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CHEMICALS FROM BIOMASS: AN ASSESSMENT OF THE POTENTIAL
FOR PRODUCTION OF CHEMICAL FEEDSTOCKS
FROM RENEWABLE RESOURCES

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ABSTRACT

This assessment of the potential for production of commodity chemicals from renewable biomass resources is based on (1) a Delphi study with 50 recognized authorities to identify key technical issues relevant to production of chemicals from biomass, and (2) a systems model based on linear programming for a commodity chemicals industry using renewable resources and coal as well as gas and petroleum-derived resources.

Results from both parts of the assessment indicate that, in the absence of gas and petroleum, coal undoubtedly would be a major source of chemicals first, followed by biomass. The most attractive biomass resources are wood, agricultural residues, and sugar and starch crops. A reasonable approximation to the current product slate for the petrochemical industry could be manufactured using only renewable resources for feedstocks. Approximately 2.5 quads [10^{15} Btu (1.055×10^{18} joules)] per year of oil and gas would be released. Further use of biomass fuels in the industry could release up to an additional 1.5 quads. However, such an industry would be unprofitable under current economic conditions with existing or near-commercial technology. As fossil resources become more expensive and biotechnology becomes more efficient, the economics will be more favorable.

Use of the chemicals industry model to evaluate process technologies is demonstrated. Processes are identified which have potential for significant added value to the system if process improvements can be made to improve the economics. Guidelines and recommendations for research and development programs to improve the attractiveness of chemicals from biomass are discussed.

1. INTRODUCTION

Until relatively recently, biomass was the prime source of organic chemicals. Distillation of hardwoods to produce charcoal also produced pyroligneous acid, methanol, acetic acid, and acetone. Naval stores such

as turpentine, rosin, pitch, and tar were obtained from softwoods. Butanol, ethanol, and several other organic chemicals were produced by fermentation from sugars and starches. The first significant nonbiomass organic chemicals were perhaps the aromatics from the by-product recovery ovens for the coking of coal in 1881. The production of organic chemicals from petroleum began in 1917 with the synthesis of isopropanol from propylene in the cracked gas stream from a petroleum refinery. Following World War II, the growth of petrochemicals resulted in the virtual disappearance of chemicals derived from both biomass and coal.

Alternative sources of organic chemical feedstocks are needed in the long term for the chemical industry. The future supply and cost of natural gas and petroleum-based chemical feedstocks are uncertain because of the finiteness of domestic reserves and the instability of foreign supplies. The use of petroleum and natural gas for fuel and feedstock to produce chemicals requires an equivalent of 7 to 8% of the U.S. consumption.¹ Because chemical feedstocks typically command higher unit prices than do fuels, the economics of processes for chemicals from biomass could result in an incentive structure favoring the use of biomass for chemical rather than fuel production.

At the request of the Biomass Energy Technology Division of the Department of Energy (DOE), we have undertaken an assessment of the potential for large-scale production of commodity chemicals from biomass to supplement chemicals production from petroleum and natural gas. The major objectives of this assessment are (1) to determine the extent to which chemicals from biomass can lessen the dependency on petroleum and natural gas resources (especially imported petroleum), and (2) to identify research and development (R&D) activities that will encourage increased production of chemicals from biomass. It is especially appropriate for DOE to sponsor this assessment for the following reasons:

1. Economic and national security can be improved by reducing national dependence on imported oil.
2. Many potentially useful products and processes will not be economically attractive to the private sector for 10 to 20 years because of continued supplies of petroleum, natural gas, and coal in the short- to mid-term.

3. Much of the needed basic research and process development work is generic in nature, and hence is not likely to provide a significant long-term competitive edge in return for investments by the private sector.
4. Biomass is truly a long-term renewable source and a significant means of collecting and storing solar energy. It is clearly in the national interest to promote maximum utilization of this resource for the well-being of all people.

To achieve the objectives of this assessment, three major activities have been carried out: (1) a Delphi study to identify important issues relevant to production of chemicals from biomass, (2) a systems analysis of a conceptual chemicals-from-biomass industry, and (3) an analysis of R&D needs. Approximately 2 person-years of effort have been devoted to these tasks. The Delphi study is described in Sect. 2 of this report; the systems analysis is covered in Sects. 3-7. R&D needs are described in Sect. 8.

2. DELPHI STUDY

The so-called Delphi technique is an iterative method whereby input on an issue is obtained from several people while minimizing the bias generated from peer interactions.² Typically, the participating consultants know that they are members of a group, but they do not know the identities of the other members. After each participant provides input on a particular issue, the organizer of the Delphi study condenses the inputs from all participants into a single statement. Each participant is asked to review this summary and is given an opportunity to modify his point of view in the light of the collective wisdom of his (unknown) colleagues. This iterative process is continued until the organizer determines that further iterations will not be useful.

We have used a similar approach to investigate a broad spectrum of technical issues. Our particular methodology and the results of the study are described in this chapter.

2.1 Methodology

A list of 85 recognized authorities in various aspects of biomass production and conversion was compiled. These authorities were invited to participate in the assessment by responding to an initial set of ten questions relating to the production of chemicals from biomass, shown in Table 1.

Fifty people responded to these assessment questions. The individual responses were condensed into an informal summary report that was sent to this 50-member panel, along with a second set of eight questions. This second set of questions is shown in Table 2. Note that the first question asks for an evaluation of the summary of the responses to the first round of questions. Responses to the second round of questions were summarized and sent to participants.

The 85 invited participants were 46% academicians, 22% industrialists, and 32% independent/government laboratory employees. The 50 participating panel members are in nearly the same proportions: 44% academicians, 26% industrialists, and 30% independent/government laboratory employees. Only

Table 1. Questions for the Delphi study, Round 1

-
1. Biomass resources: What particular biomass resources, or groups of resources, are likely to be significant for production of chemicals? Why?
 2. Chemical products: What particular chemicals, or groups of chemicals, are most attractive for production from biomass? Why?
 3. Chemicals also will be produced from coal. What are the technical issues governing optimal use of both resources? (For example: oxy-chemicals vs hydrocarbons; aromatics from coal vs lignin; gaseous vs liquid products, etc.)
 4. Please identify specific current R&D work of critical relevance to production of chemicals from biomass. Names of investigators and/or literature references would be helpful to us for overall documentation purposes.
 5. What specific additional R&D work will be critically necessary (a) in the short term, and (b) in the long term?
 6. Chemicals from biomass might be used as feedstocks for existing petrochemical-based processes (e.g., ethylene), or new processes and products might be developed around biomass-derived chemicals (e.g., lignin-based polymers). What are the pros and cons of these two approaches?
 7. There is considerable agreement that biomass processing plants will be smaller than petrochemical plants. How small is "small"? Are there noneconomic factors which might influence plant size?
 8. What time scale do you foresee for significant additional production of chemicals from biomass? If it should become highly desirable (or critical) to produce chemicals from biomass as soon as possible, what significant technical barriers (as opposed to economic barriers) now exist to immediate commercialization?
 9. Please identify ten people who, in your opinion, are leading authorities in the field of chemicals from biomass by virtue of their research work and/or familiarity with the technical issues.
 10. What literature, both general and specific in subject, would be most helpful to us for this assessment?
-

Table 2. Questions for the Delphi study, Round 2

-
1. Comments on Round 1 responses. Do you basically agree? Major points of disagreement?
 2. While use of "waste" biomass such as MSW is philosophically attractive and helps alleviate disposal problems, there also appear to be risk and uncertainty factors associated with a conversion plant dependent on perceived "wastes" as "valuable" feedstock. What are likely to be the specific problems here, and what can be done to minimize them?
 3. There are at least four major categories of biomass conversion processes: fermentation, liquefaction, gasification, and pyrolysis (fast and slow). Should one or more of these generic categories receive special R&D emphasis relative to the others for production of chemicals? Why?
 4. Describe the major technical features of an ideal multiproduct "biomass refinery."
 5. Are there circumstances under which coal-biomass dual feedstock plants might be attractive? For example?
 6. Anaerobic digestion received practically no mention in Round 1. Is methane a potentially significant chemical intermediate? Why?
 7. Are the following chemicals potentially significant as intermediates or end products? Why?
 - (a) levulinic acid
 - (b) carbon dioxide
 - (c) lignin-based polymers and cellulose-based polymers
 8.
 - (a) To what level of development should DOE sponsor new technology for chemicals from biomass? (e.g., fundamental research, bench-scale, process development unit, mini-pilot plant, pilot plant, etc.) Why?
 - (b) At what level of development will industry be able to pick up further development and implementation of new technology? What types of incentives and/or co-funding would be most useful?
-

Table 3. Participants in the Delphi study

Name	Affiliation
Alston, T. G.	Argonne National Laboratory
Antal, M. J.	Princeton University
Bellamy, W. D.	Cornell University
Blanch, H. W.	University of California, Berkeley
Bungay, H. R.	R.P.I.
Busche, R. M.	DuPont
Calvin, M.	University of California, Berkeley/L.B.L.
Clausen, E. C.	University of Arkansas
Cooney, C. L.	M.I.T.
Coffman, J.	Wright-Malta Corporation
Datta, R.	Exxon
Diebold, J.	S.E.R.I.
Dyer, G. H.	Bechtel
Eakin, D. E.	Battelle P.N.L.
Elliott, D. C.	Battelle P.N.L.
Emert, G. H.	University of Arkansas
Goldstein, I. S.	North Carolina State University
Kirk, T. K.	University of Wisconsin/F.P.L.
Klausmeier, W. H.	Argonne National Laboratory
Kuester, J. L.	Arizona State
Ladisch, M.	Purdue University
McElroy, A. D.	Midwest Research Institute
Mandels, M.	Natick
Milne, T. A.	S.E.R.I.
Myerly, R. C.	Union Carbide
Saeman, J. F.	University of Wisconsin/F.P.L.
Sarbolouki, M. N.	J.P.L.
Tanner, R. D.	Vanderbilt University
Tsuchiya, H. M.	University of Minnesota
Watkins, S. H.	Crown Zellerbach
Wiseman, A.	University of Surrey, U. K.

32 of the 50 people responded to the second set of questions. These people are identified, with permission, in Table 3. One person chose to remain anonymous.

2.2 Results

An overview of the results from both sets of questions is presented here. More details on the responses to individual questions are given in Appendix A. The following discussion is intended to be an unbiased summary of responses of panel members, not a reflection of recommendations for R&D programs:

1. Resources. Woody biomass and agricultural crops and residues are the preferred resources. There is definite interest in specialty crops and municipal solid waste. Major difficulties are the logistics of harvest and storage. However, wastes are available in inherently limited quantities, and cost increases due to perceived higher value of wastes may limit the attractiveness of these resources to venture capitalists.
2. Chemicals. Coal probably will be a major source of chemicals — perhaps before biomass. Syngas from coal will dominate over syngas from biomass. Most attractive opportunities for biomass will be oxychemicals (containing one or more oxygen atoms) and other specific chemicals easily derivable from biomass, especially in regional areas where biomass is plentiful and coal is scarce. Considerable interest is shown in aromatics and olefins from biomass in the long term.
3. Barriers. There are no insurmountable technical barriers to immediate production of some chemicals from biomass. However, most recently developed processes have not been proven at the commercial scale. Economics will be very site- and resource-specific. The projected time scale for significant chemicals will be hastened by favoring production of petrochemical feedstocks and chemical intermediates that can be used in existing facilities and markets, and by instituting favorable national policies.

4. Research and Development. Perceived R&D activities to overcome present limitations are improved separation processes, improved conversion rates and yields, improved lignocellulose conversion, genetic engineering and strain improvement, improved agronomic understanding, and process demonstrations. The goal should be efficient, complete utilization of the resource, site-optimized with respect to resource and market. No firm basis exists for favoring one or more generic conversion routes at the expense of other routes. Government support for fundamental, laboratory-scale research should have much higher priority than support for process development units and pilot plants.

3. SYSTEMS ANALYSIS

A model has been developed to simulate the interdependent nature of a conceptual chemicals industry using common biomass resources to produce a wide array of chemicals by a variety of conversion processes. The model also includes petroleum, natural gas, and coal resources and associated processes; hence the relative role of each resource can be examined under various scenario conditions. With this model, an industry-wide characterization is possible with respect to the following input conditions:

1. different oil/coal/biomass supply and cost assumptions,
2. changes in market demand for chemicals,
3. improvements in existing technology which could influence production economics, and
4. new technology that could influence the process options available to the industry.

In other words, the model provides a tool by which the economic implications of presumed results of R&D work can be explored.

3.1 Linear Programming

The model is based on linear programming, a technique employed for several decades to identify an optimal set of activities from among a larger population of competing activities.³ The petroleum industry has realized great economic benefits from linear programming in the operation of refineries to optimize the processing of numerous crude oils to meet demands for a variety of products. Some years ago, linear programming was used at Oak Ridge National Laboratory in a study for the U.S. Atomic Energy Commission to identify the nuclear reactor types and fuels that merited the greatest consideration for R&D funding. Linear programming has been used recently to analyze future U.S. energy technologies,⁴ energy from biomass,⁵ chemical feedstocks from biomass,⁶ and the U.S. petrochemical industry.⁷

A linear programming problem can be stated mathematically in the following manner:

Maximize (or minimize) $Z = \sum c_j x_j$, $j = 1, 2, \dots$
 subject to

$$\sum a_{ij} x_j \left\{ <, =, > \right\} b_i , \quad i = 1, 2, \dots$$

and $x_j \geq 0$.

Each x_j is an activity, such as "buy one metric ton of corn stalks," or "produce one metric ton of acetone from acetic acid," or "sell one metric ton of phenol." The coefficient c_j is the unit value of activity x_j . The summation of the $c_j x_j$ products is the objective function Z which, depending on the situation, may be maximized or minimized by the selection of the best set of activities. Profit is a typical objective function to be maximized, subject to a specified set of constraints.

The coefficient a_{ij} is the quantity of resource i required to do one unit of activity x_j . For example, the production of one metric ton (t) of *n*-butanol from acetaldehyde consumes 1.32 t of acetaldehyde. There is an equation in the model for each resource in the system, and also an equation for each demand for a chemical. The term $\sum a_{ij} x_j$ is subject to b_i according to a specified conditional $<, =, \text{ or } >$. For example, an inventory balance may be specified in which the quantities of a chemical consumed and sold must be less than or equal to the quantities produced and bought. In this case, b_i is zero.

In addition to determining the optimal set of activities which maximize or minimize the objective function, the linear programming algorithm also enables extensive postoptimization analysis. Valuable information is provided about:

1. the change in the value of the objective function which would result from (a) a change in a b_i by one unit, and (b) forcing one unit of a nonoptimal activity into the solution;
2. the range of values for the c_j of an optimal activity within which the activity remains at its optimal value x_j ;
3. the new value x_j of an activity if its c_j were to take the value at the upper or lower limit of this range; and

4. the identity of the nonoptimal activity that will replace an optimal activity if the c_j of the optimal activity takes a value outside this range.

This sensitivity information can aid greatly in the identification of target areas for R&D work.

3.2 Chemicals Industry Model

A comprehensive (approximate) model of a chemicals industry has been assembled in a format suitable for analysis using linear programming with the IBM Mathematical Programming System/360. The model contains three kinds of activities — purchase of raw materials, manufacture of chemicals from raw materials and intermediate chemicals, and sale of chemicals. The objective function is profit, which is to be maximized. Profit is defined simply as revenues from sales minus costs of raw materials and capital and operating costs associated with manufacture of chemicals. The dollar value of the maximum profit is not particularly significant or important for our purposes. Rather, our primary concern is the change in system profit relative to a reference case when input parameters are changed. This change in system profit is a measure of the value of the changes in input parameters.

Twenty-five primary chemical products were selected based on current production volumes and potential availabilities from coal and biomass. These chemicals account for approximately 90% of the organic chemicals production reported each spring in *Chemical and Engineering News*. Secondary products also arise from the various conversion processes in the model. There are 23 primary raw materials and 15 secondary raw materials. Ninety-five different conversion processes are available for the conversion of raw materials and chemical intermediates to products for sale. A portion of the model is shown in Fig. 1.

Four kinds of constraints are introduced to govern the activity levels for the production of these chemicals. Maximization of profit is sought by selecting the best raw materials and conversion processes, subject to the following constraints:

Fig. 1. A portion of the chemicals industry model. Other processes, raw materials, and chemicals also interact with this portion of the model.

1. For each of 25 primary chemical products, the quantities produced must equal or exceed the 1979 U.S. production (Table 4).
2. Sales of primary and secondary products cannot exceed the 1979 U.S. sales (Table 4).
3. The availabilities of raw materials are limited (Table 5).
4. The quantities of raw materials and chemical products consumed and sold cannot exceed the quantities produced and bought (materials balance constraint).

Note that the first two constraints will require production to exceed sales for some chemicals. This situation occurs frequently in the chemical industry because intermediate chemicals are converted to other chemicals which, in turn, are sold. In our model we have chosen to use an apparent sales volume equal to production for chemicals that are not feedstocks for other chemicals in the model, even though published statistics indicate that production exceeds sales. This allowance is made to obtain credit in dollars for these products. For products with opportunities for internal consumption (e.g., benzene and ethylene), the published production and sales figures are used. However, residuals of unsold chemicals may arise because of the approximate nature of the model.

No primary products may be purchased for use as feedstocks. Chemicals that are both secondary raw materials and products may be bought and sold at a common price.

Conversion processes are based on published descriptions of existing technologies, published process feasibility studies, and (in some cases) estimates developed specifically for this project. A list of processes in the model, identified by product and raw material, is given in Table 6, and a complete catalogue of material balances and economics is given in Appendix B. Processes are identified in terms of primary product and primary raw material as "Product/Raw material." A single plant capacity is specified for each process; the required total production is obtained by utilizing multiple plants. The number of plants is not restricted to integer values. This artificial flexibility has negligible economic impact unless the number of plants is small — perhaps less than five plants.

Capital costs are expressed in October 1981 dollars. The plant cost index published in *Chemical Engineering* magazine was used to adjust

Table 4. Primary products: production, sales, and price^a

Primary product	1979 U.S.		Price (\$/t)
	Production (10 ³ t)	Sales (10 ³ t)	
Acetaldehyde	1,120	224	710
Acetic acid	1,480	260	580
Acetone	1,200	1,200 ^b	680
Ammonia	17,800	17,800 ^b	220
Benzene	5,350	2,800	460
Butadiene	1,630	1,630 ^b	880
n-Butanol	348	202	790
Cyclohexane	1,100	1,090	590
Cyclohexanone	397	397 ^b	1,320
Ethanol	710	611	710
Ethylbenzene	3,830	3,830 ^b	660
Ethylene	13,600	5,280	560
Ethylene glycol	2,150	2,150 ^b	790
Ethylene oxide	2,570	2,570 ^b	990
Formaldehyde	2,710	2,710 ^b	200
Glycerol	68	68 ^b	1,800
Methanol	3,340	1,680	280
Methyl ethyl ketone	298	298 ^b	930
Phenol	1,350	738	790
Phthalic anhydride	460	460 ^b	930
Isopropanol	862	542	660
Propylene	6,440	3,340	490
Propylene oxide	1,020	1,020 ^b	900
Urea	5,420	5,420 ^b	480
p-Xylene	2,110	2,110 ^b	680

^aProduction and sales volumes obtained primarily from *Synthetic Organic Chemicals. U.S. Production and Sales, 1979*, U.S. International Trade Commission. Prices obtained primarily from *Chemical Marketing Reporter* (October 19, 1981). Data in these two sources are derived on slightly different bases and represent different periods in time. Hence this table is an approximate representation of the real market.

