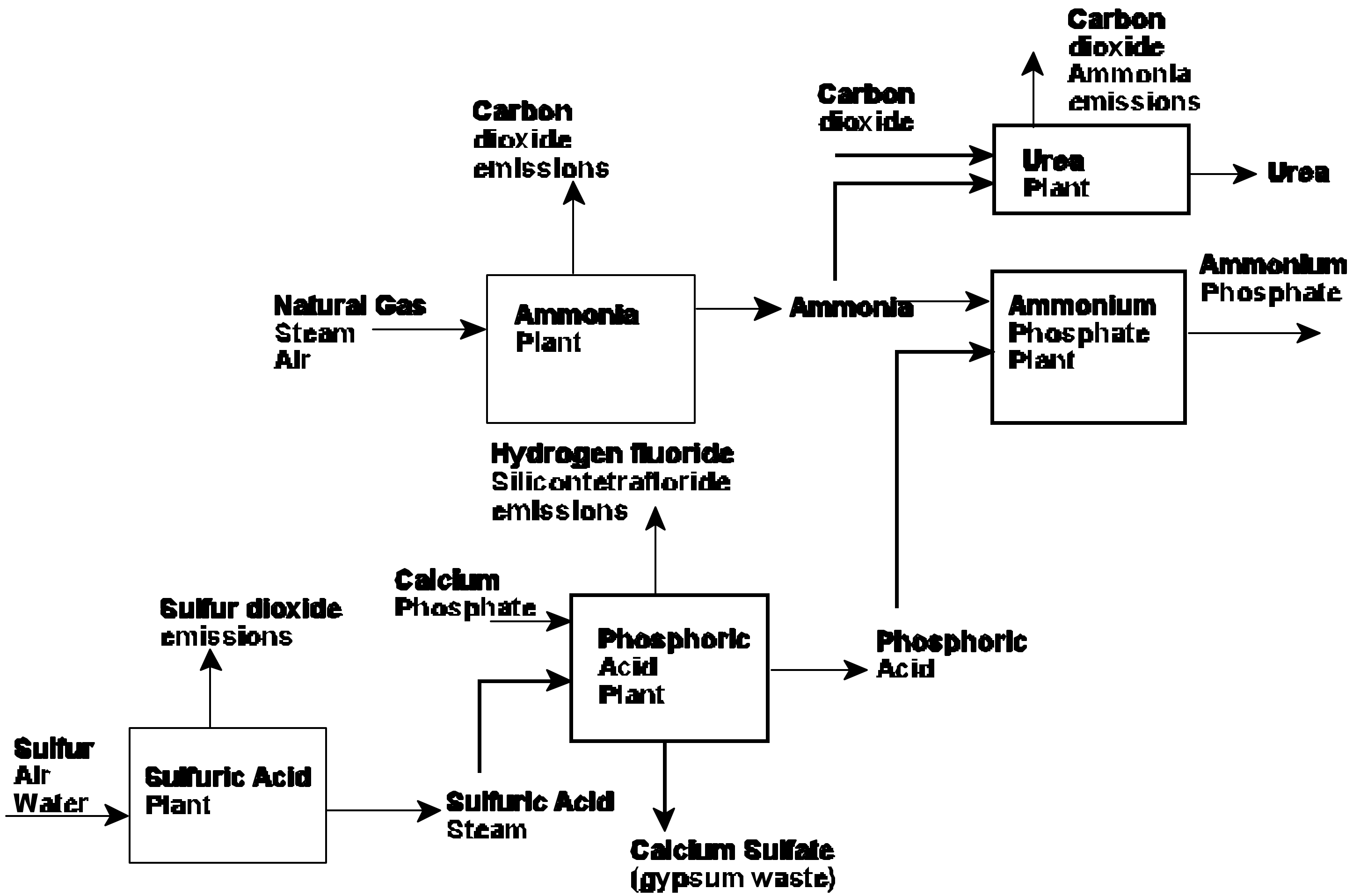


Figure 2 Schematic of Agricultural Chemicals Complex with Raw Materials, Products, Emissions and Wastes.

Agricultural Chemical Complex Expansion Evaluation

Case study by a major agricultural chemical company
- Expanding production of sulfuric and phosphoric acid capacity
- Heat recovery options
- Two locations on different sides of the Mississippi river several miles apart
- Excess ammonia capacity available

Objective expand phosphoric acid production capacity by 28%.
- Additional sulfuric acid and steam required
- Sulfuric acid can be shipped for miles and steam cannot
- Phosphoric acid evaporators require steam capacity from sulfuric acid plant
- Sulfuric acid plant produces more steam than is needed to evaporate phosphoric acid
- Some flexibility in matching sulfuric acid vs phosphoric acid production capacities within each site
- Expansion to be made in two stages
  - Stage one should be a best choice in case stage two is never justified

Agricultural Chemical Complex Expansion Evaluation

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 acid 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.

The question for the prototype to answer was what size phosphoric acid, sulfuric acid, heat recovery, and power-generation expansions should be built at each site for each stage of expansion.

Agricultural Chemical Complex Expansion Evaluation

Superstructure

- 67 different species (600 lb steam, sulfuric acid, logic switches, etc.)
- 75 processing units

Part of the superstructure for multiple sulfuric acid units for one plant site - One unit required 8-10 species

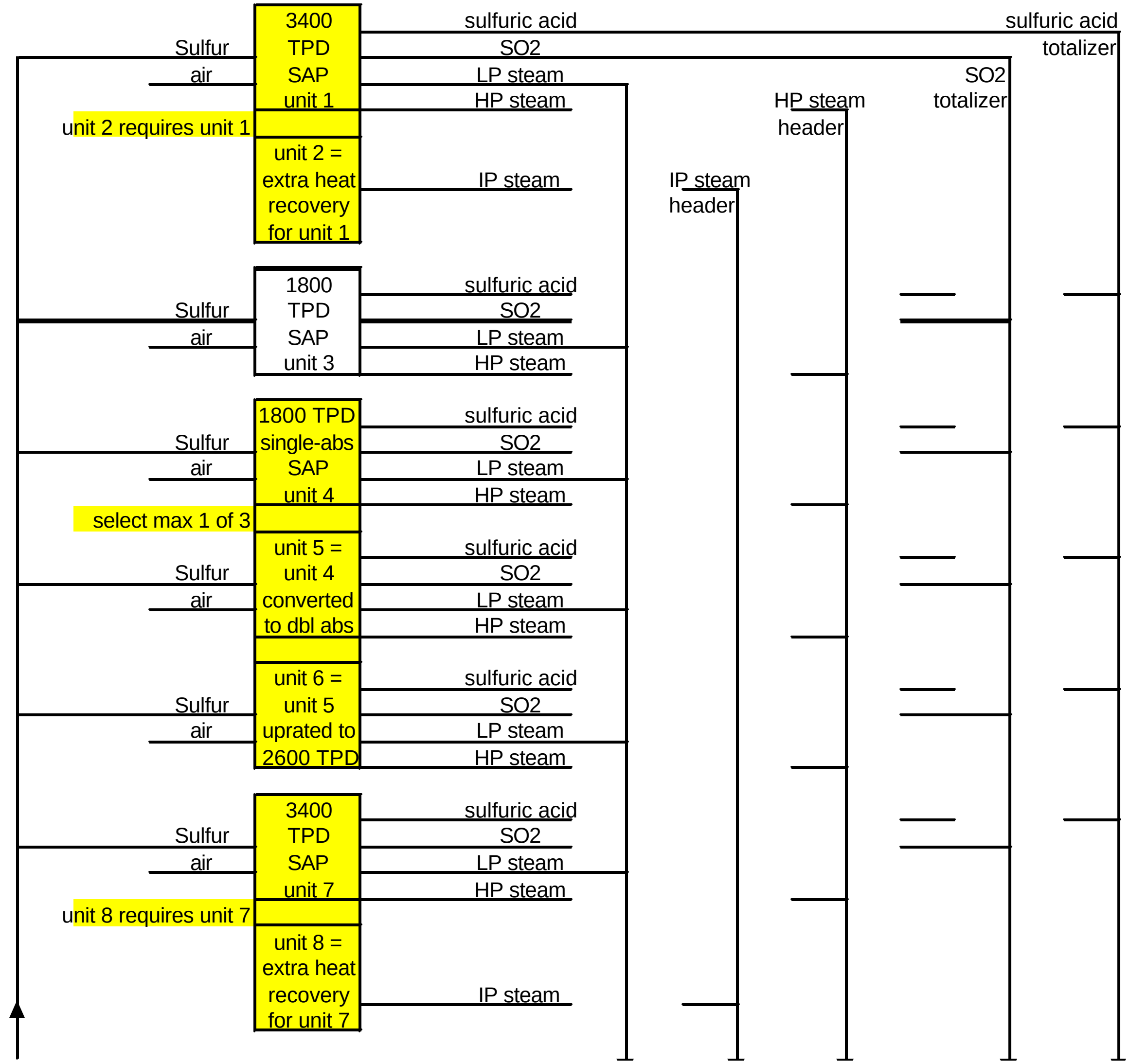


Figure 6 Part of Superstructure for SYNPHONY Sulfuric Plant Options at One of Two Plant Sites