^bEffective sales set equal to production because there is little or no opportunity for consumption of these products as feedstocks in model.

Table 5. Primary raw materials: availability and price^a

Primary raw material	Quantity available (10 ³ t)	Source ^b	Price (\$/t)	Source ^b
Aquatic biomass	40,600	a	110	d
n-Butane	1,500	b	260	f
Coal	99,999 ^c		36	g
Corn	16,400	c	120	h
Corn stover	83,300	c	45	h
Feedlot wastes	14,000	d	6.3	d
Kelp	33,100	d	d	d
Lignin, Kraft	19,000	e	41	i
Marine algae	33,100	a	70	j
Molasses	4,880	c	34	k
Municipal solid waste	9,080	c	0	c
	38,100	c	4.4	c
	62,600	c	8.8	c
Naphtha, coal	99,999 ^c		47	l
Naphtha, petroleum	99,999 ^c		32	m
Natural gas (methane)	99,999 ^c		15	f
Refinery gas	99,999 ^c		22	n
Sewage sludge	99,999 ^c		0	
Sugar beets	17,000	c	32	k,o
Sugar cane	20,500	c	25	k,o
Sulfite black liquor	370	e	0	
Sulfite waste liquor	60,800	e	0	
Sweet sorghum	52,900	c	20	k
Wheat straw	31,200	c	46	h
Wood	33,700	c	22	c
	10,600	c	33	c
	36,000	c	44	c

^aPrimary sources for data are indicated. In some cases, further assumptions and/or approximations were made, such as scaling the published price by appropriate economic indices. In the cases of municipal solid waste and wood, the lowest price material is always used first to minimize costs.

^bSources:

- a. *Cost Analysis of Aquatic Biomass Systems*, HCP/ET-4000-78, Dynatech R&D Company, 1978.
- b. *Synthetic Organic Chemicals. U.S. Production and Sales, 1979*, U.S. International Trade Commission.
- c. *The Report of the Alcohol Fuels Policy Review, Raw Material Availability Reports*, DOE/ET-0114/1, 1979.
- d. J. L. Jones et al., *Mission Analysis for the Federal Fuels from Biomass Program. Vol. V. Biochemical Conversion of Biomass to Fuels and Chemicals*, TID-29093, SRI International, 1978.
- e. *Wood Pulp Statistics*, American Paper Institute, New York.
- f. Energy Information Administration, "Monthly Energy Review," November 1981.
- g. *Coal Week* (Oct. 26, 1981).
- h. A. D. McElroy et al., *Continuation of Systems Study of Fuels from Gases and Grains: Phase 2 and Phase 3*, DSE-4042-T2, Midwest Research Institute, 1979.
- i. Price equivalent to heating value, steam coal.
- j. J. E. Sanderson et al., *Acetic Acid Production from Marine Algae*, Progress report to DOE, C00/4388-1, Dynatech R/D Company, 1977.
- k. D. A. Scantland et al., *Research Report on Development of Sweet Sorghum as an Energy Crop. Volume 3. Integration Concepts*, BMI-2054, vol. 3, Battelle Columbus Laboratories, 1980.
- l. Considered to be 50% more expensive than petroleum naphtha.
- m. *Oil & Gas J.* (Nov. 2, 1981).
- n. Based on heating value, natural gas.
- o. *Agricultural Statistics, 1980*, USDA.

^cNo significant limits for purposes of the model.

^dIncluded in the processing costs.

Table 6. Conversion processes

Product/Raw material ^a	Product/Raw material
Acetaldehyde/Ethanol	Ethanol/Molasses
Acetaldehyde/Ethylene (A)	Ethanol/Sugar beets
Acetaldehyde/Ethylene (B)	Ethanol/Sulfite waste liquor
Acetic acid/Acetaldehyde	Ethanol/Wood
Acetic acid/ <i>n</i> -Butane	Ethyl benzene/Benzene
Acetic acid/Ethanol	Ethylene/Coal
Acetic acid/Glucose	Ethylene/Ethanol
Acetic acid/Marine algae	Ethylene/Municipal solid wastes
Acetic acid/Methanol	Ethylene/Naphtha, petroleum
Acetic acid/Sulfite black liquor	Ethylene glycol/Ethylene
Acetic acid/Wood	Ethylene glycol/Ethylene oxide
Acetone/Isopropanol	Ethylene glycol/Formaldehyde
Acetone/Propylene	Ethylene oxide/Ethylene
Ammonia/Coal	Formaldehyde/Methanol
Ammonia/Methane	Glucose/Aquatic biomass
Ammonia/Wood	Glucose/Corn stover (A)
Benzene/Coal	Glucose/Corn stover (B)
Benzene/Catalytic reformat, coal	Glucose/Sugar cane
Benzene/Catalytic reformat, petroleum	Glucose/Wheat straw
Benzene/Toluene	Glucose/Wood (A)
Butadiene/ <i>n</i> -Butane	Glucose/Wood (B)
Butadiene/Ethanol	Glycerine/Glucose
<i>n</i> -Butanol/Acetaldehyde	Glycerine/Propylene
<i>n</i> -Butanol/Glucose	Hydrogen/Coal
<i>n</i> -Butanol/Molasses	Hydrogen/Methane
<i>n</i> -Butanol/Propylene	Hydrogen/Wood
<i>sec</i> -Butanol/ <i>n</i> -Butenes	Lignin, wood/Wood
<i>n</i> -Butenes/ <i>n</i> -Butanol	Methane/Coal
<i>n</i> -Butenes/ <i>sec</i> -Butanol	Methane/Feedlot wastes
<i>n</i> -Butenes/Refinery gas	Methane/Kelp
Carbon monoxide/Coal	Methane/Wheat straw
Carbon monoxide/Methane	Methane/Wood
Carbon monoxide/Wood	Methanol/Carbon dioxide
Catalytic reformat, coal/Naphtha, coal	Methanol/Coal
Catalytic reformat, petroleum/Naphtha, petroleum	Methanol/Methane
Cyclohexane/Benzene	Methanol/Wood
Cyclohexane/Naphtha, coal	Methyl ethyl ketone/ <i>sec</i> -Butanol
Cyclohexane/Naphtha, petroleum	Methyl ethyl ketone/ <i>n</i> -Butene
Cyclohexanone/Cyclohexane	Phenol/Benzene
Cyclohexanone/Phenol	Phenol/Lignin, Kraft
Ethanol/Corn	Phenol/Lignin, wood
Ethanol/Corn stover	Phthalic anhydride/Naphthalene
Ethanol/Ethylene	Phthalic anhydride/ <i>o</i> -Xylene
Ethanol/Glucose	Isopropanol/Acetone
Ethanol/Methanol	Isopropanol/Propylene
	Propylene/Isopropanol
	Propylene/Refinery gas
	Propylene oxide/Propylene
	Urea/Ammonia
	Urea/Methane

^a(A) and (B) refer to different processes.

published capital costs to this common basis. Battery limits costs were multiplied by 1.4 to obtain total plant costs. Working capital was taken to be 15% of the fixed capital for nonseasonal raw materials processes, and 25% of fixed capital for processes using seasonal raw materials. The activity cost (c_j) to build and operate a plant was taken to be the sum of operating fixed costs plus sales, administration, and research plus return on investment. Operating fixed costs were estimated as 19% of total fixed capital. Sales, administration, and research were estimated as 12% of revenues from sales of products. Return on investment was set at 25% of the fixed and working capital for established technologies and 35% for unproven technologies to reflect uncertainty and attendant financial risk. Utilities were considered separately, as shown in Appendix B. Utilities are purchased, analogous to raw materials; hence the costs can be altered easily. Unit costs used throughout this study are shown in Table 7.

Table 7. Costs for utilities

Utility	Cost (\$/unit)
Steam	\$11/t
Electricity	\$14/10 ⁹ J
Fuel	\$1.2/10 ⁹ J
Cooling water	\$0.026/m ³
Process water	\$0.42/m ³

Three categories of useful information can be obtained from solutions to the optimization problem for the simulation of this organic chemicals industry. First, the set of optimal activities is identified which maximizes the profit objective function. Second, the sensitivity of the optimal solution to all input parameters is obtained. In other words, the range is given over which the cost of each activity can vary and

still remain optimal. For nonoptimal activities, the cost is given at which the activity would become optimal. This feature enables the user of the model to interpret the significance of the optimal set of activities in light of the reliability of the input data. Mathematically optimal activities and "close but nonoptimal" activities may be essentially of equal value to the objective function within the limits of data accuracy. The result is essentially a multiplicity of optimal sets of activities. These characteristics of the model should be considered when the solutions are used to help evaluate R&D programs.

Third, a measure of the potential value of hypothetical new technologies can be obtained. Raw material requirements and product yields are postulated for the new conversion process, and the process is added to the model with zero cost (i.e., zero c_j). Raw materials are purchased, and products are sold. The activity level of the new process and the increase in system profit provide a quantitative indication of the potential value of this new hypothetical technology. The increase in system profit may be significantly greater than sales revenues less raw material costs if the levels of other activities are altered due to the presence of the new technology.

4. OPTIMAL SOLUTIONS

From the discussion of the chemical industry model in Sect. 3 and the catalog of process data in Appendix B, it can be readily appreciated that a great deal of work is necessary to compile the data for the model. Particularly for the newer, unestablished technologies, the data are estimates and subject to considerable uncertainty. Results from the model should be interpreted with these limitations in mind. However, it is quite easy to upgrade the data base as better information on processes and economics becomes available. Likewise, it is quite easy to add another conversion process and determine the effects of the availability of this process on the total system.

The point is that the model is not static — the input data can be altered (within limits) to suit the user's view of the best values for the data. With this idea in mind, the optimal solutions for four cases will be described in detail. In subsequent sections, postoptimization analyses will be described for these four cases. The particular goal will be the identification of processes with potential for significant added value to the system if R&D work could be done to improve the attractiveness of these processes. The "system" in this case includes the resource and product slates and prices shown in Tables 4 and 5. Use of the model to examine changes in the resource and product slates and prices is discussed briefly at appropriate points in Sects. 5-8.

It should be remembered that the model does not predict the future. It simply determines the optimal activities among the available activities, based on input economic data and constraints.

Only minimal interpretation of the significance of various aspects of the solutions will be given in this section. Instead, the pertinent features of the solutions will be discussed in Sects. 5, 6, and 7 in the context of opportunities for R&D programs.

4.1 Base Case

A base case is useful for two reasons: (1) it provides an opportunity to demonstrate that the model works properly under conditions when the

optimal solution is known (approximately); and (2) it provides a reference solution to aid the interpretation of other cases in which the general characteristics of the optimal solution may not be known.

An attractive situation to simulate for a base case is the current petrochemical industry. The 1979 U.S. production quantities and sales of primary chemical products are already in the model as constraints. The current raw materials and conversion processes also are known. If the model is operating properly, the optimal solution should utilize the current raw materials and processes.

However, one feature of the economic structure of the model differs from the current petrochemical industry. In the model, all chemical plants are presumed to be built in 1981 with 1981 dollars and a required 25% before-tax return on fixed and operating capital investments. Also, raw material and product prices are published "spot market" values. Thus there is no compensation in the model both for (1) old, depreciated plants built with cheap dollars, and for (2) long-term contracts for raw materials and products at lower prices.

The optimal solution for this base case is tabulated in Table 8. The required amounts of all primary chemicals are produced (with the production of even greater quantities of ethanol and propylene). The optimal set of raw materials contains butane, coal, petroleum naphtha, natural gas, and refinery gas. Coal is chosen primarily to produce carbon monoxide for butanol from propylene and acetic acid from methanol. Benzene/Coal is a multiproduct process, and it is not clear which product is pulling this activity into the optimal solution. The optimal set of processes is shown in Table 9, and the number of plants to be built and operated for each process is indicated. The number of plants may be multiplied by the plant capacity listed in Appendix B to obtain the production volume from each process.

It can be seen in Tables 8 and 9 that the optimal solution is a reasonable representation of the current raw material and process conditions. However, there is a significant discrepancy — the total system profit is negative. This condition is generated by the requirement to produce minimum quantities of all primary products and the absence of "profitable" processes in the model to manufacture some of these primary products.

Table 8. Optimal solution: chemical production
and raw material utilization

Case: Base case
Profit: -\$13.4 billion

Primary product	Quantity produced (10 ³ t)	Relative to 1979 production ^a	Primary raw material	Quantity utilized (10 ³ t)	Relative to availability ^b
Acetaldehyde		1.0	Aquatic biomass		
Acetic acid		1.0	n-Butane	1,500	1.0
Acetone		1.0	Coal	6,958	^c
Ammonia		1.0	Corn		
Benzene		1.0	Corn stover		
Butadiene		1.0	Feed lot wastes		
n-Butanol		1.0	Kelp		
Cyclohexane		1.0	Lignin, Kraft		
Cyclohexanone		1.0	Marine algae		
Ethanol	4,277	6.0	Molasses		
Ethylbenzene		1.0	Municipal solid wastes		
Ethylene		1.0	Naphtha, coal		
Ethylene glycol		1.0	Naphtha, petroleum	64,556	^c
Ethylene oxide		1.0	Natural gas	15,459	^c
Formaldehyde		1.0	(methane)		
Glycerol		1.0	Refinery gas	1,043	^c
Methanol		1.0	Sewage sludge		
Methyl ethyl ketone		1.0	Sugar beets		
Phenol		1.0	Sugar cane		
Phthalic anhydride		1.0	Sulfite black liquor		
Isopropanol		1.0	Sulfite waste liquor		
Propylene	6,944	1.1	Sweet sorghum		
Propylene oxide		1.0	Wheat straw		
Urea		1.0	Wood		
p-Xylene		1.0			

^aSee Table 4.

^bSee Table 5.

^cThese materials have unlimited availability.

Table 9. Optimal solution: optimal processes and numbers of plants

Case: Base case
Profit: -\$13.4 billion

Product/Raw material ^a	Number of plants	Product/Raw material	Number of plants
Acetaldehyde/Ethanol		Ethanol/Molasses	
Acetaldehyde/Ethylene (A)		Ethanol/Sugar beets	
Acetaldehyde/Ethylene (B)	8.2	Ethanol/Sulfite waste liquor	
Acetic acid/Acetaldehyde	8.4	Ethanol/Wood	
Acetic acid/ <i>n</i> -Butane		Ethyl benzene/Benzene	5.5
Acetic acid/Ethanol		Ethylene/Coal	
Acetic acid/Glucose		Ethylene/Ethanol	123.6
Acetic acid/Marine algae		Ethylene/Municipal solid wastes	
Acetic acid/Methanol	2.4	Ethylene/Naphtha, petroleum	24.1
Acetic acid/Sulfite black liquor		Ethylene glycol/Ethylene	11.9
Acetic acid/Wood		Ethylene glycol/Ethylene oxide	
Acetone/Isopropanol	4.2	Ethylene glycol/Formaldehyde	
Acetone/Propylene	1.5	Ethylene oxide/Ethylene	18.9
Ammonia/Coal		Formaldehyde/Methanol	59.7
Ammonia/Methane	29.7	Glucose/Aquatic biomass	
Ammonia/Wood		Glucose/Corn stover (A)	
Benzene/Coal	0.6	Glucose/Corn stover (B)	
Benzene/Catalytic reformat, coal		Glucose/Sugar cane	
Benzene/Catalytic reformat, petroleum	11.7	Glucose/Wheat straw	
Benzene/Toluene	34.5	Glucose/Wood (A)	
Butadiene/ <i>n</i> -Butane	18.1	Glucose/Wood (B)	
Butadiene/Ethanol		Glycerine/Glucose	
<i>n</i> -Butanol/Acetaldehyde		Glycerine/Propylene	1.5
<i>n</i> -Butanol/Glucose		Hydrogen/Coal	
<i>n</i> -Butanol/Molasses		Hydrogen/Methane	
<i>n</i> -Butanol/Propylene	5.1	Hydrogen/Wood	
<i>sec</i> -Butanol/ <i>n</i> -Butenes	5.6	Lignin, wood/Wood	
<i>n</i> -Butenes/ <i>n</i> -Butanol		Methane/Coal	
<i>n</i> -Butenes/ <i>sec</i> -Butanol		Methane/Feedlot wastes	
<i>n</i> -Butenes/Refinery gas	4.3	Methane/Kelp	
Carbon monoxide/Coal	10.1	Methane/Wheat straw	
Carbon monoxide/Methane		Methane/Wood	
Carbon monoxide/Wood		Methanol/Carbon dioxide	
Catalytic reformat, coal/Naphtha, coal		Methanol/Coal	
Catalytic reformat, petroleum/Naphtha, petroleum	44.2	Methanol/Methane	5.6
Cyclohexane/Benzene		Methanol/Wood	
Cyclohexane/Naphtha, coal		Methyl ethyl ketone/ <i>sec</i> -Butanol	
Cyclohexane/Naphtha, petroleum	7.3	Methyl ethyl ketone/ <i>n</i> -Butene	6.6
Cyclohexanone/Cyclohexane		Phenol/Benzene	13.2
Cyclohexanone/Phenol	13.2	Phenol/Lignin, Kraft	
Ethanol/Corn		Phenol/Lignin, wood	
Ethanol/Corn stover		Phthalic anhydride/Naphthalene	
Ethanol/Ethylene	15.7	Phthalic anhydride/ <i>o</i> -Xylene	9.2
Ethanol/Glucose		Isopropanol/Acetone	
Ethanol/Methanol		Isopropanol/Propylene	3.2
		Propylene/Isopropanol	
		Propylene/Refinery gas	
		Propylene oxide/Propylene	10.2
		Urea/Ammonia	
		Urea/Methane	14.8

^a(A) and (B) refer to different processes.

The origin of the negative maximum profit can be seen clearly by considering a modified base case. The requirement to equal or exceed the 1979 production volumes for primary products is relaxed and changed to an equal or less-than constraint. The results are shown in Tables 10 and 11. Now the profit is positive and is approximately 16% of revenues from sales of primary and secondary products. However, several primary products are not manufactured. No acetaldehyde, ammonia, and ethylene and derivatives are produced. In addition, less than the 1979 volumes of other primary chemicals are produced. The absence of acetaldehyde, ammonia, and ethylene is caused by the lack of profitable processes in the model for these chemicals. This condition can be verified easily by inspecting the process data in Appendix B. Both ethylene and ammonia are large-volume products that impose substantial costs when production is required.