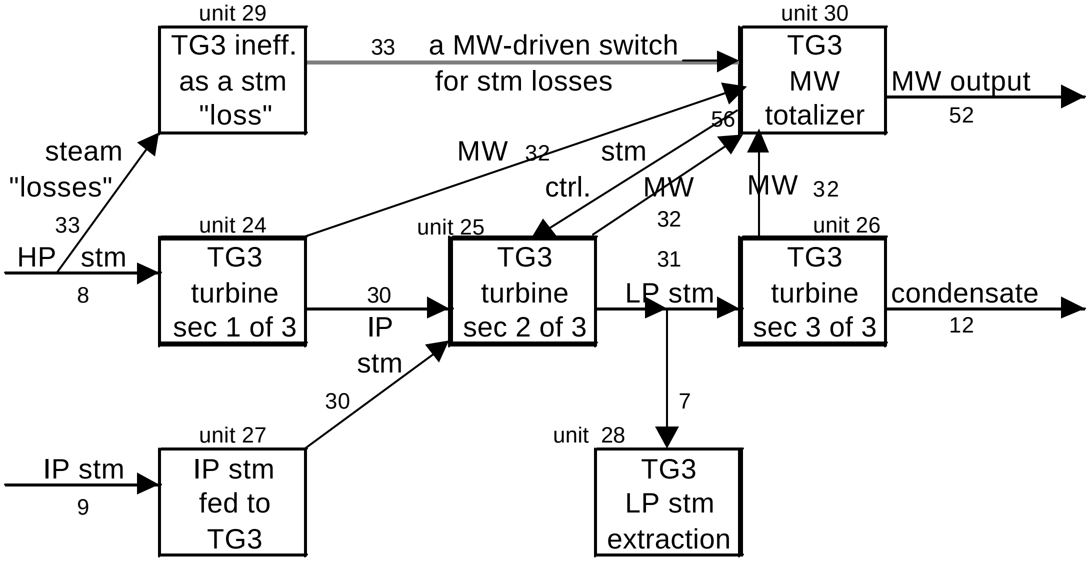
Agricultural Chemical Complex Expansion Evaluation

New turbo-generator

10 species and 7 units to model.

SYNPHONY used for MINLP

Computing time for any one case - less than 15 seconds on a Pentium II PC.



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 7 Representation of a Turbo-Generator in SYNPHONY

Agricultural Chemical Complex Expansion Evaluation

- 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.

- 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.

- 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 phosphoric acid 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.

Agricultural Chemical Complex Expansion Evaluation

- 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.

- In conclusion, the prototype 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. Its capability was demonstrated by duplicating and expanding an industrial case study

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

Dow AgricoScience (Blau and Kuenker, 1998)

Delivering nutrients to crops will lead to the best economic, environmental and sustainable development solutions for agricultural chemicals rather than focusing on the products themselves.

Agricultural Chemical Complex

Based on the plants in the Baton Rouge - New Orleans Mississippi river corridor Information provided by the cooperating companies and other published sources

Representative of the current operations and practices in the agricultural chemical industry

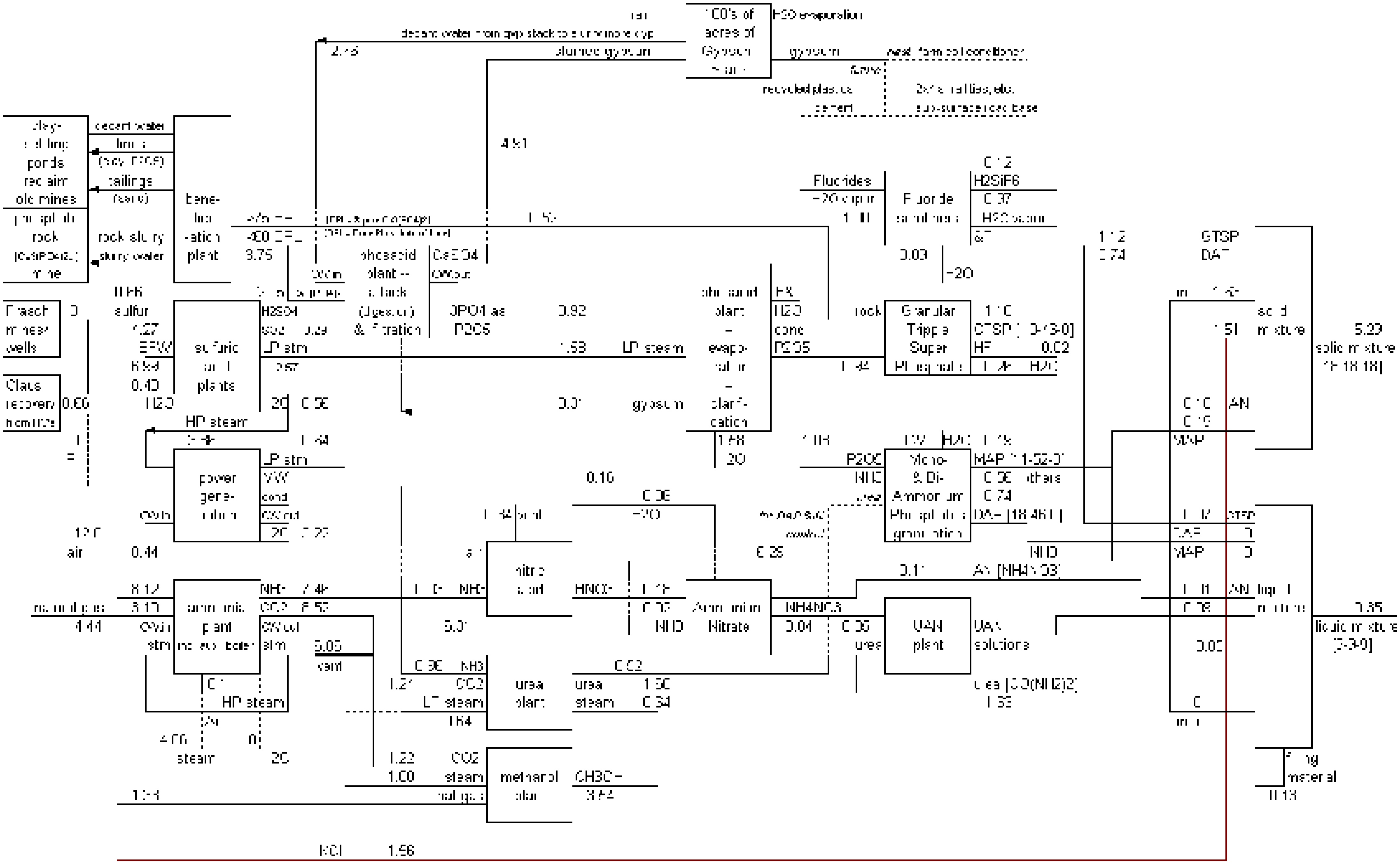


Figure 6 Agricultural Chemical Complex Based on Plants in the Baton Rouge-New Orleans Mississippi River Corridor, Base Case. Flowrates are TPY

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

10 production units and associated utilities for power, steam and cooling water

PRODUCTS
solid mixture [18% N - 18% P_2O_5 - 18% K_2O]
liquid mixture [9-9-9]
ammonia
methanol

RAW MATERIALS
air
water
natural gas
sulfur
phosphate rock
potassium chloride

INTERMEDIATES
sulfuric acid
phosphoric acid
ammonia
nitric acid
urea
carbon dioxide

EMISSIONS
sulfur dioxide
nitrogen oxides,
ammonia
methanol
silicon tetrafluoride
hydrogen fluoride
gypsum

BLENDING COMPOUNDS
mono-ammonium phosphate (MAP) [11-52-0]
di-ammonium phosphate (DAP)[18-46-0],
granular triple super phosphate (GTSP) [0-46-0]
urea [46-0-0]
ammonium nitrate [34-0-0],
UAN [~30-0-0]

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

Superstructure

Additional plants
- Alternate ways to produce intermediates, consume wastes and greenhouse gases and conserve energy
- Leading to a complex with less environmental impacts and improved sustainability