It would be possible, of course, to adjust the input data for these processes in order to make them profitable to simulate the current chemical industry. However, arbitrary adjustments of this nature would alter the uniform economic basis of the model. For similar reasons, it is not desirable to arbitrarily change the prices of raw materials and primary products. A much more desirable position is recognition that the model is acting properly. It is generally acknowledged, for example, that a profitable ethylene plant cannot be built today based on current technology.⁸

One more feature of the first base case (in which minimum production of all primary products is required) needs to be discussed. Table 9 indicates that both ethanol from ethylene and ethylene from ethanol are optimal activities. This "loop" results from (1) the availability of processes to form such a loop, (2) requirements to produce (not sell) minimum quantities of ethanol and ethylene, and (3) less favorable economics for production of ethylene and ethanol by other routes.

The essential correctness of this interpretation has been verified by increasing the process cost for ethylene from ethanol to a very high value to make this process ridiculously unattractive. In this case no ethylene was produced from ethanol. This result indicates that the loop is created by economics as the profit is maximized (albeit negative), and not an artifact created by the structure of the model. Since the availability of ethylene from ethanol is desirable for subsequent cases to be

Table 10. Optimal solution: chemical production and raw material utilization

Case: Modified base case — no production requirements
Profit: \$2.5 billion

Primary product	Quantity produced (10 ³ t)	Relative to 1979 production ^a	Primary raw material	Quantity utilized (10 ³ t)	Relative to availability ^b
Acetaldehyde			Aquatic biomass		
Acetic acid	260	0.2	n-Butane		
Acetone	1,200	1.0	Coal	96.9	^c
Ammonia			Corn		
Benzene	859	0.2	Corn stover		
Butadiene	858	0.5	Feed lot wastes		
n-Butanol	202	0.6	Kelp		
Cyclohexane	1,100	1.0	Lignin, Kraft		
Cyclohexanone	397	1.0	Marine algae		
Ethanol			Molasses		
Ethylbenzene	392	0.1	Municipal solid wastes		
Ethylene			Naphtha, coal		
Ethylene glycol			Naphtha, petroleum	12,603	^c
Ethylene oxide			Natural gas (methane)	3,354	^c
Formaldehyde	2,710	1.0	Refinery gas	9,248	^c
Glycerol	68	1.0	Sewage sludge		
Methanol	2,856	0.9	Sugar beets		
Methyl ethyl ketone	298	1.0	Sugar cane		
Phenol	920	0.7	Sulfite black liquor		
Phthalic anhydride	460	1.0	Sulfite waste liquor		
Isopropanol	542	0.6	Sweet sorghum		
Propylene	5,099	0.8	Wheat straw		
Propylene oxide	120	0.1	Wood		
Urea	5,420	1.0			
p-Xylene	873	0.4			

^aSee Table 4.

^bSee Table 5.

^cThese materials have unlimited availability.

Table 11. Optimal solution: optimal processes
and numbers of plantsCase: Modified base case — no production requirements
Profit: \$2.5 billion

Product/Raw material ^a	Number of plants	Product/Raw material	Number of plants
Acetaldehyde/Ethanol		Ethanol/Molasses	
Acetaldehyde/Ethylene (A)		Ethanol/Sugar beets	
Acetaldehyde/Ethylene (B)		Ethanol/Sulfite waste liquor	
Acetic acid/Acetaldehyde		Ethanol/Wood	
Acetic acid/ <i>n</i> -Butane	1.9	Ethyl benzene/Benzene	
Acetic acid/Ethanol		Ethylene/Coal	
Acetic acid/Glucose		Ethylene/Ethanol	
Acetic acid/Marine algae		Ethylene/Municipal solid wastes	
Acetic acid/Methanol		Ethylene/Naphtha, petroleum	
Acetic acid/Sulfite black liquor		Ethylene glycol/Ethylene	
Acetic acid/Wood		Ethylene glycol/Ethylene oxide	
Acetone/Isopropanol		Ethylene glycol/Formaldehyde	
Acetone/Propylene	9.3	Ethylene oxide/Ethylene	
Ammonia/Coal		Formaldehyde/Methanol	59.7
Ammonia/Methane		Glucose/Aquatic biomass	
Ammonia/Wood		Glucose/Corn stover (A)	
Benzene/Coal		Glucose/Corn stover (B)	
Benzene/Catalytic reformat, coal		Glucose/Sugar cane	
Benzene/Catalytic reformat, petroleum	4.8	Glucose/Wheat straw	
Benzene/Toluene		Glucose/Wood (A)	
Butadiene/ <i>n</i> -Butane	9.5	Glucose/Wood (B)	
Butadiene/Ethanol		Glycerine/Glucose	
<i>n</i> -Butanol/Acetaldehyde		Glycerine/Propylene	1.5
<i>n</i> -Butanol/Glucose		Hydrogen/Coal	
<i>n</i> -Butanol/Molasses		Hydrogen/Methane	
<i>n</i> -Butanol/Propylene	3.0	Hydrogen/Wood	
<i>sec</i> -Butanol/ <i>n</i> -Butenes	5.6	Lignin, wood/Wood	
<i>n</i> -Butenes/ <i>n</i> -Butanol		Methane/Coal	
<i>n</i> -Butenes/ <i>sec</i> -Butanol		Methane/Feedlot wastes	
<i>n</i> -Butenes/Refinery gas	10.2	Methane/Kelp	
Carbon monoxide/Coal	2.8	Methane/Wheat straw	
Carbon monoxide/Methane		Methane/Wood	
Carbon monoxide/Wood		Methanol/Carbon dioxide	
Catalytic reformat, coal/ Naphtha, coal		Methanol/Coal	
Catalytic reformat, petroleum/ Naphtha, petroleum	18.3	Methanol/Methane	4.8
Cyclohexane/Benzene		Methanol/Wood	
Cyclohexane/Naphtha, coal		Methyl ethyl ketone/ <i>sec</i> -Butanol	
Cyclohexane/Naphtha, petroleum	7.3	Methyl ethyl ketone/ <i>n</i> -Butene	6.6
Cyclohexanone/Cyclohexane	0.1	Phenol/Benzene	9.2
Cyclohexanone/Phenol	12.9	Phenol/Lignin, Kraft	
Ethanol/Corn		Phenol/Lignin, wood	
Ethanol/Corn stover		Phthalic anhydride/Naphthalene	
Ethanol/Ethylene		Phthalic anhydride/ <i>o</i> -Xylene	9.2
Ethanol/Glucose		Isopropanol/Acetone	
Ethanol/Methanol		Isopropanol/Propylene	2.0
		Propylene/Isopropanol	
		Propylene/Refinery gas	28.2
		Propylene oxide/Propylene	1.2
		Urea/Ammonia	
		Urea/Methane	14.8

^a(A) and (B) refer to different processes.

studied, it was decided to accept this peculiar loop behavior for current model demonstration purposes and interpret solutions to the model accordingly. The model should be modified to eliminate such process loops for future studies.

These two base cases demonstrate that the model will satisfactorily simulate the current chemical industry. Sensitivity analyses of these two cases will be described later. First, the optimal solutions for three more special cases will be described. Each of these cases will be compared with the first base case (hereafter called simply the base case), which requires minimum production of all primary products.

4.2 Increased Petroleum/Natural Gas/Butane Costs

This case considers a 100% increase in the prices of petroleum naphtha, natural gas, butane, and refinery gas. All other economic factors and constraints are identical to the base case. This case is selected to simulate a (severe) increase in petroleum price, while other costs remain constant. It can be argued that such a divergence is unlikely. This case represents a limit. Probable conditions will lie somewhere between a limiting case such as this case and the base case.

The optimal solution is shown in Tables 12 and 13. The change in system profit is — \$9.5 billion (i.e., the profit is more negative by \$9.5 billion).

The following major changes are relative to the base case:

1. Substantial coal is used for the production of benzene and ethylene as primary products. Several other primary chemicals are produced in these processes. The excess production of *n*-butanol occurs in this manner.
2. No petroleum naphtha is used. Natural gas consumption is reduced slightly, while refinery gas consumption is doubled. The latter is due to the addition of propylene from refinery gas to replace propylene obtained as a by-product from the Ethylene/Petroleum naphtha process. Butane use is unaltered at the limit of availability. The net reduction in consumption of petroleum, natural gas, and refinery gas is 67.5×10^9 kg, with a value of ~\$21 billion.

Table 12. Optimal solution: chemical production and raw material utilization

Case: Prices of butane, petroleum naphtha, natural gas,
and refinery gas increased 100%
Profit: -\$23.0 billion

Primary product	Quantity produced (10 ³ t)	Relative to 1979 production ^a	Primary raw material	Quantity utilized (10 ³ t)	Relative to availability ^b
Acetaldehyde		1.0	Aquatic biomass		
Acetic acid		1.0	<i>n</i> -Butane	1,500	1.0
Acetone		1.0	Coal	139,746	^c
Ammonia		1.0	Corn		
Benzene		1.0	Corn stover		
Butadiene		1.0	Feed lot wastes		
<i>n</i> -Butanol	3,752	10.8	Kelp		
Cyclohexane		1.0	Lignin, Kraft		
Cyclohexanone		1.0	Marine algae		
Ethanol	7,332	10.3	Molasses		
Ethylbenzene		1.0	Municipal solid wastes		
Ethylene		1.0	Naphtha, coal	21,562	^c
Ethylene glycol		1.0	Naphtha, petroleum		
Ethylene oxide		1.0	Natural gas (methane)	14,139	^c
Formaldehyde		1.0	Refinery gas	2,670	^c
Glycerol		1.0	Sewage sludge		
Methanol		1.0	Sugar beets	17,000	1.0
Methyl ethyl ketone		1.0	Sugar cane	14,750	0.7
Phenol		1.0	Sulfite black liquor		
Phthalic anhydride		1.0	Sulfite waste liquor		
Isopropanol		1.0	Sweet sorghum	11,080	0.2
Propylene		1.0	Wheat straw		
Propylene oxide		1.0	Wood		
Urea		1.0			
<i>p</i> -Xylene		1.0			

^aSee Table 4.

^bSee Table 5.

^cThese materials have unlimited availability.

Table 13. Optimal solution: optimal processes
and numbers of plants

Case: Prices of butane, petroleum naphtha, natural gas,
and refinery gas increased 100%
Profit: -\$23.0 billion

Product/Raw material ^a	Number of plants	Product/Raw material	Number of plants
Acetaldehyde/Ethanol		Ethanol/Molasses	
Acetaldehyde/Ethylene (A)		Ethanol/Sugar beets	33.1
Acetaldehyde/Ethylene (B)	8.2	Ethanol/Sulfite waste liquor	
Acetic acid/Acetaldehyde	8.4	Ethanol/Wood	
Acetic acid/ <i>n</i> -Butane		Ethyl benzene/Benzene	5.5
Acetic acid/Ethanol		Ethylene/Coal	38.5
Acetic acid/Glucose		Ethylene/Ethanol	211.9
Acetic acid/Marine algae		Ethylene/Municipal solid wastes	
Acetic acid/Methanol	2.4	Ethylene/Naphtha, petroleum	
Acetic acid/Sulfite black liquor		Ethylene glycol/Ethylene	11.9
Acetic acid/Wood		Ethylene glycol/Ethylene oxide	
Acetone/Isopropanol		Ethylene glycol/Formaldehyde	
Acetone/Propylene	5.7	Ethylene oxide/Ethylene	18.9
Ammonia/Coal		Formaldehyde/Methanol	59.7
Ammonia/Methane	19.7	Glucose/Aquatic biomass	
Ammonia/Wood		Glucose/Corn stover (A)	
Benzene/Coal	0.6	Glucose/Corn stover (B)	
Benzene/Catalytic reformat, coal	11.7	Glucose/Sugar cane	
Benzene/Catalytic reformat, petroleum		Glucose/Wheat straw	
Benzene/Toluene	34.1	Glucose/Wood (A)	
Butadiene/ <i>n</i> -Butane	18.1	Glucose/Wood (B)	
Butadiene/Ethanol		Glycerine/Glucose	
<i>n</i> -Butanol/Acetaldehyde		Glycerine/Propylene	1.5
<i>n</i> -Butanol/Glucose		Hydrogen/Coal	
<i>n</i> -Butanol/Molasses		Hydrogen/Methane	
<i>n</i> -Butanol/Propylene		Hydrogen/Wood	
<i>sec</i> -Butanol/ <i>n</i> -Butenes	5.5	Lignin, wood/Wood	
<i>n</i> -Butenes/ <i>n</i> -Butanol	21.5	Methane/Coal	
<i>n</i> -Butenes/ <i>sec</i> -Butanol		Methane/Feedlot wastes	
<i>n</i> -Butenes/Refinery gas	5.9	Methane/Kelp	
Carbon monoxide/Coal	5.2	Methane/Wheat straw	
Carbon monoxide/Methane		Methane/Wood	
Carbon monoxide/Wood		Methanol/Carbon dioxide	
Catalytic reformat, coal/Naphtha, coal	34.3	Methanol/Coal	
Catalytic reformat, petroleum/Naphtha, petroleum		Methanol/Methane	5.6
Cyclohexane/Benzene	11.0	Methanol/Wood	
Cyclohexane/Naphtha, coal		Methyl ethyl ketone/ <i>sec</i> -Butanol	
Cyclohexane/Naphtha, petroleum		Methyl ethyl ketone/ <i>n</i> -Butene	6.6
Cyclohexanone/Cyclohexane		Phenol/Benzene	13.2
Cyclohexanone/Phenol	13.2	Phenol/Lignin, Kraft	
Ethanol/Corn		Phenol/Lignin, wood	
Ethanol/Corn stover		Phthalic anhydride/Naphthalene	
Ethanol/Ethylene	15.7	Phthalic anhydride/ <i>o</i> -Xylene	9.2
Ethanol/Glucose		Isopropanol/Acetone	
Ethanol/Methanol		Isopropanol/Propylene	3.2
		Propylene/Isopropanol	10.6
		Propylene/Refinery gas	5.2
		Propylene oxide/Propylene	10.2
		Urea/Ammonia	15.9
		Urea/Methane	

^a(A) and (B) refer to different processes.

3. Ethanol from sugar beets enters the optimal solution. (This process is actually a multiple feedstock process utilizing sugar beets, sugar cane, and sweet sorghum.) The total availability of sugar beets is used. The ethylene/ethanol loop persists; the demise of petroleum naphtha coincides with the entry of ethanol from sugar beets as a source of ethylene and derivatives.
4. Major alterations in the set of optimal conversion processes include benzene from coal; catalytic reformat from coal instead of petroleum processes; loss of *n*-butanol from propylene and acetone from isopropanol; urea from ammonia instead of methane; addition of propylene from refinery gas; cyclohexane from benzene instead of petroleum naphtha. (Note: Some of these changes may effectively represent multiple optima. This possibility will be addressed in Sect. 5.) Ethanol from sugar beets is added, and a propylene/isopropanol loop occurs analogous to the ethylene/ethanol loop.

4.3 Increased Costs and Decreased Availabilities of Petroleum/Natural Gas/Butane

It is reasonable to expect that increased costs for raw materials will lead to decreased consumption of these raw materials. This result was obtained to a significant degree in the previous case. Coal utilization was increased to compensate for the decrease in petroleum feedstocks, and sugars from biomass became important. Another way to simulate these conditions is to reduce availabilities and increase costs simultaneously. In the case examined here, prices of petroleum and natural gas feedstocks are doubled as in Subsect. 4.2, and the availabilities of these raw materials are set at 50% of the quantities utilized in the base case.

The optimal solution is shown in Tables 14 and 15. The change in system profit is — \$10.8 billion, only slightly more negative than the change when only prices were doubled. One major change occurs in resource utilization — wood, rather than methane, is used to produce ammonia. Coal utilization is up slightly, while butane, natural gas, and refinery gas are utilized at the (reduced) limits of availability.

Table 14. Optimal solution: chemical production and raw material utilization

Case: Prices of butane, petroleum naphtha, natural gas, and refinery gas increased 100%, and availabilities of these resources reduced to 50% of utilization in the base case

Profit: -\$24.3 billion

Primary product	Quantity produced (10 ³ t)	Relative to 1979 production ^a	Primary raw material	Quantity utilized (10 ³ t)	Relative to availability ^b
Acetaldehyde		1.0	Aquatic biomass		
Acetic acid		1.0	<i>n</i> -Butane	750	1.0
Acetone		1.0	Coal	151,315	^c
Ammonia		1.0	Corn		
Benzene		1.0	Corn stover		
Butadiene		1.0	Feed lot wastes		
<i>n</i> -Butanol	4,065	11.7	Kelp		
Cyclohexane		1.0	Lignin, Kraft		
Cyclohexanone		1.0	Marine algae		
Ethanol	7,332	10.3	Molasses		
Ethylbenzene		1.0	Municipal solid wastes		
Ethylene		1.0	Naphtha, coal	21,561	^c
Ethylene glycol		1.0	Naphtha, petroleum		
Ethylene oxide		1.0	Natural gas (methane)	7,730	1.0
Formaldehyde		1.0	Refinery gas	522	1.0
Glycerol		1.0	Sewage sludge		
Methanol		1.0	Sugar beets	17,000	1.0
Methyl ethyl ketone		1.0	Sugar cane	14,750	0.7
Phenol		1.0	Sulfite black liquor		
Phthalic anhydride		1.0	Sulfite waste liquor		
Isopropanol	1,617	1.9	Sweet sorghum	11,080	0.2
Propylene		1.0	Wheat straw		
Propylene oxide		1.0	Wood	15,052	0.2
Urea		1.0			
<i>p</i> -Xylene		1.0			

^aSee Table 4.

^bSee Table 5.

^cThese materials have unlimited availability.