Phosphoric acid
- Electric furnace process which produces calcium oxide
- HCl which produces calcium chloride rather than gypsum

Potassium chloride
- Trona process
- IMCC process
- Sylvinite ore plant

Ammonium sulfate

Acetic acid from methane and carbon dioxide

Multi-Plant, Multi-Product Agricultural Chemical Complex

Four options for obtaining phosphoric acid

Four options for obtaining potassium chloride

Two options for sulfuric acid

Ammonium sulfate plant

Acetic acid plant

Economic, environmental and sustainable costs and credits

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

Value added or profit margin (difference between sales and the cost of raw materials) for economic model

Environmental Costs

- 67% of the raw material costs
- Based on the data provided by Amoco, DuPont and Novartis in the AIChE/CRWRT report

Sustainable Costs

- Cost of \$3.25 per ton was charged as a cost to plants that emitted carbon dioxide
- Based on the data provided by from the study of power generation in the AIChE/CRWRT report
- Credit of \$6.50 per ton to plants that consumed carbon dioxide
- Credit of \$6.50 per ton for steam by the sulfuric acid plant when carbon dioxide emissions were reduced by not having to produce steam in the boilers.

Multi-Plant, Multi-Product Agricultural Chemical Complex

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

Raw Materials	Cost ($/T)
Natural Gas	40
Phosphate Rock	
wet process	27
electrofurnace	24
HCl process	25
HCl	50
Sulfur	
Frasch	42
Claus	38
Brine	2
Searles Lake KCl ore	15
Sylvinite	45

Raw Materials	Cost ($/T)
Market cost for short term purchase	
KCl	101
H3PO4	176
H2SO4	86
Credit for CO_2 Consumption	6.50
Deficit for CO_2 Production	3.25

Products	Price($/T)
Ammonia	190
Methanol	96
Acetic Acid	45
Solid Mixture	160
Liquid Mixture	60
HP Steam	10
IP Steam	6.40