Table 15. Optimal solution: optimal processes and numbers of plants

Case: Prices of butane, petroleum naphtha, natural gas, and refinery gas increased 100% and availabilities of these resources reduced to 50% of utilization in the base case
 Profit: -\$24.3 billion

Product/Raw material ^a	Number of plants	Product/Raw material	Number of plants
Acetaldehyde/Ethanol		Ethanol/Molasses	
Acetaldehyde/Ethylene (A)		Ethanol/Sugar beets	33.1
Acetaldehyde/Ethylene (B)	8.2	Ethanol/Sulfite waste liquor	
Acetic acid/Acetaldehyde	1.2	Ethanol/Wood	
Acetic acid/ <i>n</i> -Butane		Ethyl benzene/Benzene	5.5
Acetic acid/Ethanol		Ethylene/Coal	41.7
Acetic acid/Glucose		Ethylene/Ethanol	173.8
Acetic acid/Marine algae		Ethylene/Municipal solid wastes	
Acetic acid/Methanol	9.7	Ethylene/Naphtha, petroleum	
Acetic acid/Sulfite black liquor		Ethylene glycol/Ethylene	11.9
Acetic acid/Wood		Ethylene glycol/Ethylene oxide	
Acetone/Isopropanol		Ethylene glycol/Formaldehyde	
Acetone/Propylene	5.7	Ethylene oxide/Ethylene	18.9
Ammonia/Coal		Formaldehyde/Methanol	59.7
Ammonia/Methane	15.2	Glucose/Aquatic biomass	
Ammonia/Wood	66.7	Glucose/Corn stover (A)	
Benzene/Coal	0.6	Glucose/Corn stover (B)	
Benzene/Catalytic reformat, coal	11.7	Glucose/Sugar cane	
Benzene/Catalytic reformat, petroleum		Glucose/Wheat straw	
Benzene/Toluene	34.1	Glucose/Wood (A)	
Butadiene/ <i>n</i> -Butane	10.6	Glucose/Wood (B)	
Butadiene/Ethanol	16.8	Glycerine/Glucose	1.5
<i>n</i> -Butanol/Acetaldehyde		Glycerine/Propylene	
<i>n</i> -Butanol/Glucose		Hydrogen/Coal	
<i>n</i> -Butanol/Molasses		Hydrogen/Methane	
<i>n</i> -Butanol/Propylene		Hydrogen/Wood	
<i>sec</i> -Butanol/ <i>n</i> -Butenes	5.6	Lignin, wood/Wood	
<i>n</i> -Butenes/ <i>n</i> -Butanol	40.2	Methane/Coal	
<i>n</i> -Butenes/ <i>sec</i> -Butanol		Methane/Feedlot wastes	
<i>n</i> -Butenes/Refinery gas	2.2	Methane/Kelp	
Carbon monoxide/Coal	20.8	Methane/Wheat straw	
Carbon monoxide/Methane		Methane/Wood	
Carbon monoxide/Wood		Methanol/Carbon dioxide	1.4
Catalytic reformat, coal/Naphtha, coal	34.3	Methanol/Coal	
Catalytic reformat, petroleum/Naphtha, petroleum		Methanol/Methane	4.8
Cyclohexane/Benzene	11.0	Methanol/Wood	
Cyclohexane/Naphtha, coal		Methyl ethyl ketone/ <i>sec</i> -Butanol	
Cyclohexane/Naphtha, petroleum		Methyl ethyl ketone/ <i>n</i> -Butene	6.6
Cyclohexanone/Cyclohexane		Phenol/Benzene	13.2
Cyclohexanone/Phenol	13.2	Phenol/Lignin, Kraft	
Ethanol/Corn		Phenol/Lignin, wood	
Ethanol/Corn stover		Phthalic anhydride/Naphthalene	
Ethanol/Ethylene	15.7	Phthalic anhydride/ <i>o</i> -Xylene	9.2
Ethanol/Glucose		Isopropanol/Acetone	
Ethanol/Methanol		Isopropanol/Propylene	5.9
		Propylene/Isopropanol	35.7
		Propylene/Refinery gas	
		Propylene oxide/Propylene	10.2
		Urea/Ammonia	15.9
		Urea/Methane	

^a(A) and (B) refer to different processes.

Several changes occur in process selection compared to the price-increase-only case. Acetic acid from methanol is increased, and acetic acid from acetaldehyde is decreased. Ammonia from wood shows up strong, and ammonia from methane is decreased. Butadiene from ethanol is added. Carbon monoxide is increased. Methanol from carbon dioxide appears at a low level, and propylene from refinery gas is deleted. (Again, some of these changes may be essentially multiple optima.)

4.4 No Fossil Raw Materials

It certainly is possible to restrict the availabilities and alter the prices of fossil raw materials according to various schemes to simulate hypothetical future conditions. But for purposes of illustration, and to establish a limit, the case of zero availability of all fossil resources (including coal) will be examined here. Although this situation is quite unrealistic, it does represent a worst-case condition and provides insight for subsequent studies of more probable conditions (including altered product slates and prices).

The optimal solution is shown in Tables 16 and 17. The constraints are modified slightly from the base case, however. No solution could be obtained to produce the minimal quantities of all primary products. The two chemicals which could not be produced in sufficient quantities using technologies in the model were phthalic anhydride and *p*-xylene. This difficulty arose from the lack of adequate technologies in the model, and not from a resource limitation. In order to obtain a solution for a chemical industry with no fossil resources, the production requirements for phthalic anhydride and *p*-xylene were eliminated. As can be seen in Table 16, phthalic anhydride and *p*-xylene are not produced.

Several significant features of the optimal solution are the following:

1. Wood is clearly the dominant resource. Approximately 70% of the estimated supply is used. The total supply of Kraft lignin and a significant fraction of the corn supply are used. (Recall that the sugar beets/sugar cane/sweet sorghum process for ethanol also was present in previous cases.)

Table 16. Optimal solution: chemical production
and raw material utilization

Case: No fossil raw materials
Profit: -\$38.9 billion

Primary product	Quantity produced (10 ³ t)	Relative to 1979 production ^a	Primary raw material	Quantity utilized (10 ³ t)	Relative to availability ^b
Acetaldehyde	2,098	1.9	Aquatic biomass		
Acetic acid		1.0	<i>n</i> -Butane		
Acetone	1,967	1.6	Coal		
Ammonia		1.0	Corn	4,597	0.3
Benzene		1.0	Corn stover		
Butadiene		1.0	Feed lot wastes		
<i>n</i> -Butanol	3,934	11.3	Kelp		
Cyclohexane		1.0	Lignin, Kraft	19,000	1.0
Cyclohexanone		1.0	Marine algae		
Ethanol	25,777	36.3	Molasses		
Ethylbenzene		1.0	Municipal solid wastes		
Ethylene		1.0	Naphtha, coal		
Ethylene glycol		1.0	Naphtha, petroleum		
Ethylene oxide		1.0	Natural gas (methane)		
Formaldehyde		1.0	Refinery gas		
Glycerol		1.0	Sewage sludge		
Methanol		1.0	Sugar beets	17,000	1.0
Methyl ethyl ketone	7,470	5.5	Sugar cane	14,750	0.7
Phenol	0	0	Sulfite black liquor		
Phthalic anhydride	9,692	11.2	Sulfite waste liquor		
Isopropanol		1.0	Sweet sorghum	11,080	0.2
Propylene		1.0	Wheat straw	128,310	0.7
Propylene oxide		1.0	Wood		
Urea		1.0			
<i>p</i> -Xylene	0	0			

^aSee Table 4.

^bSee Table 5.

Table 17. Optimal solution: optimal processes and numbers of plants

Case: No fossil raw materials
Profit: -\$38.9 billion

Product/Raw material ^a	Number of plants	Product/Raw material	Number of plants
Acetaldehyde/Ethanol		Ethanol/Molasses	
Acetaldehyde/Ethylene (A)		Ethanol/Sugar beets	33.1
Acetaldehyde/Ethylene (B)	15.4	Ethanol/Sulfite waste liquor	
Acetic acid/Acetaldehyde		Ethanol/Wood	
Acetic acid/ <i>n</i> -Butane		Ethyl benzene/Benzene	7.3
Acetic acid/Ethanol		Ethylene/Coal	
Acetic acid/Glucose		Ethylene/Ethanol	680.0
Acetic acid/Marine algae		Ethylene/Municipal solid wastes	
Acetic acid/Methanol	10.9	Ethylene/Naphtha, petroleum	
Acetic acid/Sulfite black liquor		Ethylene glycol/Ethylene	11.9
Acetic acid/Wood		Ethylene glycol/Ethylene oxide	
Acetone/Isopropanol		Ethylene glycol/Formaldehyde	
Acetone/Propylene		Ethylene oxide/Ethylene	18.9
Ammonia/Coal		Formaldehyde/Methanol	59.7
Ammonia/Methane		Glucose/Aquatic biomass	
Ammonia/Wood	136.9	Glucose/Corn stover (A)	
Benzene/Coal		Glucose/Corn stover (B)	
Benzene/Catalytic reformat, coal		Glucose/Sugar cane	
Benzene/Catalytic reformat, petroleum		Glucose/Wheat straw	
Benzene/Toluene		Glucose/Wood (A)	
Butadiene/ <i>n</i> -Butane		Glucose/Wood (B)	1182.8
Butadiene/Ethanol	40.7	Glycerine/Glucose	5.0
<i>n</i> -Butanol/Acetaldehyde		Glycerine/Propylene	
<i>n</i> -Butanol/Glucose	56.2	Hydrogen/Coal	
<i>n</i> -Butanol/Molasses		Hydrogen/Methane	
<i>n</i> -Butanol/Propylene		Hydrogen/Wood	
<i>sec</i> -Butanol/ <i>n</i> -Butenes	5.5	Lignin, wood/Wood	
<i>n</i> -Butenes/ <i>n</i> -Butanol	51.0	Methane/Coal	
<i>n</i> -Butenes/ <i>sec</i> -Butanol		Methane/Feedlot wastes	
<i>n</i> -Butenes/Refinery gas		Methane/Kelp	
Carbon monoxide/Coal		Methane/Wheat straw	
Carbon monoxide/Methane		Methane/Wood	22.9
Carbon monoxide/Wood	23.3	Methanol/Carbon dioxide	3.5
Catalytic reformat, coal/Naphtha, coal		Methanol/Coal	
Catalytic reformat, petroleum/Naphtha, petroleum		Methanol/Methane	3.7
Cyclohexane/Benzene	11.0	Methanol/Wood	
Cyclohexane/Naphtha, coal		Methyl ethyl ketone/ <i>sec</i> -Butanol	
Cyclohexane/Naphtha, petroleum		Methyl ethyl ketone/ <i>n</i> -Butene	6.6
Cyclohexanone/Cyclohexane		Phenol/Benzene	
Cyclohexanone/Phenol	13.2	Phenol/Lignin, Kraft	129.3
Ethanol/Corn	7.4	Phenol/Lignin, wood	123.1
Ethanol/Corn stover		Phthalic anhydride/Naphthalene	
Ethanol/Ethylene	37.1	Phthalic anhydride/ <i>o</i> -Xylene	
Ethanol/Glucose	138.6	Isopropanol/Acetone	29.9
Ethanol/Methanol		Isopropanol/Propylene	28.2
		Propylene/Isopropanol	322.0
		Propylene/Refinery gas	
		Propylene oxide/Propylene	10.2
		Urea/Ammonia	15.9
		Urea/Methane	

^a(A) and (B) refer to different processes.

2. There is overproduction of several products. Isopropanol, phenol, ethanol, and *n*-butanol have the most extensive overproduction. However, ethanol and isopropanol are in alcohol/olefin loops which contribute to overproduction of these products.
3. Ammonia, methane, and carbon monoxide are produced from wood, along with the intermediate feedstocks glucose and lignin.

The presence of the two alcohol/olefin loops creates the possibility that material is cycled to meet the production requirements and the raw material needs are understated in the optimal solution. In the worst case of no fossil resources, no ethylene, ethanol, propylene, or isopropanol is sold; however, ethylene derivatives are sold to the extent of 34% of the ethylene production, and propylene oxide is sold to the extent of 13% of the propylene production. Therefore, at least these portions of the raw materials are consumed. Since these two olefins are a substantial fraction of the total chemical production, total consumption of resources might increase significantly and additional conversion processes utilizing additional raw materials might be required if these loops were avoided. Further modifications to the model are needed to eliminate these two loops and yet maintain flexibility for process selection.

5. POSTOPTIMIZATION ANALYSIS

A vast amount of parameter sensitivity information is provided with the optimal solution. The basic nature of this information has been described in Subsect. 3.1. In this section one portion of the sensitivity information is used to identify conversion processes that may have significant potential if the necessary R&D goals can be accomplished. Other analyses that would be useful to identify promising processes will be mentioned at the end of the section.

Each conversion process in the model falls into one of three categories with respect to the optimal solution for a given input condition:

1. The process is optimal and has a nonzero level of activity.
2. The process has a zero level of activity, but would become optimal and have a nonzero level of activity if the cost were reduced to a specified value.
3. The process has a zero level of activity, and reduction of the cost to zero will not produce a nonzero level of activity.

Category 1 processes are clearly already good, although reduction of costs would increase profit. Category 3 processes are lost causes, so to speak; nothing can be done to make these processes attractive. This is an approximation, of course, because the process description (yields, etc.) could be improved, which might improve the economics sufficiently to move the process from category 3 to category 2, or even to category 1. However, processes already in category 2 would require more modest improvements and hence will probably be more attractive from this point of view.

Processes in category 2 are listed in Tables 18, 19, and 20 for three of the cases discussed in Sect. 3. For each process the percent reduction in cost (c_j , as described in Subsects. 3.1 and 3.2) needed to achieve optimality and the percent of the primary chemical production requirement that would be manufactured by this process are also shown. These data pertain to only one process at a time.

In the tables, the processes with the most potential are those which could produce a substantial fraction of the chemical product demand, particularly for chemicals with relatively high demand. The required reduction in cost is a measure of the research and development which would be needed

Table 18. Cost reductions needed for inactive processes to become active

Case: Base case

Process	Reduction in cost (%)	Production requirement for primary product from this process ^a (%)
Ammonia/Coal	46	100
Ammonia/Wood	44	100
Acetic acid/Butane	86	<1
Acetic acid/Wood	17	<1
n-Butanol/Acetaldehyde	92	58
Cyclohexane/Benzene	68	1
Carbon monoxide/Wood	31	101
Carbon monoxide/Methane	4	102
Ethanol/Methanol	3	33
Ethylene/Coal	7	3
Methane/Wood	85	68
Methanol/Carbon dioxide	54	32
Methanol/Coal	55	9
Methanol/Wood	57	9
Methyl ethyl ketone/ sec-Butanol	10	88
Phenol/Kraft lignin	13	64

^aFor chemicals which have no specified production requirements, the percent of actual production or utilization in the optimal solution is given.

Table 19. Cost reductions needed for inactive processes to become active

Case: Increased costs and decreased availabilities of petroleum, natural gas, and butane

Process ^a	Reduction in cost (%)	Production requirement for primary product from this process ^b (%)
Acetaldehyde/Ethylene (A)	11	100
Acetic acid/Wood	5	6
Acetone/Isopropanol	35	32
Ammonia/Coal	3	49
Carbon monoxide/Methane	53	100
Carbon monoxide/Wood	23	100
Cyclohexane/Coal naphtha	30	1
Ethanol/Corn	14	31
Ethanol/Glucose	20	31
Ethanol/Wood	46	31
Ethylene/Petroleum naphtha	74	16
Methanol/Coal	14	86
Methanol/Wood	22	87
Methane/Wood	24	79
Phenol/Kraft lignin	16	17

^a(A) and (B) refer to different processes.

^bFor chemicals which have no specified production requirements, the percent of actual production or utilization in the optimal solution is given.

Table 20. Cost reductions needed for inactive processes to become active

Case: No fossil raw materials

Process ^a	Reduction in cost (%)	Production requirement for primary product from this process ^b (%)
Acetic acid/Acetaldehyde	77	24
Acetic acid/Wood	26	6
Ammonia/Methane	35	100
Carbon monoxide/Methane	20	100
Ethanol/Sulfite waste liquor	<1	56
Ethanol/Wood	48	140
Glucose/Wood (A)	73	1
Hydrogen/Wood	56	^c
Methanol/Wood	8	67

^a(A) and (B) refer to different processes.

^bFor chemicals which have no specified production requirements, the percent of actual production or utilization in the optimal solution is given.

^cDifficult to determine since hydrogen is produced and consumed by several processes.

to get the process into the optimal solution. However, the prices of raw materials and products will also influence the optimality of processes in the system since the objective function is total system profit. The potential effects of changes in prices of raw materials and products should be considered before conclusions are drawn for particular processes.

5.1 Base Case (Table 18)

There are several processes for which reductions in cost of 20% or less are needed for these processes to become active. While these processes might be candidates for R&D work, the uncertainty in the economic data may exceed the indicated reduction in cost. These processes may essentially be alternate optimal activities from a practical standpoint. For example, in the optimal solution for the base case discussed in Subsect. 4.1, carbon monoxide from coal was an optimal process. However, from Table 18, it can be seen that all of the required carbon monoxide would be produced from methane if the cost of the process were reduced by only 4%. In this case the discrimination in the model between coal and methane for production of carbon monoxide is mathematical and not an indication of process merit.

Biomass feedstock processes that may have potential value as indicated by this type of analysis are ammonia from wood, carbon monoxide from wood, methane from wood, and methanol from carbon dioxide. Phenol from Kraft lignin is also a candidate since a significant portion of the phenol could be produced by this route, although the needed process improvements probably fall within the uncertainty of the economic data.

5.2 Increased Costs and Decreased Availabilities of Petroleum, Natural Gas, and Butane (Table 19)

Biomass feedstock processes which may have potential in this case are carbon monoxide from wood, ethanol from wood, and methane from wood. It should be noted that ammonia from wood and methanol from carbon dioxide, which were identified in the base case discussion, are now in the optimal solution. Acetone from isopropanol might be a candidate if

significant quantities of isopropanol from fermentation should become available.

5.3 No Fossil Raw Materials (Table 20)

Processes that might be appropriate targets for R&D programs are ammonia from methane, carbon monoxide from methane, ethanol from wood, and methanol from wood. However, there is no opportunity here to displace petroleum since no petroleum is used in the optimal solution. A more appropriate approach would be to identify processes in the optimal solution which could be improved. An example of this analysis will be given in Subsect. 5.5 below.

5.4 Overall Evaluation of Inactive Processes

The inactive processes that may have potential according to the criteria used in Subsects. 5.1–5.3 are listed in Table 21. The potential importance and value of 9 of the 10 processes improves as petroleum and fossil raw materials are withdrawn from the system. The exception is acetone from isopropanol, which decreases in value.

It should be mentioned that no value is placed on carbon dioxide by-product in the model, which may influence the attractiveness of the Methanol/Carbon dioxide process. In the base case and no-fossil-raw-materials case, no carbon dioxide is bought; however, it is bought (at \$71/t) in the intermediate case. It would be possible to work through the optimal solution and determine which processes (if any) are consuming carbon dioxide in addition to Methanol/Carbon dioxide, but this has not been done.

5.5 Additional Postoptimization Analyses

Several other types of valuable postoptimization analyses have not been pursued in this study, but are well within the capabilities of the systems model. For example, the activity level for some optimal processes would increase to a new level if the cost of the process were decreased

Table 21. Summary of inactive processes which may have potential value^a

Process	Base case	Increased cost and decreased availability for petroleum et al.	No fossil raw materials
Ammonia/Methane	+	+	*
Ammonia/Wood	*	+	+
Acetone/Isopropanol	+	*	—
Carbon monoxide/Wood	*	*	+
Carbon monoxide/Methane	*/+	*	*
Ethanol/Wood	—	*	*
Methane/Wood	*	*	+
Methanol/Carbon dioxide	*	+	+
Methanol/Wood	—	*	*
Phenol/Kraft lignin	*	*/+	+

^a+ means optimal; * means potential value (see text); */+ means nonoptimal but very close (see text); — means nonoptimal and of little interest because of highly unattractive economics or small production potential.

to a specified value. This information is similar to the information on nonoptimal processes and can be used in a similar manner. Prospects for achieving the necessary cost reduction through research and development could be weighed against the benefits to the system if the process were optimal at the higher activity level. Since these processes are already optimal, it can be argued that there would be sufficient incentive for the private sector to improve these processes, and government support for research and development should not have high priority. On the other hand, this approach could be used to evaluate optimal processes in "future scenarios" to determine if R&D work might increase the contributions of these processes and improve the optimal solutions. For example, consider the Ethanol/Glucose process in the case of no fossil raw materials. The optimal activity level is 138.6 plants (Table 17). If the cost of this process were reduced by only 6%, the activity level would increase by 10% to 152.4 plants.

It was mentioned earlier that prices of raw materials and products can influence the optimality of processes. The sensitivity of the optimal solution to prices can be determined in the same manner as the sensitivity to process costs. Nonoptimal raw materials that would become optimal if the prices were decreased to specified values can be identified. In many cases, a new optimal process would be added to utilize this raw material. Prices that would give increased utilization of already optimal raw materials also can be identified.

The model could be restructured to require utilization of certain raw materials instead of production of certain chemicals. In this form, the optimal product slate could be determined for different input conditions, and the relationships between process economics and product slates could be studied.

6. HYPOTHETICAL TECHNOLOGIES

In Sect. 5 postoptimization analysis was used to characterize non-optimal activities in terms of the economic improvements needed in order to make these activities optimal. Another approach is to alter the economics of a nonoptimal activity in such a manner that the activity appears quite attractive and is included in the optimal set of activities. The change in total system profit (relative to a base case condition) is a measure of the potential value of this activity to the system.

This approach is especially useful for "gleam-in-the-eye" technologies for which no process description and economics are available. A process is hypothesized which has certain raw material requirements and yields certain products. Rather than estimate the capital and operating cost of this conversion process, the costs are simply set at an arbitrary reference value of zero. In most cases this process will appear economically attractive under these conditions and will be optimal in the solution. The increase in system profit relative to profit without this process is an indication of the upper limit of value of this process.

Of course, no real process can be operated at zero cost. However, the postoptimization analysis will indicate the upper limit for the cost of the process, beyond which the process is no longer optimal. This cost limit is a goal for R&D work; if a real process can be developed which can be built and operated for X dollars or less, it will be optimal. (Please note that the model does not determine the probability of successful development of such a process; this determination requires a human decision!)

Although the discussion to this point has focused on hypothetical new technologies, this approach can also be used with technologies that are already in the model. The cost of a particular process can be artificially set at zero in order to induce optimality and maximum profit, and the upper limit of cost which will maintain optimality can be determined. Essentially the same information can be obtained by the postoptimization analysis described in Sect. 5, but with one important addition in the present case. Since a second solution to the model has been obtained, the change in profit in response to the change in process cost can be calculated.

Three examples will be discussed to demonstrate the utility of this analysis for hypothetical new technologies and for technologies already in the model.

6.1 Benzene from Wood Lignin

Wood lignin is a potential source of aromatic chemicals and will be available in large quantities if hexose and pentose sugars are produced from lignocellulosic materials. Some process development work has been done to produce phenol (plus some benzene) from lignin, and the model contains a process based on this work. However, there is no established technology to convert phenol to benzene. Consequently, there is the potential for a large mismatch between the quantities of phenol and benzene produced and the nonfuel markets for these chemicals. This inefficiency could be resolved by either (1) altering the relative yields of phenol and benzene from the current process, (2) introducing a new process to convert phenol to benzene, or (3) introducing a new process to produce primarily benzene from wood lignin.

All of these options could be assessed using the LP model. By way of illustration, only option (3) will be discussed here.

Consider a hypothetical process to convert 1 kg of lignin to 0.48 kg of benzene, 0.26 kg of propylene, and 0.26 kg of carbon dioxide. Clearly this process is highly ideal, but therefore represents an upper limit. Lignin will be purchased at \$40/t, which is approximately the fuel value. This lignin is presumed to be available in unlimited quantities as a by-product from wood sugar processes. Economic contributions of the wood sugar processes to the model exist, but will not be considered at this time. All other inputs to the model are identical to the base case described in Subsect. 4.1.

Major features of the optimal solution are listed in Table 22, column (A). The increase in profit is \$312/t of benzene produced from lignin. Other significant changes in the optimal solution relative to the base case include:

- Benzene/Coal is no longer optimal. This process produces both benzene and propylene, as does the new benzene from lignin process, so appears to be needed no longer.

Table 22. Hypothetical Benzene/Wood Lignin: Effect of process cost on optimal solution

	(A)	(B)	(C)
Process Cost	\$0	\$2 per t of Lignin	\$140 per t of Lignin
Increase in Profit over Base Case	\$1455 million	\$1437 million	\$474 million
Benzene produced from Wood Lignin	4668×10^3 t	3360×10^3 t	3025×10^3 t
Changes relative to base case	<ul style="list-style-type: none"> • Benzene/Coal deleted • Benzene/Toluene reduced to 5.4 from 34.5 • Cyclohexane/Benzene replaces Cyclohexane/Petroleum naphtha • Urea/Ammonia replaces Urea/Methane 	<ul style="list-style-type: none"> • (same) • Benzene/Toluene reduced to 19.9 from 34.5 • (same) • Both Urea/Ammonia and Urea/Methane are optimal 	<ul style="list-style-type: none"> • (same) • (same) • Both Cyclohexane/Benzene and Cyclohexane/Petroleum naphtha are optimal • (same)

- Benzene/Toluene is reduced substantially, due no doubt to an alternate attractive route for benzene production.
- Cyclohexane/Benzene replaces Cyclohexane/Petroleum naphtha, probably due to a relatively inexpensive supply of benzene.
- Urea/Ammonia replaces Urea/Methane due to a subtle by-product interaction. Methane is a by-product from Benzene/Coal, which was optimal in the base case but nonoptimal in this present benzene-from-lignin problem. The loss of this "free" by-product methane causes Urea/Ammonia to be more attractive than Urea/Methane.

Postoptimization analysis shows that if the process cost is changed from zero to \$1.55 per t of lignin, benzene production by this process will decline from 4.668 million t to 3.36 million t. A second case was run in which the process cost was set at \$2 per t of lignin. The results of this analysis are shown in Table 22, column (B). The increase in system profit is \$428 per t of benzene produced from lignin. Note that the unit profit is up, but the total system profit is slightly less improved relative to the zero cost process.

Post optimization analysis now shows that the activity level of benzene from wood lignin will change again if the process cost is increased to \$135 per t of lignin. A third case was run in which the process cost was set at \$140 per t of lignin. The results are summarized in Table 22, column (C). The increase in system profit dropped to \$474 million, or \$157 per t of benzene from lignin. Cyclohexane is produced from both benzene and petroleum naphtha.

If the process cost is increased to \$144 per t of lignin, the solution will change again. A fourth case was run with a process cost of \$145 per t of lignin. Increase in system profit was \$445 million, and production of benzene from lignin was 2.3 million t (not shown in Table 22). The cost limit above which this process is not optimal was determined to be \$295 per t of lignin.

These process costs may be compared with the process cost for the Phenol/Lignin process in the model, which is \$227 per t of lignin consumed.

6.2 Ethylene from Wood Sugars

Ethylene is a dominant chemical in the current petrochemical industry. It can be produced from biomass resources via dehydration of fermentation ethanol, and perhaps could be produced via rapid pyrolysis if process development work were successful. However, it is known that certain microorganisms can ferment sugars directly to ethylene.⁹ Although the yield currently is low, perhaps the yield could be improved through strain and process development.

Consider a hypothetical process to convert 1 kg of wood to 0.32 kg of ethylene, 0.20 kg of lignin, 0.45 kg of carbon dioxide, and 0.03 kg of water. This stoichiometry is representative of a probable upper limit for the yield of ethylene. No credit will be taken for by-product lignin and carbon dioxide, although both will be available for conversion to other chemicals.

The optimal solutions are summarized in Table 23 for several conditions. The substantial increases in system profit at zero process cost are not surprising in view of the dominant role of ethylene in the chemical industry. The profit increase is less, of course, at higher process costs. The upper limit on process cost which still maintains this process in the optimal solution was found to be \$500 per t of wood in the base case, and \$565/t in the no-fossil-resources case. If a process could be developed that could be operated for less than these limits, profit would increase and more ethylene would be produced from wood.

These process costs may be compared with the process cost for ethylene from ethanol from wood in the model, which is ~\$160 per t of wood. However, the yield of ethylene from these combined processes is only 8% compared to 32% for the hypothetical process.

6.3 Methanol from Carbon Dioxide

This process is already in the model and has been mentioned briefly in Sect. 5. It involves the combination of 1.5 kg of carbon dioxide and 0.22 kg of hydrogen to produce 1.0 kg of methanol. It is not optimal in the base case, but would become optimal if the process cost were reduced

by 54% (see Table 18). To determine the increase in system profit if this cost reduction could be accomplished, the process cost in the model was reduced by 55%. System profit increased \$102 million and 1.35×10^6 t of methanol were produced by this process.

Table 23. Hypothetical Ethylene/Wood: Effect of process cost on optimal solution

	Base case		No fossil resources	
	I	II	I	II
Process cost, per t of wood	\$0	\$500	\$0	\$565
Increase in profit over reference condition	\$18.4 billion	\$35 million	\$24.3 billion	\$57 million
Ethylene produced from wood, t	13.6×10^6	1.2×10^6	44.8×10^6	8.0×10^6

7. RESEARCH AND DEVELOPMENT

In this section, the use of the model to identify goals and guide R&D programs will be discussed. Because the scope must necessarily be limited in this report, the optimal solutions and postoptimization analyses presented in Sects. 4, 5, and 6 will be used to illustrate the utility of the model.

7.1 Excess Production of Primary Products

In the base case (Subsect. 4.1 and Table 8), there is a negligible production of primary chemicals above the specified minimum quantities. This situation is expected because the base case is a simulation of the current industry, which does in fact produce the specified minimum quantities.

The situation changes, however, when the input conditions are altered. In the case of increased raw material costs (Subsects. 4.2, 4.3, and Tables 12 and 14), there is significant excess production of *n*-butanol. (Recall that the excess ethanol and isopropanol are converted to olefins.) Similarly, in the cases of no fossil resources (Subsect. 4.4 and Table 16), there is excess production of acetaldehyde, acetone, *n*-butanol, and phenol.

Production in excess of the minimum quantities is a sign of inefficient and/or inappropriate technologies. Opportunities to improve the optimal solution through R&D programs exist in two areas:

1. New uses for those chemicals produced in excess in order to establish new markets for additional revenues. New technologies may be needed to convert these chemicals into marketable products.
2. Alterations to existing technologies and development of new technologies to avoid excess production.

Both of these areas focus on the extent to which the product slate can be matched. Implicit in this approach is the choice of a desirable, probable, or otherwise appropriate product slate. Alternatively, the utilization of raw materials could be specified and the product slate determined by the optimization process. This approach was mentioned briefly in Sect. 5.

7.2 Process Improvement

In Sect. 5 several nonoptimal processes were identified which could become optimal if process improvements could be made to improve the economics. These processes include Ammonia/Wood, Carbon monoxide/Wood, Ethanol/Wood, Methanol/Carbon dioxide, Methanol/Wood, and Phenol/Kraft lignin (Table 21). Methanol from carbon dioxide was examined in more detail in Subsect. 6.2 to assess the increase in system profit if these improvements could be realized. In this particular case, a reduction of 55% in the process cost led to optimality for this process in the base case and an increase of \$102 million in system profit. This information on potential value must be combined with the probability of achieving the needed technical advances and the associated R&D costs in order to decide if a R&D program should be instituted.

7.3 New Technologies

The potential value of hypothetical or conceptual technologies can be estimated. An idealized process for benzene from lignin was evaluated in Subsect. 6.1. This analysis could be especially useful to establish a rank order of several technologies that ostensibly are similar, or of R&D programs competing for financial and personnel resources.

For example, consider the three processes evaluated in Sect. 6. At the maximum process costs that maintain optimality for these processes, Methanol/Carbon dioxide increases the system profit by \$102 million, whereas Benzene/Wood lignin increases the system profit by \$47 million and Ethylene/Wood increases the system profit by \$35 million. On this basis, it could be argued that Methanol/Carbon dioxide has more potential.

Processes can also be compared and rank-ordered with respect to displacement of fossil raw materials. Table 24 shows that Methanol/Carbon dioxide, Benzene/Lignin, and Ethylene/Wood each displace about 4% of the petroleum naphtha used in the base case. Methanol/Carbon dioxide displaces more natural gas (about 4.7% of base case consumption) than do Benzene/Lignin and Ethylene/Wood since the latter have no direct ties to natural gas processes. Methanol/Carbon dioxide also displaces 66% of the coal

used in the base case because Carbon monoxide/Coal is no longer optimal. Since Carbon monoxide/Coal is preferred only marginally over Carbon monoxide/Methane in the base case, this coal displacement may be considered equivalent to natural gas displacement.

Similar analyses could be done, of course, using other reference conditions instead of the base case of Subsect. 4.1.

Table 24. Utilization of fossil raw materials
for four cases

Raw material	Consumption (10 ³ t)			Base case
	Methanol/ Carbon dioxide	Benzene/ Lignin	Ethylene/ Wood	
Butane	1,500	1,500	1,500	1,500
Coal	2,366	6,958	6,958	6,958
Natural gas	14,734	15,100	14,948	15,459
Petroleum naphtha	62,118	61,948	61,948	64,556
Refinery gas	1,043	1,043	1,043	1,043

8. CONCLUSIONS AND RECOMMENDATIONS

Several conclusions may be drawn from the integrated results of the Delphi study and the systems model. When current costs are used in the model, a satisfactory approximation of the current chemical industry is obtained when the current uneconomical status of several processes (new plants) are considered. A twofold increase in the cost of petroleum and natural gas relative to process costs and product prices in the model leads to a reduction to zero in the use of petroleum naphtha. Approximately 140×10^9 kg of coal per year is used to produce naphtha to replace the 64×10^9 kg of petroleum naphtha used under current conditions. Total system profit declines approximately \$10 billion per year relative to current conditions, which is approximately 25% of sales revenues. These numbers give an indication of the cost of continuing to produce the current product slate at petroleum costs double current values in a relative sense. In view of the substantial cost, it seems highly unlikely that this scenario will occur. Significant alterations in the product slate surely would occur to help mitigate the increased costs of petroleum feedstocks.

The time may be near when olefins from alcohols from biomass may be competitive with olefins from petroleum and gas resources when the basis for comparison is the construction and operation of new plants. Sufficient supplies of alcohol raw materials will have to be assured, of course. While technology to convert ethanol to ethylene is available, similar technology to convert isopropanol to propylene needs further development. The present study points out the potential utility of such technology.

A reasonable approximation to our current product slate could be produced from renewable resources without the use of petroleum, gas, or coal as feedstocks. The primary resource would be wood. Such an industry would be highly unprofitable, however, because revenues from sales would recover only 35% of the costs at current market prices. The utility of this scenario is rather to define a limiting case. There are numerous opportunities to improve economics by process improvements through research and development. The dollar value to the system for particular process improvements can be estimated by using the systems model.

Many processes are under development for the recovery of oils and hydrocarbon liquids from specialty crops such as jojoba, guayule, sunflower seeds, euphorbia, etc. These processes have not been considered in this assessment because it is not clear at this time how the products would fit into the commodity chemicals industry. The same argument applies to biomass liquefaction. The potential value of these processes to a commodity chemicals industry could be assessed using the model if additional refining and separations technologies were hypothesized.

A critical factor in the assessment of the potential for production of chemicals (and fuels) from biomass is the total quantity of resource which can be produced economically on a renewable basis. This factor equals and may exceed in importance the biomass conversion issues addressed in this present assessment. It appears that sufficient biomass resources are available to meet the demand for all chemicals presently made from petroleum and natural gas, although the costs of these resources and competition for fuel and food uses are largely unknown. Improved fundamental understanding and techniques for biomass production should be a high priority in the national biomass program. However, a major barrier to immediate increased use of biomass is the lack of proven economical conversion processes. The recommendations discussed below pertain only to biomass conversion and utilization for chemicals.

8.1 Lignocellulose Conversion

Lignocellulose is the most abundant renewable resource available today, and will be the most abundant renewable resource in the short- to mid-term. Hence increased utilization of lignocellulose is one preferred strategy for increased production of chemicals from biomass. From a process development perspective, the goal should be the total utilization of the resource delivered to the conversion plant to yield products of the highest possible value. It is unlikely that there will be a single optimum process to achieve this goal. However, the following problem areas need significant R&D work in order to provide options for future process designs:

1. Pretreatment and hydrolysis to convert lignocellulose to less-refractory materials. Significant progress has been made in this area in recent years, which has encouraged further process development. Work is needed on direct hydrolysis and solubilization without extensive pretreatment, isolation of stable cellulase enzymes in larger quantities, and simultaneous hydrolysis and fermentation in a single reactor unit. In general, any R&D that enhances the conversion of lignocellulose to less-refractory materials is a good investment.
2. Higher-value, non-fuel uses for lignin. Work is needed on selective depolymerization of lignin to yield aromatic chemicals as a high priority, and on development of new polymeric materials. Development of higher-value uses for lignin does not imply that it cannot also be used for fuel for process energy. The goal is to provide various options to permit future process selection that will be optimal for the specific resource and site location.
3. New microbial systems. New strains of organisms and mixed cultures are needed which will convert lignocellulose fractions to desirable products at greater rates and yields. Traditional isolation and selection procedures, as well as genetic alterations, will be useful.

8.2 New Reactor Designs

Biomass conversion by thermal, physical, and biological means presents problems that are not necessarily overcome in an optimal manner by conventional technology. In a general sense, there are opportunities for improving yields, product distributions, and process economics from the development of new generic reactors for biomass conversion. Desirable work includes improved means for immobilization and retention of cells and biological components in reactors; stabilization, kinetics, and physical properties of immobilized constituents; minimization of end-product inhibition by novel reactor design and contacting schemes; combination of various unit operations in a single reactor (such as extractive fermentation and simultaneous hydrolysis and fermentation); development of enzymatic and nonenzymatic catalytic systems, especially near-ambient temperature systems; and use of solar energy for process energy.