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

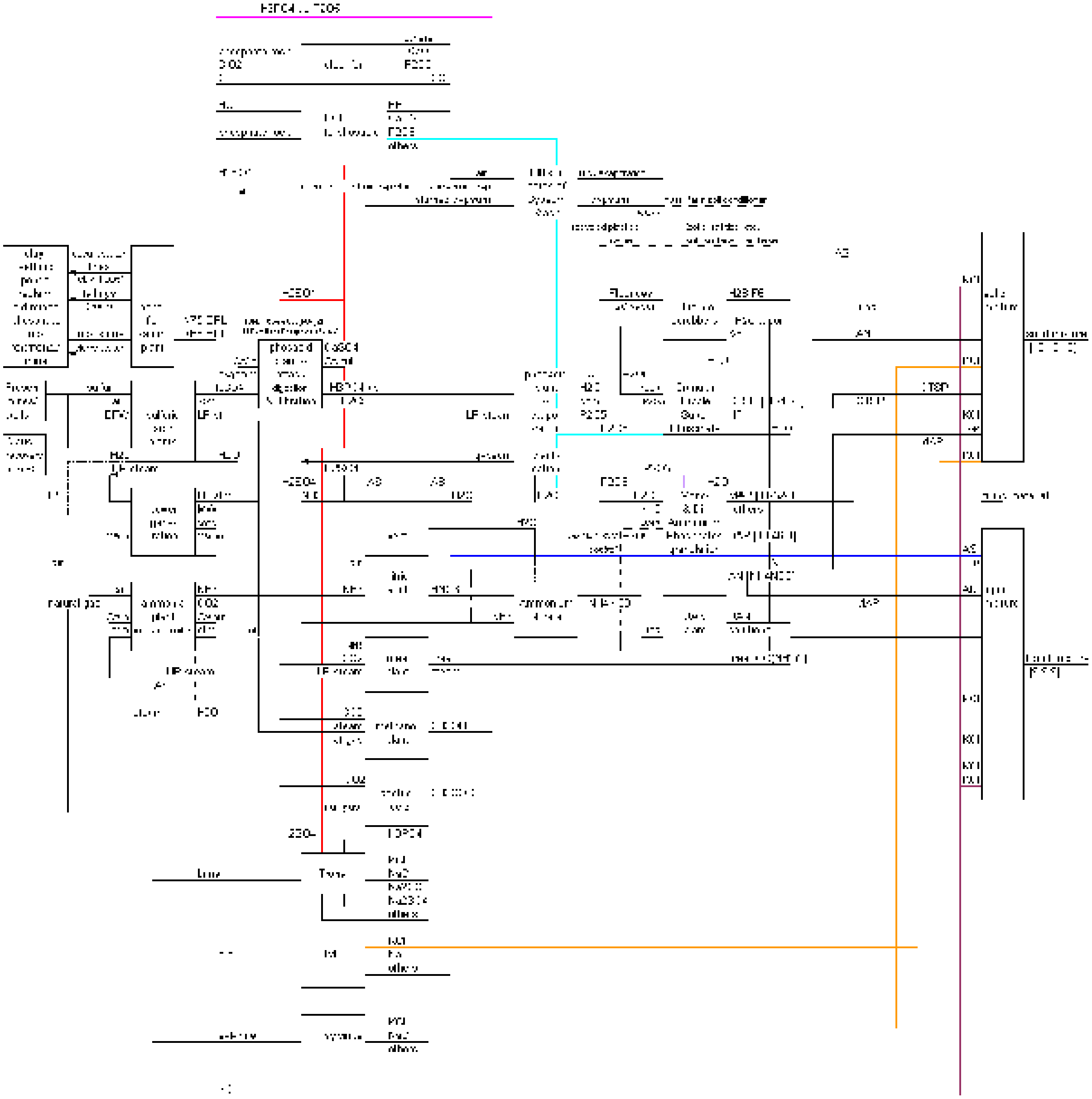


Figure 7 Superstructure for the Agricultural Chemical Complex

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

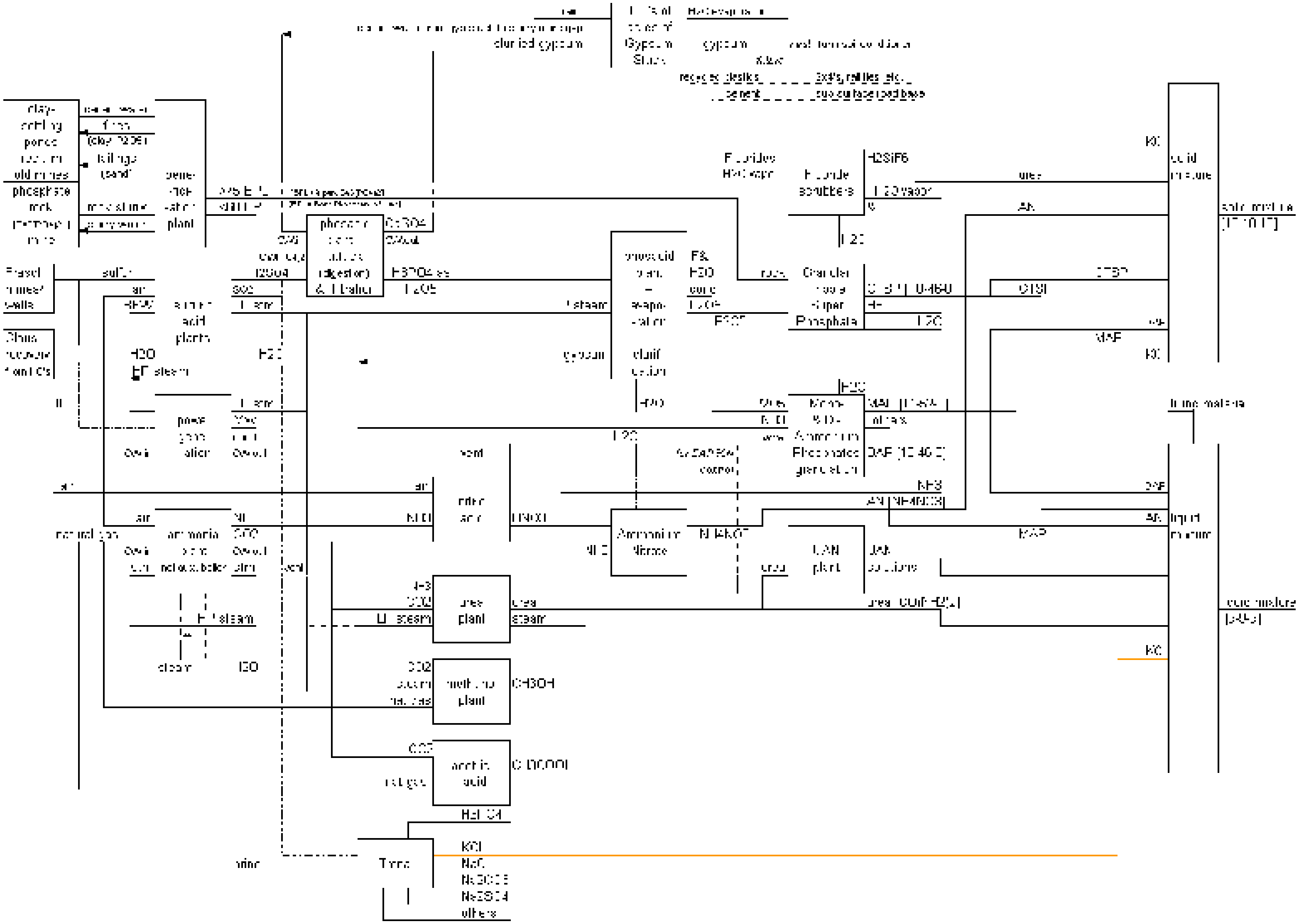


Figure 8 Optimal Configuration of the Agricultural Chemical Complex

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

		Base Case	Optimal Structure
Profit (million $/yr)		1,691	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			

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

Comparison of the base case and the optimal solution

Profit increased about 10%
- Including environmental and sustainability costs
- Carbon dioxide consumption credit and the new acetic acid plant were sufficient to outweigh the other costs

Sulfuric acid production rate increased
Production rates for the products in the optimal solution at their upper limit which was set at the base case values
Best to obtain KCl from the Trona plant
Acetic acid plant was operating at the upper limit
Profit declines an additional 7.0% if acetic acid plant was not included in the computation of the profit
Ammonium sulfate plant not optimal to operate

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.

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

		Optimal Structure				
	Base Case	Case 1	Case 2	Case 3	Case 4	Case 5
Profit($/yr)	1.96E+09	1.82E+09	1.71E+09	1.82E+09	1.83E+09	1.44E+09
Plant name	Capacity (TPY)	Capacity (TPY)	Capacity (TPY)	Capacity (TPY)	Capacity (TPY)	Capacity (TPY)