8.3 Product Separation and Purification

Many current conversion technologies produce either a broad mix of chemical compounds in roughly similar quantities or a dilute aqueous solution of one or two primary products. In both cases more efficient and effective separation technologies are badly needed to improve the attractiveness of these overall processes. It is unlikely that a single separation technique will be optimal in all cases. Processes are needed which are (1) operated at ambient temperature; (2) combined with other operations (e.g., extractive fermentation); and (3) based on new separations, large-scale chromatography, novel solvent extraction schemes, etc.

8.4 Rapid Pyrolysis

Thermochemical conversion of biomass by very rapid pyrolysis offers an opportunity for direct production of olefins. This capability is one of the most attractive features of this process. However, only small yields of olefins have been produced to date. It remains to be determined whether significantly improved yields of olefins can be achieved by advanced reactor designs, improved heat transfer, catalytic reactors, etc. The learning curve appears to be very steep at this time. A well-conceived and efficiently executed research program focused on basic chemistry and reactor design could produce large dividends.

8.5 Non-CO₂-Producing Processes

Many fermentations and thermochemical processes convert a significant portion of the biomass resource to CO₂. Carbon dioxide is not a high-value product, although it does have some value when relatively pure. When CO₂ is produced, the maximum theoretical yield of preferred chemicals is reduced considerably. This is a particular disadvantage because raw materials costs are a major fraction of the total cost for many biomass conversion processes. Production of low- or no-value CO₂ simply inflates the effective cost of the raw materials.

Fermentations that do not produce CO₂ should be studied. Examples include organic acid fermentations. It is probable that higher overall rates and process yields can be obtained compared to CO₂-producing fermentations, which will contribute to the total biomass utilization goal. Organism selection, reactor designs, and product recovery and upgrading should be studied. Minimization of CO₂ production in thermal processes also should be sought, although some CO₂ may result from partial combustion to provide energy for the process.

8.6 CO₂-Consuming Processes

An alternative approach is to develop high-value uses for CO₂. There is some activity in this direction, exemplified by CO₂-containing polymers and CO₂-enriched photosynthesis environments to recycle the CO₂ back to biomass. At one time, fermentation CO₂ was used on a commercial scale to produce methanol. The quantity of CO₂ currently produced from fossil fuel use is tremendous. In addition, the no-fossil-resources model (Subsect. 4.4) produces \$1.2 billion worth of CO₂ (at \$71 per t) that is unsold and unutilized.

The prospects for successful development of high-value uses are difficult to assess. Innovative and imaginative concepts should be sought and supported. Examples might include new synthesis routes to established chemicals and new chemical products such as polymers. A general strategy might be to seek chemical syntheses in which carbon and oxygen are added to produce higher-value chemicals. Novel reactor designs and/or catalysts might permit the utilization of CO₂. Perhaps methods could be found to combine CO₂ and H₂ to produce oxychemicals if there were a readily available supply of cheap hydrogen. Enriched atmospheres for photosynthesis might receive limited support for fundamental rate and efficiency studies.

8.7 New Bioconversion Processes

The potential utility of new bioconversion processes is illustrated by the Ethylene/Wood fermentation process discussed in Subsect. 6.2. Microbial processes offer the opportunity for high specificity and high

yields, especially if carbon dioxide production can be avoided. Current activities in so-called genetic engineering, strain improvement, and mixed culture work may lead to attractive new processes when combined with advances in reactor designs and product separations.

8.8 Chemicals Industry Model

Several applications of the model to assess and evaluate technologies have been illustrated in this report. Further work is needed to assess new technologies and process improvements under different input conditions in order to identify specific R&D work having high potential payoff in a more universal context. In addition, studies of the resource base and various product slates would be especially valuable in order to obtain a more complete picture of the prospects for increased chemicals from biomass. The model also should be expanded to include biomass fuel markets.

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APPENDIXES

APPENDIX A: RESPONSES TO DELPHI STUDY QUESTIONS

The individual responses to each question have been condensed into a format to highlight the consensus as well as dissenting points of view and miscellaneous comments. The numbers of respondents favoring the various points of view are indicated.

1. Biomass resources: What particular biomass resources, or groups of resources, are likely to be significant for production of chemicals? Why?

<u>Resource</u>	<u>Short-term</u>	<u>Mid-term</u>	<u>Long-term</u>	<u>Unspecified</u>
"Wood," Lignocellulosics	1	2	3	21
Forestry residues	3	2		11
Woody plantations			5	5
Agricultural residues	5	2	1	19
Sugar & starch crops	5	1		7
Corn	3			4
Municipal solid waste	1			11
Special crops		1	2	11
Algae			3	5
Pulp mill wastes	1			3
Manure				4
Peat				1

Frequent comments:

- Wood — Flexible harvest, abundant, tolerant of weather variations, potential for coppicing, use of marginal land, high growth and yields
- Agricultural residues — Available now, large volume, but seasonal, difficult to collect, soil maintenance need
- Sugar & starch crops — Available now, potential for high yields and high value chemicals, but competition with food uses
- Municipal solid waste — Available now, a "waste," but heterogeneous and contaminated
- The key concept is "high value at low cost." (quote from one person)

2. Chemical products: What particular chemicals, or groups of chemicals, are most attractive for production from biomass? Why?

<u>Frequently mentioned</u>		<u>Less frequently mentioned</u>	
Alcohols	17	Polyols	5
Aromatics	15	Specialty chemicals	5
Olefins	14	Fermentation products	4
Organic acids	10	Proteins	3
Natural	8	Amino acids	2
hydrocarbons		Esters	2
Cellulose	7	Ketones	2
Fuels	7	Naval stores	2
Sugars	6	Resins	1

- Over 25 individual chemicals were named.
- Rationale for these choices generally appeared again in response to later questions.

3. Chemicals also will be produced from coal. What are the technical issues governing optimal use of both resources? (For example: oxychemicals vs hydrocarbons; aromatics from coal vs lignin; gaseous vs liquid products, etc.)

Frequently mentioned issues

Regional availability — use what is available locally

Renewable — biomass preferred over coal

Environment — sulfur, NO_x and CO₂ from coal; biomass cleaner

Syngas — coal a heavy favorite (compared to biomass)

Current economics — coal a heavy favorite, especially for syngas and methanol

Oxychemicals — biomass a heavy favorite

Aromatics — strong for coal; mixed for biomass (compared to coal)

- Fuel needs and economy of scale favor coal, while there is a definite interest in selected chemicals from biomass.
- Biomass is considerably more reactive than coal, and easier to gasify or liquefy.
- Both coal and biomass probably will be important, and an "either/or" mentality should be avoided.

4. Please identify specific current R&D work of critical relevance to production of chemicals from biomass. Names of investigators and/or literature references would be helpful to us for overall documentation purposes.

A large number of specific projects were mentioned.

<u>R&D area</u>	<u>Number of groups mentioned</u>
Cellulose hydrolysis	18
Fermentations	11
Ethanol	7
Acetone/butanol	6
Acetic acid	4
Gasification	8
Separations	7
Production of biomass	5
Pretreatment of lignocelluloses	3
Lignin processing	3
Liquefaction	3
Genetic manipulation	3
Syngas to chemicals	3

Other research areas mentioned include hemicellulose utilization, ethanol tolerance, and production of particular chemicals.

5. What specific additional R&D work will be critically necessary (a) in the short term, and (b) in the long term?

<u>R&D area</u>	<u>Short-term</u>	<u>Long-term</u>	<u>Unspecified</u>
Lignocellulose conversion	11	10	9
Product separations	11	4	5
Species development and genetic engineering	3	11	7
Fermentation yields and rates	5	7	3
Gasification-syngas and olefins	5	8	3

Additional areas mentioned included agronomy, collection, harvesting, storage, and economic analyses.

Comments:

"Develop and demonstrate known technologies with real feedstocks."

"No more uneconomical demonstration units!"

"More R&D money!"

"Hold a conference on research needs."

6. Chemicals from biomass might be used as feedstocks for existing petrochemical-based processes (e.g., ethylene), or new processes and products might be developed around biomass-derived chemicals (e.g., lignin-based polymers). What are the pros and cons of these two approaches?

A clear majority of respondents said that intermediate chemical feedstocks for existing petrochemical-based processes should be the primary objective. The principal reasons are the use of existing facilities (perhaps fully depreciated) and established markets and infrastructure to gain market penetration quickly.

"Both" also was a common response — the two approaches are not exclusive, but complementary. By-product and co-product opportunities for new products will arise naturally. Optimal product slates in both cases will depend on local utilization markets.

There was a significant anti-petrochemicals sentiment as well. These arguments against producing petrochemical feedstocks from biomass are:

- wasteful duplication — stick with petroleum.
- biomass has no clear advantage, other than renewable.
- savings in petroleum will be insignificant.
- large-scale coal facilities will compete better.
- product slate favors olefins from petroleum and oxy-chemicals from biomass; new products approach may favor better utilization of biomass.

Several pure economic arguments also were made. It is easier to form capital for known marketable products (favors petrochemical feedstocks and intermediates), and it is difficult to form capital for utilization of "wastes."

7. There is considerable agreement that biomass processing plants will be smaller than petrochemical plants. How small is "small"? Are there non-economic factors which might influence plant size?

Availability of biomass feedstock for the plant was mentioned by over half the respondents. This barrier encompasses transportation, storage, handling, inventories, and other logistics.

There was a strong "overall economics" argument: petroleum prices will escalate; scale factors; value-added; small plants are labor-intensive; particular product market.

Other comments:

"Satellite groups and mobile conversion units are attractive."

"Plants should be large enough to utilize energy-recovery equipment."

"Pulp mills provide a good example of what can and cannot be done."

"Environmental factors and national security considerations may favor small plants."

8. What time scale do you foresee for significant additional production of chemicals from biomass? If it should become highly desirable (or critical) to produce chemicals from biomass as soon as possible, what significant technical barriers (as opposed to economic barriers) now exist to immediate commercialization?

Some (but not all) of the 5-year estimates are based on adoption of Japanese/German/USSR technology, and reflect the time required to build plants.

Barriers

None (9), but "clumsy processes," "non-optimal"

Processes are unproven at commercial scale (12)

Improved yields and separations (14)

Agronomics (7)

Market/capital/labor and other economic matters (11)

Several references were made to funding levels, national goals and policies, and competition from coal and petroleum.

9. Please identify ten people, who, in your opinion, are leading authorities in the field of chemicals from biomass by virtue of their research work and/or familiarity with the technical issues.

Twenty-three people received four or more citations:

<u>Name</u>	<u>Affiliation</u>	<u>Citations</u>
Wang, D. I. C.	M.I.T.	22
Tsao, G. T.	Purdue U.	15
Humphrey, A. E.	Lehigh U.	14
Goldstein, I. S.	N.C. State	14
Cooney, C. L.	M.I.T.	11
Wilke, C. R.	U.C. Berkeley	11
Lipinsky, E. S.	Battelle Columbus	8
Busche, R. M.	DuPont	7
Pye, E. K.	U. Penn.	7
Shafizadeh, F.	U. Montana	7
Katzen, R.	R. Katzen Assoc.	6
Ladisch, M.	Purdue U.	6
Blanch, H. W.	U.C. Berkeley	5
Emert, G. H.	U. Arkansas	5
Goheen, D. W.	Crown Zellerbach	5
Saeman, J. F.	U. Wisconsin/F.P.L.	5
Zaborsky, O.	N.S.F.	5
Bungay, H. R.	R.P.I.	4
Elliott, D. C.	Battelle P.N.L.	4
Jones, J. L.	S.R.I.	4
Klass, D. L.	I.G.T.	4
Sarkanen, K.	U. Washington	4
Villet, R.	S.E.R.I.	4

9. (Continued)

The following people received three or fewer citations. Affiliations and spelling of names have not been verified.

<u>Name</u>	<u>Affiliation</u>	<u>Name</u>	<u>Affiliation</u>
Amon, W. F.	Cetus	Erickson, K. E.	Swedish Forest Products
Anderson, D. B.	Battelle P.N.L.	Eveleigh, D. E.	Rutgers
Antal, M. J.	Princeton U.	Falkehag, I.	Mt. Pleasant, N. C.
Bailey, R.	U. W. Va.	Feldman, H.	Battelle Columbus
Baker, A.	F.P.L.	Findley	
Baker, E. G.	Battelle P.N.L.	Finn, R.	Cornell U.
Batter, T. R.	Battelle P.N.L.	Flanigan, V.	U. Missouri
Beck, S. R.	Texas Tech	Fletcher, W.	Dow Chemical
Bellamy, W. D.	Cornell U.	Flickinger, M.	Fredrick Cancer Research
Beneman, J. R.	U.C. Berkeley	Foster, K.	Office Arid Land Research
Bird, C.		Frankiewicz, T.	Oxy Research
Bouner, J.	Cal. Tech.	Fry, M. W.	Frysville, Ephrata
Brandon, O.	Harnwell (U.K.)	Fulmer R. W.	Cargill Research Ctr.
Brink, D.	U.C. Berkeley	Gaddy, J. L.	U. Arkansas
Buchanon, J.	N.R.R.L.	Gaden, E. L.	U. Virginia
Chambers, R.	Auburn U.	Gaspar, E.	P.R.C.
Chang, H. -M.	N.C. State	Gavalas, G.	Cal Tech.
Charles, M.	Lehigh U.	Ghose, T.	Indian Inst. Tech.
Chum, H. L.	S.E.R.I.	Glasser, W.	V.P.I.
Coffman, J.	Wright-Malta Corp.	Gratzl, J. S.	N. C. State
Coughlin, R. W.	U. Connecticut	Gregor, H.	Columbia U.
Del Gobbs, N.	DOE	Grethlein, H.	Dartmouth
Detroy, R.	N.R.R.L.	Gung, C. S.	Purdue U.
Diebold, J.	S.E.R.I.	Halligan, J.	U. Arkansas
Douglas, L.	S.E.R.I.	Harris, J. F.	F.P.L.
Dunlop, A.	U. Missouri	Hearon, W. M.	Boise Cascade
Eakin, D. E.	Battelle P.N.L.	Herbert, H. L.	I.T.T. Rayonier
Engstrom, S.	Royal Institute, Sweden	Herrick, F.	I.T.T. Rayonier
Ergun, S.	L.B.L.	Hesseltine, C.	U.S.D.A.
Hillman, C. W.	Battelle Columbus	Moo-Young, M.	U. W. Ontario
Hiraoka, M.	Diamond Shamrock	Moreira, A.	Colorado State
Howard, J.	Kyoto, U.	Mudge, L. K.	Battelle P.N.L.
Huang, H. T.		Mun, P. K.	ARCO
Inman, R. E.	Arco Ventures	Nystrom, J.	A. D. Little
Jewell, W.	Cornell	Pearl, I.	Inst. Paper Chemistry
Jones, M.	Hydrocarbon Research	Pollack, J.	Louisiana State
Jonson, J. D.	U. Arizona	Pyne, J. W.	
King, C.	DuPont	Radovich, J.	U. Oklahoma
Kirk, T. K.	U. Wisconsin/F.P.L.	Raymond,	Weyerhaeuser
Kirwan, D. J.	U. Virginia	Reed, T. B.	S.E.R.I.
Kohan, S. M.	E.P.R.I.	Reilly, P. J.	Iowa State
Kuester, J. L.	Arizona State	Root, D.	Weyerhaeuser
Kriegar, B.	U. Washington	Rowe, J. W.	F.P.L.

9. (Continued)

<u>Name</u>	<u>Affiliation</u>	<u>Name</u>	<u>Affiliation</u>
Laskin, A. I.	Exxon	Russell, J. A.	Battelle P.N.L.
Lee, Y. Y.	Auburn	Ryu, D.	Korea
Lilly, M.	U. C. London	Schuerch, C.	Syracuse U.
Ljungdahl, L. G.	U. Georgia	Scott, C. D.	O.R.N.L.
Lopez, E.		Sealock, L. J.	Battelle P.N.L.
Lovin, A.		Siebert, M.	
Ludwig, C. H.	Georgia Pacific	Schiefelbein, G.	Battelle P.N.L.
Lynch, J.		Silver, R.	Gulf
Mateles, R.	Stauffer Chem.	Sinsky, A. J.	M.I.T.
Mandels, M.	Natick	Smiley, K.	U.S.D.A.
Marchessault, R. H.	U. Montreal	Smith, L.	S.E.R.I.
McCarthy, J.	U. Washington	Soltes, E. J.	Texas A & M
Medeiros, D. J.	ARCO	Spano, L.	Natick
Mendel, D. A.	S.R.I.	Spivey, M. J.	Nat. Chem. Prod.
Milne, T. A.	S.E.R.I.	Sweed, N.	Oxirane
Modell, M.	M.I.T.	Switer, C.	S.E.R.I.
Tong, G.	Stone and Webster	Whistler, R.	Purdue
Tornabene, T. G.	Colorado State	Weisz, P.	Mobil
Tsuchiya, H. M.	U. Minnesota	Wilhelm, D. J.	S.R.I.
Wan,	Battelle P.N.L.	Wise, D.	Dynatech R&D
Ward, R.	United Nations	Wolfe, R. S.	U. Illinois
Wayman, M.	U. Toronto	Yang, V.	
Weiss, C. H.	Chem. Systems	Zarbe, J.	F.P.L.
Welch,		Zeikus, J. G.	U. Wisconsin

10. What literature, both general and specific in subject, would be most helpful to us for this assessment?

A number of people graciously supplied reprints and extensive reference lists. These lists are not included at this time since they might reveal the identities of some of the respondents. In addition to specific journal papers, the following more general suggestions were received.

(a) Reports and publications from

Department of Energy	MBT Division of ACS
Office of Technology Assessment	Battelle Laboratories
Institute of Gas Technology	National Research Council/NAS
Solar Energy Research Institute	American Institute of Chemical Engineers
Stanford Research Institute	Forest Products Laboratory
Mitre Corporation	CRC Press
Jet Propulsion Laboratory	Technical Association of the Pulp and Paper Industry
Noyes Data Corporation	

10. (Continued)

(b) Periodicals

<i>Biomass Digest</i>	<i>Alcohol Week</i>
<i>Biotechnology & Bioengineering</i>	<i>Biofuels Reporter</i>
<i>Biotechnology Letters</i>	<i>Biomass Refining Newsletter</i>
<i>Chemtech</i>	<i>Applied & Environmental Microbiology</i>

(c) Particular books and reports

<i>Chemrawn I Conference</i>	<i>Bungay, Energy, the Biomass Options</i>
<i>Bioenergy 80</i>	
<i>Bioenergy Directory</i>	<i>Goldstein, Organic Chemicals from Biomass</i>
	<i>Zaborsky, Biosolar Handbook</i>

ROUND 2

1. Comments on Round 1 responses. Do you basically agree? Major points of disagreement?

Most respondents basically agreed with the Round 1 Summary.

Most comments emphasized certain features in the Summary, or reiterated a minority view.

Selected Comments:

- Economics will be very much site- and resource-specific.
- Economical processes are being developed now, but these are not the processes described in the technical literature.

2. While use of "waste" biomass such as MSW is philosophically attractive and helps alleviate disposal problems, there also appear to be risk and uncertainty factors associated with a conversion plant dependent on perceived "wastes" as "valuable" feedstock. What are likely to be the specific problems here, and what can be done to minimize them?

2. (Continued)

"What is the business?"

- Eliminate waste to nothing?
- Produce product at a profit and expand the business?

"Golden Garbage" — a "waste" immediately becomes a valuable "by-product" when a demand arises for it.

Solutions:

- Burn wastes for fuel.
- Long-term contracts for wastes, perhaps tied to the cost of fuel.

3. There are at least four major categories of biomass conversion processes: fermentation, liquefaction, gasification, and pyrolysis (fast and slow). Should one or more of these generic categories receive special R&D emphasis relative to the others for production of chemicals? Why?

Fermentation	16 + 2 -	High-value specialty chemicals, most advanced, alternative to thermal processes, <u>but</u> cannot compete with coal.
Gasification	7 + 3 -	Good yields, uniform product, feed flexibility, <u>but</u> cannot compete with coal.
Pyrolysis	2 + 7 -	Steep learning curve, opportunity for olefins, <u>but</u> complex product slate, will not compete with coal.
Liquefaction	5 + 6 -	Fuel production, "efficient" process, <u>but</u> complex product slate, will not compete with coal.
No preference	9	All will be significant in specific situations, as determined by economics.

"In R&D, pursue the most advantageous, not just the most available."

4. Describe the major technical features of an ideal multiproduct "biomass refinery."

- Complete utilization of resource, no wastes.
- Efficient processes with high yields.
- Energy self-sufficient, with waste heat recovery.
- Site-optimized with respect to resources and markets.
- Single product (may not be possible).
- Flexibility to utilize various resources and produce various product slates.

5. Are there circumstances under which coal-biomass dual feedstock plants might be attractive? For example?

- Burn coal for process energy for biomass conversion (9).
- Co-gasify or liquefy coal and biomass to smooth feedstock supply, reduce feedstock vulnerability, lower emissions, and gain economy of scale for biomass (9).
- No — "too dissimilar" (10).

6. Anaerobic digestion received practically no mention in Round 1. Is methane a potentially significant chemical intermediate? Why?

- Too expensive relative to natural gas.
- Must go through syngas to make chemicals; there are better ways to make syngas.
- Potential for conversion of wet, low-lignin feeds, such as marine biomass, manure, sewage sludge.
- Recover acids rather than methane.

7. Are the following chemicals potentially significant as intermediates or end products? Why?
- (a) levulinic acid
 - (b) carbon dioxide
 - (c) lignin-based polymers and cellulose-based polymers

Attractive conceptually, but serious marketing and practical drawbacks.

Currently low value, supply exceeds demand.

8. (a) To what level of development should DOE sponsor new technology for chemicals from biomass? (e.g., fundamental research, bench-scale, process development unit, mini-pilot plant, pilot plant, etc.) Why?
- (b) At what level of development will industry be able to pick up further development and implementation of new technology? What types of incentives and/or co-funding would be most useful?

<u>Fundamental/bench/lab scale</u>		<u>Process Development Unit/Pilot Plant</u>	
Academic	(8)	Academic	(2)
Industrial	(4)	Industrial	(0)
Independent/ government labs	<u>(6)</u>	Independent/ government labs	<u>(2)</u>
Total	18	Total	4

Other comments

Whatever is needed (industrial and independent viewpoints)

Demonstrate growth of purpose crops (industrial viewpoint)

Less support as process approaches commercialization (academic viewpoint)

None (industrial viewpoint)

Arguments

Exclusive license/patent positions are needed.

Reasonable expectation of reasonable return on investment is needed.

Industry needs to see product coming from a plant.

APPENDIX B: MATERIAL BALANCES AND ECONOMICS FOR CONVERSION PROCESSES
(The source of data for each process is given in the list of references following the individual process data sheets.)

PRIMARY PRODUCT: Acetaldehyde

SOURCE: 1

PRIMARY RAW MATERIAL: Ethanol

PLANT CAPACITY: 40×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$21.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetaldehyde, t	1.0	Ethanol, t	1.2	Steam, t	3.5
Hydrogen, t	0.045			Electricity, 10^9 J	0.72
				Fuel, 10^9 J	2.1
				Cooling water, m^3	65

PRIMARY PRODUCT: Acetaldehyde

SOURCE: 2

PRIMARY RAW MATERIAL: Ethylene (A)

PLANT CAPACITY: 30×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$10.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetaldehyde, t	1.0	Ethylene, t	0.67	Steam, t	1.2
		Hydrochloric acid (31%), t	0.091	Electricity, 10^9 J	1.33
				Cooling water, m^3	200
				Process water, m^3	1.7

PRIMARY PRODUCT: Acetaldehyde

SOURCE: 3

PRIMARY RAW MATERIAL: Ethylene (B)

PLANT CAPACITY: 136×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$46.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetaldehyde	1.0	Ethylene	0.68	Fuel, 10^9 J	10.0

PRIMARY PRODUCT: Acetic Acid

SOURCE: 3

PRIMARY RAW MATERIAL: Acetaldehyde

PLANT CAPACITY: 136×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$45.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Acetaldehyde	0.78	Fuel, 10^9 J	13.2
Methyl Acetate	0.04				

PRIMARY PRODUCT: Acetic Acid

SOURCE: 3

PRIMARY RAW MATERIAL: n-Butane

PLANT CAPACITY: 136×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$84.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	n-Butane	0.83	Fuel, 10^9 J	9.6
Formic Acid	0.03				

PRIMARY PRODUCT: Acetic Acid

SOURCE: 4

PRIMARY RAW MATERIAL: Ethanol

PLANT CAPACITY: 3×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$3.84 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Ethanol	0.95	Steam, t	12
		Ethyl Acetate	0.015	Electricity, 10^3 J	2.0
				Cooling water, m^3	480
				Process water, m^3	10

PRIMARY PRODUCT: Acetic Acid

SOURCE: 5

PRIMARY RAW MATERIAL: Glucose

PLANT CAPACITY: 75.6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$34.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Glucose	1.20	Steam, t	19.0
Sodium Sulfate	1.25	Sodium Hydroxide	0.474	Electricity,	0.87
		Sulfuric Acid	0.76	10^3 J	
		Ammonia	0.0022	Cooling water,	145
				m^3	

PRIMARY PRODUCT: Acetic Acid

SOURCE: 6

PRIMARY RAW MATERIAL: Marine Algae

PLANT CAPACITY: 119×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$17.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Marine Algae	2.50	Fuel, 10^9 J	2.2
		Sewage Sludge	2.50		

PRIMARY PRODUCT: Acetic Acid

SOURCE: 3

PRIMARY RAW MATERIAL: Methanol

PLANT CAPACITY: 136×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$45.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Methanol	0.58	Fuel, 10^9 J	12.3
		Carbon Monoxide	0.61		

PRIMARY PRODUCT: Acetic Acid

SOURCE: 1

PRIMARY RAW MATERIAL: Sulfite Black Liquor

PLANT CAPACITY: 5.5×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$6.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Sulfite Black	68	Steam, t	9.0
Formic Acid	0.11	Liquor		Electricity,	0.18
Sodium Sulfate	1.4	Sulfuric Acid	0.93	10^9 J	
		Methyl Ethyl	0.03	Cooling water,	10
		Ketone		m^3	

PRIMARY PRODUCT: Acetic Acid

SOURCE: 1

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 0.90×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$2.6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetic Acid	1.0	Wood	33.3	Electricity, 10^9 J	1.2
Charcoal	8.33				
Methanol	0.35				
Fuel Liquid	1.90				

PRIMARY PRODUCT: Acetone

SOURCE: 3

PRIMARY RAW MATERIAL: Isopropanol

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$16.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetone	1.0	Isopropanol	1.11	Fuel, 10^9 J	15

PRIMARY PRODUCT: Acetone

SOURCE: 3

PRIMARY RAW MATERIAL: Propylene

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$34 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Acetone	1.0	Propylene	0.85	Fuel, 10^9 J	35
		Hydrogen	0.08	Process water, m^3	0.43
		Chloride			
		Sodium	0.01		
		Hydroxide			

PRIMARY PRODUCT: Ammonia

SOURCE: 7

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 599×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$391 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ammonia	1.0	Coal	1.77	Steam, t	3.3
Sulfur	0.065			Electricity, 10^9 J	0.15
				Cooling water m^3	410
				Process water, m^3	29

PRIMARY PRODUCT: Ammonia

SOURCE: 7

PRIMARY RAW MATERIAL: Methane

PLANT CAPACITY: 599×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$194 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ammonia	1.0	Methane	0.70	Steam, t	-0.66
				Electricity, 10^9 J	0.36
				Cooling water, m^3	400
				Process water, m^3	0.9

PRIMARY PRODUCT: Ammonia

SOURCE: 8

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 130×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$66 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ammonia	1.0	Wood	1.73	Steam, t	1.3
				Electricity, 10^9 J	4.3
				Cooling water, m^3	43

PRIMARY PRODUCT: Benzene

SOURCE: 9

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 283×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$2200 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Benzene	1.0	Coal	39.9	Fuel, 10^9 J	-181
Ethylene	1.12				
Propylene	0.31				
Naphthalene	0.55				
Phenol	0.19				
o-Cresol	0.066				
m,p-Cresol	0.21				
Xylenols	0.23				
Carbon Black	0.17				
Feedstock					
Coke Briquettes	10.4				
Ammonia	0.14				
Sulfur	0.69				

PRIMARY PRODUCT: Benzene

SOURCE: 10

PRIMARY RAW MATERIAL: Catalytic Reformate, Coal

PLANT CAPACITY: 179×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$59.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Benzene	1.0	Catalytic Reformate, Coal	9.44	Steam, t	0.060
Toluene	2.6			Electricity,	1.7
Ethyl Benzene	0.455			10^9 J	
p-xylene	1.0			Fuel, 10^9 J	30.8
Pyrolysis	3.3			Cooling water,	430
Gasoline				m^3	
o-xylene	1.07				

PRIMARY PRODUCT: Benzene

SOURCE: 10

PRIMARY RAW MATERIAL: Catalytic Reformate, Petroleum

PLANT CAPACITY: 178×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$64.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Benzene	1.0	Catalytic Reformate, Petroleum	12.3	Steam, t	0.078
Toluene	2.6			Electricity, 10^9 J	1.75
Ethyl Benzene	0.46			Fuel, 10^9 J	31.8
p-Xylene	1.02			Cooling water m^3	434
o-Xylene	1.07				
Pyrolysis Gasoline	6.15				

PRIMARY PRODUCT: Benzene

SOURCE: 3

PRIMARY RAW MATERIAL: Toluene

PLANT CAPACITY: 90×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Benzene	1.0	Toluene	1.20	Fuel, 10^9 J	3.64
Methane	0.24	Hydrogen	0.07		

PRIMARY PRODUCT: Butadiene

SOURCE: 3

PRIMARY RAW MATERIAL: n-Butane

PLANT CAPACITY: 90×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$72.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Butadiene	1.0	n-Butane	1.9	Fuel, 10^9 J	29.5

PRIMARY PRODUCT: Butadiene

SOURCE: 1

PRIMARY RAW MATERIAL: Ethanol

PLANT CAPACITY: 40×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$87 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Butadiene	1.0	Ethanol	1.38	Steam, t	30
		Acetaldehyde	1.15	Electricity, 10^9 J	0.004
				Cooling water, m^3	144
				Process water, m^3	2.5

PRIMARY PRODUCT: n-Butanol

SOURCE: 1

PRIMARY RAW MATERIAL: Acetaldehyde

PLANT CAPACITY: 30×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$34.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butanol	1.0	Acetaldehyde	1.45	Steam, t	2.3
n-Butyraldehyde	0.17	Sodium Hydroxide	0.03	Electricity, 10^9 J	5.9
		Acetic Acid	0.045	Cooling water, m^3	4.0
		Hydrogen	0.07		

PRIMARY PRODUCT: n-Butanol

SOURCE: 10,18,35

PRIMARY RAW MATERIAL: Glucose

PLANT CAPACITY: 70×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$22.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butanol	1.0	Glucose	5.2	Steam, t	14.6
Acetone	0.5			Electricity, 10^9 J	6.3
Ethanol	0.18			Cooling water, m^3	436
Carbon Dioxide	2.1				
Hydrogen	0.065				

PRIMARY PRODUCT: n-Butanol

SOURCE: 1

PRIMARY RAW MATERIAL: Molasses

PLANT CAPACITY: 6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$20.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butanol	1.0	Molasses	9.5	Steam, t	20
Acetone	0.50	Ammonium Sulfate	0.67	Electricity, 10^9 J	0.36
Ethanol	0.17			Cooling water, m^3	417
Hydrogen	0.90			Process water, m^3	45
Carbon Dioxide	1.33				

PRIMARY PRODUCT: n-Butanol

SOURCE: 3

PRIMARY RAW MATERIAL: Propylene

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$38.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butanol	1.0	Propylene	0.92	Fuel, 10^9 J	19.5
Fuel Liquid	0.38	Carbon Monoxide	0.54		
Isobutanol	0.14	Hydrogen	0.07		

PRIMARY PRODUCT: s-Butanol

SOURCE: 3

PRIMARY RAW MATERIAL: n-Butenes

PLANT CAPACITY: 45×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$15 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
s-Butanol	1.0	n-Butenes	1.14	Fuel, 10^9 J	32.2
Fuel Liquid	0.33	Sodium Hydroxide	0.02		
		Sulfuric Acid	0.01		

PRIMARY PRODUCT: n-Butenes

SOURCE: 10

PRIMARY RAW MATERIAL: n-Butanol

PLANT CAPACITY: 20×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butenes	1.0	n-Butanol	1.4	Steam, t	1.26
				Electricity, 10^9 J	0.76
				Fuel, 10^9 J	1.8
				Cooling water, m^3	63
				Process water, m^3	0.34

PRIMARY PRODUCT: n-Butenes

SOURCE: 10

PRIMARY RAW MATERIAL: s-Butanol

PLANT CAPACITY: 20×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butenes	1.0	s-Butanol	1.4	Steam, t	1.26
				Electricity, 10^9 J	0.76
				Fuel, 10^9 J	1.8
				Cooling water, m^3	6.3
				Process water, m^3	0.34

PRIMARY PRODUCT: n-Butenes

SOURCE: 10,11

PRIMARY RAW MATERIAL: Refinery Gas

PLANT CAPACITY: 100×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
n-Butenes	1.0	Refinery Gas	2.4	Fuel, 10^9 J	1.5
n-Butane	1.4				

PRIMARY PRODUCT: Carbon Monoxide

SOURCE: 10

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 38.7×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$19.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Carbon Monoxide	1.0	Coal	0.9	Steam, t	0.97
Hydrogen	0.046			Electricity, 10^9 J	77
Sulfur	0.030			Cooling water, m^3	167
				Process water, m^3	11

PRIMARY PRODUCT: Carbon Monoxide

SOURCE: 3

PRIMARY RAW MATERIAL: Methane

PLANT CAPACITY: 160×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$40 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Carbon Monoxide	1.0	Methane	0.64	Fuel, 10^9 J	23.6
Hydrogen	0.23				

PRIMARY PRODUCT: Carbon Monoxide

SOURCE: 8, 10, 12

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 38.7×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$19 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Carbon Monoxide	1.0	Wood	1.27	Steam, t	1.5
Hydrogen	0.16			Electricity, 10^9 J	4.7
				Cooling Water, m^3	57.8

PRIMARY PRODUCT: Catalytic Reformate, Coal

SOURCE: 13

PRIMARY RAW MATERIAL: Naphtha, Coal

PLANT CAPACITY: 577×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$11.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Catalytic Reformate	1.0	Coal Naphtha	1.1	Steam, t	0.12
Hydrogen	0.019			Electricity, 10^9 J	0.1
Propane	0.02			Fuel, 10^9 J	2.3
n-Butane	0.039			Cooling water, m^3	20.4

PRIMARY PRODUCT: Catalytic Reformate, Petroleum

SOURCE: 13

PRIMARY RAW MATERIAL: Naphtha, Petroleum

PLANT CAPACITY: 577×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$11.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Catalytic Reformate	1.0	Petroleum	1.1	Steam, t	0.12
Hydrogen	0.019	Naphtha		Electricity, 10^9 J	0.1
Propane	0.02			Fuel, 10^9 J	2.3
n-Butane	0.039			Cooling water, m^3	20.4

PRIMARY PRODUCT: Cyclohexane

SOURCE: 3

PRIMARY RAW MATERIAL: Benzene

PLANT CAPACITY: 100×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$12.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Cyclohexane	1.0	Benzene	0.94	Fuel, 10^9 J	-0.455
		Hydrogen	0.07		

PRIMARY PRODUCT: Cyclohexane

SOURCE: 10

PRIMARY RAW MATERIAL: Naphtha, Coal

PLANT CAPACITY: 150×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$4.57 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Cyclohexane	1.0	Coal Naphtha	1.0	Steam, t Electricity, 10^9 J Cooling water, m^3	3.2 0.01 170

PRIMARY PRODUCT: Cyclohexane

SOURCE: 10

PRIMARY RAW MATERIAL: Naphtha, Petroleum

PLANT CAPACITY: 150×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$5.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Cyclohexane	1.0	Petroleum Naphtha	1.0	Steam, t Electricity, 10^9 J Cooling water, m^3	4.8 0.014 265

PRIMARY PRODUCT: Cyclohexanone

SOURCE: 3

PRIMARY RAW MATERIAL: Cyclohexane

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$47.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Cyclohexanone	1.0	Cyclohexane	1.05	Fuel, 10^9 J	15.4
Hydrogen	0.02				

PRIMARY PRODUCT: Cyclohexanone

SOURCE: 10

PRIMARY RAW MATERIAL: Phenol

PLANT CAPACITY: 30×10^3 metric tons (t) primary product/year .