Profit	1.96E+09	1.82E+09	1.71E+09	1.82E+09	1.83E+09	1.44E+09
Ammonia	7.46E+06	7.46E+06	7.46E+06	7.46E+06	7.46E+06	7.46E+06
Nitric Acid	1.00E+05	1.00E+05	1.00E+05	1.00E+05	1.00E+05	1.00E+05
Ammonium Nitrate	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05	1.27E+05
Urea	1.69E+06	1.69E+06	1.69E+06	1.69E+06	1.69E+06	5.14E+04
Methanol	3.55E+06	3.55E+06	3.55E+06	3.55E+06	3.55E+06	3.55E+06
UAN	9.06E+04	9.06E+04	9.06E+04	9.06E+04	9.06E+04	9.06E+04
MAP	1.89E+05	1.89E+05	1.89E+05	1.89E+05	1.89E+05	1.00E+04
DAP	7.38E+05	7.38E+05	7.38E+05	7.38E+05	7.38E+05	1.21E+05
GTSP	1.19E+06	1.19E+06	1.19E+06	1.19E+06	1.19E+06	6.38E+04
Sulfuric Acid (S4)	6.61E+05	6.73E+05	6.61E+05	6.61E+05	1.21E+04	1.11E+03
Phosphate Rock(S13ROCK)	2.55E+06	2.55E+06	2.55E+06	2.55E+06	0	0
Phosphate Rock(S12+S13ROCK)	3.06E+06	3.06E+06	3.06E+06	3.06E+06	5.17E+05	2.78E+04
Phosphorous Acid	9.19E+05	9.19E+05	9.19E+05	9.19E+05	0	0
Electric furnace (S109)	na	0	0	0	0	0
HCl to Phosacid (S85)	na	0	0	0	1.94E+06	1.93E+05
Ammonium Sulfate	na	0	0	0	0	0
Acetic Acid	na	9.00E+04	9.00E+04	9.00E+04	9.00E+04	9.00E+04
Trona (S93)	na	3.97E+07	0	0	3.97E+07	3.65E+06
IMCC (S89)	na	0	9.78E+06	0	0	0
Sylvinite (S101)	na	0	0	3.65E+06	0	0
Direct Buying P2O5 (S153)	na	0	0	0	0	0
Direct Buying KCl (S156)	1.56E+06	0	0	0	0	0
Direct Buying H2SO4 (S159)	na	0	0	0	0	0
Solid Mixture (S140)	5.29E+06	5.29E+06	5.29E+06	5.29E+06	5.29E+06	3.50E+05
Liquid Mixture (S141)	3.49E+05	3.49E+05	3.49E+05	3.49E+05	3.49E+05	3.02E+05