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Cyclohexanone	1.0	Phenol	0.96	Fuel, 10^9 J	-0.47
		Hydrogen	0.04		

PRIMARY PRODUCT: Ethanol

SOURCE: 10, 14

PRIMARY RAW MATERIAL: Corn

PLANT CAPACITY: 211×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$112 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Corn	3.0	Fuel, 10^9 J	9.6
Distillers Grains	0.76	Barlet Malt	0.7		
Carbon Dioxide	0.7				

PRIMARY PRODUCT: Ethanol

SOURCE: 15

PRIMARY RAW MATERIAL: Corn Stover

PLANT CAPACITY: 30.8×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$55.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Corn Stover	13.4	Fuel, 10^9 J	54.5
Carbon Dioxide	1.3				
Pentose	1.2				

PRIMARY PRODUCT: Ethanol

SOURCE: 3

PRIMARY RAW MATERIAL: Ethylene

PLANT CAPACITY: 272×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$160 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Ethylene	0.75	Fuel, 10^9 J	33.7

PRIMARY PRODUCT: Ethanol

SOURCE: 16

PRIMARY RAW MATERIAL: Glucose

PLANT CAPACITY: 74.7×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$36 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Glucose	2.0	Steam, t	7
Carbon Dioxide	1.0			Electricity, 10^9 J	3
				Cooling water, m^3	205

PRIMARY PRODUCT: Ethanol

SOURCE: 10

PRIMARY RAW MATERIAL: Methanol

PLANT CAPACITY: 318×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$100 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Methanol	1.26	Steam, t	1.9
Methyl Acetate	0.33	Carbon Monoxide	1.22	Electricity, 10^9 J	3.5
		Hydrogen	0.17	Cooling water, m^3	200

PRIMARY PRODUCT: Ethanol

SOURCE: 1

PRIMARY RAW MATERIAL: Molasses

PLANT CAPACITY: 32×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$34.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Molasses	4.54	Steam, t	5.75
Carbon Dioxide	1.0	Sulfuric Acid	0.03	Electricity, 10^9 J	0.27
		Ammonium Sulfate	0.0095	Cooling water, m^3	275
				Process water, m^3	10.8

PRIMARY PRODUCT: Ethanol

SOURCE: 17

PRIMARY RAW MATERIAL: Sugar Beets

PLANT CAPACITY: 92.3×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$36.6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Sugar Beets	5.6	Fuel, 10^9 J	26.4
Carbon Dioxide	1.0	Sugar Cane	4.8		
		Sweet Sorghum	3.6		
		(integrated multi- feedstock process)			

PRIMARY PRODUCT: Ethanol

SOURCE: 10, 18

PRIMARY RAW MATERIAL: Sulfite Waste Liquor

PLANT CAPACITY: 15.4×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$12.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Sulfite Waste	153	Steam, t	22
Methanol	0.05	Liquor		Electricity,	1.75
Carbon Dioxide	0.77	Lime (Calcium Oxide)	0.52	10^9 J	
		Sulfuric Acid	0.022		

PRIMARY PRODUCT: Ethanol

SOURCE: 19

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 75.4×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$122 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethanol	1.0	Wood	7.5	Cooling water,	700
Carbon Dioxide	1.0	Sulfuric Acid	0.1	m ³	
		Calcium Oxide	0.09	Process water,	46
				m ³	

PRIMARY PRODUCT: Ethylbenzene

SOURCE: 3

PRIMARY RAW MATERIAL: Benzene

PLANT CAPACITY: 522×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$47.6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylbenzene	1.0	Benzene	0.74	Fuel, 10 ⁹ J	0.9
Fuel Liquid	0.01	Ethylene	0.27		

PRIMARY PRODUCT: Ethylene

SOURCE: 20

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 238×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$766 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene	1.0	Coal	14.4	Steam, t	11.0
Propylene	0.57			Electricity, 10^9 J	0.76
n-Butanol	0.4			Fuel, 10^9 J	12.4
Pyrolysis	2.83			Cooling water, m^3	3520
Gasoline				Process water, m^3	115

PRIMARY PRODUCT: Ethylene

SOURCE: 1

PRIMARY RAW MATERIAL: Ethanol

PLANT CAPACITY: 20×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene	1.0	Ethanol	1.73	Steam, t	1.26
				Electricity, 10^9 J	0.75
				Fuel, 10^9 J	1.8
				Cooling water, m^3	63
				Process water, m^3	0.34

PRIMARY PRODUCT: Ethylene

SOURCE: 10

PRIMARY RAW MATERIAL: Municipal Solid Wastes

PLANT CAPACITY: 2.6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$10.9 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene	1.0	Municipal Solid Waste	12.6	Electricity, 10^9 J	24
Ferrous Metal	0.83			Process water, m^3	7.3
Non-Ferrous Metal	0.2				
Fuel Liquid	2.3				

PRIMARY PRODUCT: Ethylene

SOURCE: 3

PRIMARY RAW MATERIAL: Naphtha, Petroleum

PLANT CAPACITY: 454×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$430 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene	1.0	Naphtha, Petroleum	3.25	Fuel, 10^9 J	12.5
Propylene	0.63				
n-Butenes	0.37				
Pyrolysis Gasoline	0.62				
Fuel Liquid	0.05				

PRIMARY PRODUCT: Ethylene Glycol

SOURCE: 3

PRIMARY RAW MATERIAL: Ethylene

PLANT CAPACITY: 180×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$107 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene Glycol	1.0	Ethylene	0.5	Fuel, 10^9 J	29
		Acetic Acid	0.03		
		Methane	0.02		

PRIMARY PRODUCT: Ethylene Glycol

SOURCE: 3

PRIMARY RAW MATERIAL: Ethylene Oxide

PLANT CAPACITY: 180×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$41.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene Glycol	1.0	Ethylene Oxide	0.87	Fuel, 10^9 J	15.0
Diethylene Glycol	0.11				
Triethylene Glycol	0.03				

PRIMARY PRODUCT: Ethylene Glycol

SOURCE: 10, 18

PRIMARY RAW MATERIAL: Formaldehyde

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$57.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene Glycol	1.0	Formaldehyde	0.65	Fuel, 10^9 J	24.5
		Carbon Monoxide	0.60	Process water,	0.01
		Methanol	0.03	m^3	
		Hydrogen	0.086		

PRIMARY PRODUCT: Ethylene Oxide

SOURCE: 3

PRIMARY RAW MATERIAL: Ethylene

PLANT CAPACITY: 136×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$128 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Ethylene Oxide	1.0	Ethylene	0.96	Fuel, 10^9 J	-3.2

PRIMARY PRODUCT: Formaldehyde (37 wt%)

SOURCE: 21

PRIMARY RAW MATERIAL: Methanol

PLANT CAPACITY: 45.4×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Formaldehyde	1.0	Methanol	0.43	Steam, t	-0.56
				Electricity, 10^9 J	0.3
				Cooling water, m^3	23
				Process water, m^3	5.7

PRIMARY PRODUCT: Glucose

SOURCE: 16

PRIMARY RAW MATERIAL: Aquatic Biomass

PLANT CAPACITY: 150×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$36 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Aquatic Biomass	2.45	Steam, t	1.6
		Sulfuric Acid	0.15	Electricity, 10^9 J	0.4
		Limestone	0.17		

PRIMARY PRODUCT: Glucose

SOURCE: 22

PRIMARY RAW MATERIAL: Corn Stover (A)

PLANT CAPACITY: 150×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$61 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Corn Stover	3.12	Steam, t	6.8
Pentose	1.4	Sulfuric Acid	0.28	Electricity,	0.83
Lignin, Kraft	0.94	Calcium Oxide	0.13	10^9 J	
		Methanol	0.06	Fuel, 10^9 J	20
				Process water,	21.5
				m^3	

PRIMARY PRODUCT: Glucose

SOURCE: 5

PRIMARY RAW MATERIAL: Corn Stover (B)

PLANT CAPACITY: 91×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$15.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Corn Stover	3.82	Steam, t	1.0
		Sodium Hydroxide	0.072	Electricity,	0.7
		Ammonia	0.006	10^9 J	
		Yeast	0.003	Cooling water,	78
				m^3	

PRIMARY PRODUCT: Glucose

SOURCE: 16

PRIMARY RAW MATERIAL: Sugar Cane

PLANT CAPACITY: 150×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$60.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Sugar Cane	10.8	Steam, t Electricity, 10^9 J Process water, m^3	3.6 0.05 1.5

PRIMARY PRODUCT: Glucose

SOURCE: 16

PRIMARY RAW MATERIAL: Wheat Straw

PLANT CAPACITY: 150×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$110 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Wheat Straw Sulfuric Acid Newsprint	6.54 0.21 0.27	Steam, t Electricity, 10^9 J Cooling water, m^3 Process water, m^3	4.4 5.45 100 45

PRIMARY PRODUCT: Glucose

SOURCE: 1

PRIMARY RAW MATERIAL: Wood (A)

PLANT CAPACITY: 16×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$7.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Wood	3.13	Steam, t	3.5
Pentose	0.25	Sulfuric Acid	0.25	Electricity, 10^9 J	0.07
Wood Lignin	0.94	Calcium Oxide	0.14	Cooling water, m^3	0.31
				Process water, m^3	12.5

PRIMARY PRODUCT: Glucose

SOURCE: 23

PRIMARY RAW MATERIAL: Wood (B)

PLANT CAPACITY: 34.7×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$2.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glucose	1.0	Wood	2.2	Steam, t	0.6
Pentose	0.18				
Wood Lignin	0.44				

PRIMARY PRODUCT: Glycerine

SOURCE: 10, 18

PRIMARY RAW MATERIAL: Glucose

PLANT CAPACITY: 13.6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$18 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glycerine	1.0	Glucose	3.0	Steam, t Electricity, 10^9 J Cooling water, m^3	9.0 3.9 270

PRIMARY PRODUCT: Glycerine

SOURCE: 3

PRIMARY RAW MATERIAL: Propylene

PLANT CAPACITY: 45×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$57.6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Glycerine	1.0	Propylene	0.73	Fuel, 10^9 J	53
Dichloro- propylene	0.27	Chlorine	2.25		
Hydrogen	0.56	Sodium	0.50		
Chloride		Hydroxide			
		Calcium Oxide	0.78		
		Toluene	0.01		

PRIMARY PRODUCT: Hydrogen

SOURCE: 7

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 83.8×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$290 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Hydrogen	1.0	Coal	8.5	Steam, t	12.8
Sulfur	0.29			Electricity, 10^9 J	0.5
				Cooling water, m^3	1620
				Process water, m^3	114

PRIMARY PRODUCT: Hydrogen

SOURCE: 7

PRIMARY RAW MATERIAL: Methane

PLANT CAPACITY: 83.8×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$74.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Hydrogen	1.0	Methane	3.3	Steam, t	-6.1
				Electricity, 10^9 J	1.5
				Cooling water, m^3	200
				Process water, m^3	14.2

PRIMARY PRODUCT: Hydrogen

SOURCE: 10

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 104×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$140 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Hydrogen	1.0	Wood	10.6	Steam, t	5.1
				Electricity, 10^9 J	7.1
				Fuel, 10^9 J	14.3
				Cooling water, m^3	155
				Process water, m^3	10.5

PRIMARY PRODUCT: Lignin, Wood

SOURCE: 24

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 76.6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$122 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Lignin, Wood	1.0	Wood	4.8	Steam, t	32
Furfural	0.46	Hydrochloric Acid	0.9	Electricity, 10^9 J	4.9
Acetic Acid	0.20	Calcium Oxide	1.4		
Ethanol	0.91	Calcium Chloride	0.19		

PRIMARY PRODUCT: Methane

SOURCE: 25

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 1670×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$1500 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methane	1.0	Coal	3.6	Fuel, 10^9 J	-4.24
Sulfur	0.031			Process water,	13.7
Ammonia	0.032			m^3	

PRIMARY PRODUCT: Methane

SOURCE: 26

PRIMARY RAW MATERIAL: Feedlot Wastes

PLANT CAPACITY: 6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$21.6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methane	1.0	Feedlot Wastes	11.2	Steam, t	6.6
Distillers	1.5			Electricity,	3.6
Grains				10^9 J	
(equivalent)				Fuel, 10^9 J	0.73
				Process water,	21.7
				m^3	

PRIMARY PRODUCT: Methane

SOURCE: 10, 27

PRIMARY RAW MATERIAL: Kelp

PLANT CAPACITY: 20×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$3000 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methane	1.0	Kelp (wet) Calcium Chloride	180 0.8	(None)	

PRIMARY PRODUCT: Methane

SOURCE: 28

PRIMARY RAW MATERIAL: Wheat Straw

PLANT CAPACITY: 9.3×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$18 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methane	1.0	Wheat Straw Sodium Hydroxide	16.0 0.80	Electricity, 10^9 J Process water, m^3	2.8 150

PRIMARY PRODUCT: Methane

SOURCE: 8

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 71×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$37.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methane	1.0	Wood	3.2	Electricity, 10^9 J Cooling water, m^3	2.1 6.6

PRIMARY PRODUCT: Methanol

SOURCE: 3, 29

PRIMARY RAW MATERIAL: Carbon Dioxide

PLANT CAPACITY: 320×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$96.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methanol	1.0	Carbon Dioxide Hydrogen	1.50 0.22	Steam, t Electricity, 10^9 J Cooling water, m^3	1.8 3.4 190

PRIMARY PRODUCT: Methanol

SOURCE: 7

PRIMARY RAW MATERIAL: Coal

PLANT CAPACITY: 600×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$416 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methanol	1.0	Coal	1.7	Steam, t	3
Sulfur	0.06			Electricity, 10^9 J	0.44
				Cooling water, m^3	374
				Process water, m^3	26.2

PRIMARY PRODUCT: Methanol

SOURCE: 7

PRIMARY RAW MATERIAL: Methane

PLANT CAPACITY: 600×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$160 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methanol	1.0	Methane	0.71	Electricity, 10^9 J	0.3
				Cooling water, m^3	255
				Process water, m^3	0.9

PRIMARY PRODUCT: Methanol

SOURCE: 8

PRIMARY RAW MATERIAL: Wood

PLANT CAPACITY: 88.7×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$57 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methanol	1.0	Wood	2.54	Electricity, 10^9 J	3.1
				Cooling water, m^3	10.7

PRIMARY PRODUCT: Methyl Ethyl Ketone

SOURCE: 3

PRIMARY RAW MATERIAL: s-Butanol

PLANT CAPACITY: 45×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$10.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methyl Ethyl Ketone	1.0	s-Butanol	1.1	Fuel, 10^9 J	45.5

PRIMARY PRODUCT: Methyl Ethyl Ketone

SOURCE: 3

PRIMARY RAW MATERIAL: n-Butene

PLANT CAPACITY: 45×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$35.6 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Methyl Ethyl Ketone	1.0	n-Butene	0.84	Fuel, 10^9 J	22
Sec-Butyl Ether	0.12				

PRIMARY PRODUCT: Phenol

SOURCE: 30

PRIMARY RAW MATERIAL: Benzene

PLANT CAPACITY: 100×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$78 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Phenol	1.0	Benzene	0.93	Steam, t	0.05
Acetone	0.62	Propylene	0.53	Electricity, 10^9 J	1.5
				Fuel, 10^9 J	17.2
				Cooling water, m^3	260
				Process water, m^3	0.51

PRIMARY PRODUCT: Phenol

SOURCE: 31

PRIMARY RAW MATERIAL: Lignin, Kraft

PLANT CAPACITY: 29.6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$49 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Phenol	1.0	Lignin, Kraft	5.0	Electricity,	3.4
Benzene	0.72			10^9 J	
Sulfur	0.05			Process water,	2.7
Fuel Liquid	0.54			m^3	

PRIMARY PRODUCT: Phenol

SOURCE: 10, 31

PRIMARY RAW MATERIAL: Lignin, Wood

PLANT CAPACITY: 29.6×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$49 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Phenol	1.0	Lignin, Wood	5.0	Electricity,	3.4
Benzene	0.72			10^9 J	
Fuel Liquid	0.54			Process water,	2.7
				m^3	

PRIMARY PRODUCT: Phthalic Anhydride

SOURCE: 32

PRIMARY RAW MATERIAL: Naphthalene

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$44.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Phthalic Anhydride	1.0	Naphthalene	1.0	Steam, t	-3.9
				Electricity, 10^9 J	0.24
				Fuel, 10^9 J	2.32
				Cooling water, m^3	83.5
				Process water, m^3	9.2

PRIMARY PRODUCT: Phthalic Anhydride

SOURCE: 32

PRIMARY RAW MATERIAL: o-Xylene

PLANT CAPACITY: 50×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$23.8 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Phthalic Anhydride	1.0	o-Xylene	0.93	Steam, t	-3.5
				Electricity, 10^9 J	0.54
				Fuel, 10^9 J	2.2
				Process water, m^3	3.7

PRIMARY PRODUCT: Isopropanol

SOURCE: 10

PRIMARY RAW MATERIAL: Acetone

PLANT CAPACITY: 68×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$2.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Isopropanol	1.0	Acetone	0.97	Steam, t	0.95
		Hydrogen	0.033	Electricity, 10^9 J	0.03
				Fuel, 10^9 J	1.75
				Cooling water, m^3	130

PRIMARY PRODUCT: Isopropanol

SOURCE: 3

PRIMARY RAW MATERIAL: Propylene

PLANT CAPACITY: 272×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$82.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Isopropanol	1.0	Propylene	0.73	Fuel, 10^9 J	18

PRIMARY PRODUCT: Propylene

SOURCE: 10

PRIMARY RAW MATERIAL: Isopropanol

PLANT CAPACITY: 20×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8.2 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Propylene	1.0	Isopropanol	1.5	Steam, t	1.3
				Electricity, 10^9 J	0.76
				Fuel, 10^9 J	1.8
				Cooling water, m^3	63
				Process water, m^3	0.34

PRIMARY PRODUCT: Propylene

SOURCE: 3

PRIMARY RAW MATERIAL: Refinery Gas

PLANT CAPACITY: 180×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$8.3 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Propylene	1.0	Refinery Gas	1.33	Fuel, 10^9 J	0.45
Propane	0.33				

PRIMARY PRODUCT: Propylene Oxide

SOURCE: 33

PRIMARY RAW MATERIAL: Propylene

PLANT CAPACITY: 100×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$47.5 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Propylene Oxide	1.0	Propylene	0.82	Steam, t	5.0
Dichloro- propylenes	0.11	Chlorine	1.46	Electricity, 10^9 J	0.4
		Lime (Calcium Oxide)	1.1	Fuel, 10^9 J	-5.8
				Cooling water, m^3	220
				Process water, m^3	45

PRIMARY PRODUCT: Urea

SOURCE: 3

PRIMARY RAW MATERIAL: Ammonia

PLANT CAPACITY: 340×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$82.7 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Urea	1.0	Ammonia	0.57	Fuel, 10^9 J	3.2
		Carbon Dioxide	0.74		

PRIMARY PRODUCT: Urea

SOURCE: 34

PRIMARY RAW MATERIAL: Methane

PLANT CAPACITY: 365×10^3 metric tons (t) primary product/year

TOTAL FIXED CAPITAL AS OF OCTOBER 1981: \$161 million

Product	Per t of primary product	Raw material	Per t of primary product	Utility	Per t of primary product
Urea	1.0	Methane	0.24	Fuel, 10^9 J	10.7
				Cooling water, m^3	0.27
				Process water, m^3	1.4

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