Table 3Evaluation of Sensitivity to Prices and Costs for Plants in the Agricultutal Chemical Complex

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

Brief sensitivity study
- Test the capability of the system
- Four cases - changing the cost of raw materials and sales price of products

Case 1 Is the optimal structure

Case 2, Cost of brine to Trona plant was increased by 90%
- Trona plant was replaced with IMCC plant in the optimal solution
- Trona plant consumes sulfuric acid, and the IMCC plant does not
- Profit was about 6% less

Case 3, Cost of sylvinite was decreased by 52%
- Trona plant was replaced with Sylvinite plant
- Profit was essentially the same

Case 4, Cost of phosphate rock was decreased by 50% for the HCl plant and the cost of HCl was decreased 80%
- Unrealistic reductions, the HCl plant replaced the wet-process plant
- Sulfuric acid production rate was 98% less.
- Profit was essentially

Case 5 Cost of phosphate rock (<68BPL) was increased by an unrealistic 360%
- Decrease in all related products
- Profit declined 21%

In summary, this brief sensitivity study gave results that were intuitively to be expected and demonstrated additional capabilities of the system.

Summary of Results from Two Evaluations with the System

Multi-Plant, Multi-Product Agricultural Chemical Complex Evaluation

Based on the plants in the Baton Rouge - New Orleans Mississippi river corridor.

Information provided by the cooperating companies and other published sources.

Representative of the current operations in the agricultural chemical industry

Results

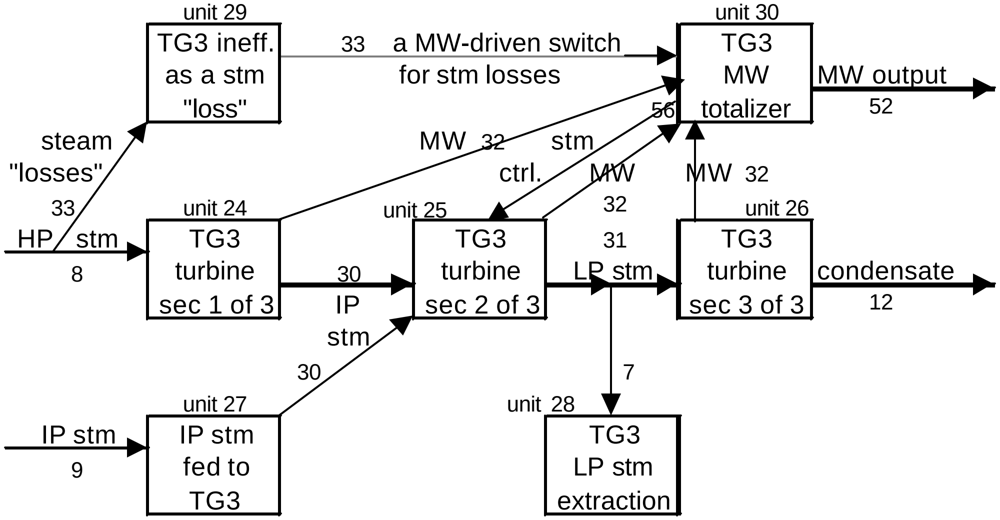
Demonstrates capability of the system to select an optimum configuration of plants in an agricultural chemical complex and incorporate economic, environmental and sustainable costs.

Summary of Results from Two Evaluations with the System

Agricultural Chemical Complex Expansion Evaluation

System selected the optimum site required for new phosphoric and sulfuric acids production capacities and selected, sited, and sized the optional heat-recovery and power-generation facilities.

Its capability was demonstrated by duplicating and expanding an industrial case study



Conclusions

Prototype of a chemical complex analysis system has been developed

Capability demonstrated

- Duplicating and expanding an industrial case study
  - 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
- Application to an agricultural chemical complex
  - Optimal configuration of plants determined based on economic, environmental and sustainable costs

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

Applications to other chemical complexes continuing

System and users manual will be available from the Mineral Processing Research Institute web site www.mpri.lsu.edu