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THE ECONOMICS OF FOREST CHEMICALS:  
PROCESS DEVELOPMENT AND ECONOMICS ANALYSIS

by

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**THE ECONOMICS OF FOREST CHEMICALS:  
PROCESS DEVELOPMENT AND ECONOMICS ANALYSIS**

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## SUMMARY

The abundance of natural resources in Canada tends to support a resource-based <sup>exports</sup> economy, and it is recognized that excessive industrial activity goes towards the export of resources in an undeveloped form, instead of in higher value <sup>added</sup> products. A case is the forest products industries, comprising of paper and allied products, and the wood industries. The vast forest reserves, and the statistics of employment, production and exports, reveal these industries to be highly significant part of the Canadian economy. The vulnerability of these industries has been demonstrated by recent protectionist actions taken by the US government, emphasising the need for a diversification of products, as well as for a switch to products of a higher value added.

Canada, as most western industrialized nations, relies largely on petroleum, not only for energy, but also as a chemical base upon which the manufacture of innumerable consumer goods depends. The OPEC oil embargoes stimulated R&D into alternative energy sources in many countries, to lessen this dependence on a depleting and politically controlled resource. The current fall in the price of oil may temporarily have diminished, in some respects, the urgency of this search for alternatives.

At the same time, the independent need for a more advanced exploitation of resources has compelled the pursuit of new technology, in particular for the forest industry. The Forintek Biomass Conversion Project serves that objective. A similar

research project is the work at the Solar Energy Research Institute (SERI), Colorado, and so also is the French 'Carburol' plan (Chem. Eng., 19 March, 1984, p. 49), with its commitment to a plant depending in part on Canadian technology.

The concentration on biotechnology, a trend taking place in other parts of the world, and in other economic sectors, is important for the future of the forest industries. Broadly, it fits a necessary direction for the Canadian economy. The concern in Canada with this technology, and the R&D needed to have a state of the art research capability, and to offer and share in development elsewhere, is highly suitable. It is necessary to be in touch with similar activities in other countries, so as to be able to evaluate their significance in the Canadian context. The records and analytical work at Forintek should advance that capability.

In the economics of a new technology, as this one which is a subject of fundamental R&D, obscurities are inevitable. It may be that for some questions, only the future has the answer. But with designs of processes, an analysis of process characteristics and market conditions can tell about profitability; this enables plants to be built, and also provides indicators for further R&D.

In the Forintek Project, basic processes, undergoing development or already established, become components in an integrated bioconversion process, which may eventually be expanded into a larger design, and a proposal for a plant facility.

It is important to be able to anticipate the performance of a process in economics terms, under various market conditions. A

computer simulation of the process serves this requirement, and optimized management, when the process is embodied in an operating plant. With one integrated process that is being considered at Forintek, it has been shown we have succeeded in simulating it on the linear activity system model, and formulating the optimization as a linear programming problem. That has been done despite process parameters having a non-linear response, and in such a way that an optimal setting of such parameters is determined at the same time.

As auxiliary to the R&D, the future prospect includes continual repetition of such a type of economic exploration. A long run organization for it, and appropriate facilities, will be essential for its on-going, cumulative usefulness. A part of that, of primary importance, is the development of a data base, with a design that suits the work.

The program used for LP computations at Forintek, as with other programs that were available formerly, had not been ideal. We now use another that serves convenience for analysis, in harmony with needs for the organized recording and documentation of technical and economic data. It permits, while remaining in the same framework as the data, the carrying out of economic analysis and recording of its results. For a part of this facility, the program reads an LP problem from an area in a spreadsheet, and writes the results to designated rows and columns extending that area. The availability of this type of program will greatly facilitate subsequent work, firstly for storage of data in an intelligible and usable form; for carrying out analysis based on

it; finally, for recording the results in their proper relation to the data, and in a most effective way for documenting and communicating their significance. With data that has been assembled, we have an LP model for one integrated process, with 165 variables and 62 constraints, and 1,260 non-zero coefficients. The model has been transferred into the spreadsheet framework. There will be a great enhancement of the position for reviewing it, interpreting and communicating the results, and building further on it.

The R&D in the biotechnology area will broaden the already significant contribution that the forest products industries make to Canada's economy, in that potential products would be of a more highly processed form and thus increase the value added of this industry.

## Acknowledgements

This paper would not have been possible without the supervision of Professors S.N. Afriat and J. Kuiper whose guidance and patience proved invaluable. Additionally, the opportunity granted to me by Forintek Canada Corporation to work on their biomass conversion model offered me the chance to apply my knowledge in a practical manner. Special thanks to Dr. A. Schuler, Dr. J. Saddler, M. Mes-Hartress, Q. Nguyen and the Biotechnology Department of Forintek Canada Corporation.

The forest is a peculiar organism of unlimited kindness and benevolence that makes no demands for its sustenance and extends generously the products of its life activity; it affords protection to all beings, offering shade even to the axeman who destroys it.

*Gautama Buddha*



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## 1.0 INTRODUCTION : THE CANADIAN FORESTRY INDUSTRY

Until the late 1800's, the forest, as a provider of wood fuel, satisfied most of the world's modest energy needs. The industrial revolution in Europe, and population increase, produced a demand for energy and agricultural land that depleted the forests on the continent. To meet their energy requirements, it was necessary to turn to coal, which over the next 30 years replaced wood as the primary energy source. A higher energy density, a greater ease of transportation, handling and storage, and its availability, represented advantages of coal over wood.

The mid-1900's introduced the petroleum era, in which oil gained supremacy as the world's major energy provider. It was cleaner and cheaper, and easier to transport and store than coal, and more versatile. Its applications as a fuel source, in the transportation sector, electrification, home heating, and the multitude of petrochemical products, industrial chemicals, solvents, paints, cosmetics, synthetic materials, drugs, plastics, cellophane, explosives, photo films, celluloid, shatterproof glass, sponges, phonograph records, cassette tapes, artificial hair etc. seemed unlimited. Thus brought about the sweeping changes in lifestyle, technological development and affluence which are the characteristics of modern industrialized societies.

By 1980, petroleum satisfied 45% of the world's primary energy requirements, besides being the provider of the multitude of petroleum-based consumer products. With OPEC countries accounting for one third of its production, and the embargoes of the 1970's,

petroleum became a politicized economic commodity. Interruptions in supply and escalating prices awakened the western world to their dependence on a depleting resource controlled by a few, and in some cases anti-western, nations. How these world trends apply to Canada are illustrated in Figure 1.1.

To lessen the dependence, attention has been given to other energy options. Renewable sources such as solar, wind, hydraulic, geothermal, tidal and forest biomass are recognized as contributing to the world's energy requirements on a sustainable basis.

In less than a century, coming full-circle, the forest again makes a significant contribution to energy requirements. Forest biomass, like petroleum, is also used as a chemical base in the manufacture of many consumer goods.

This paper examines forest biomass as a chemical resource, with a view to analysis of the economic performance of conversion processes now under R&D.

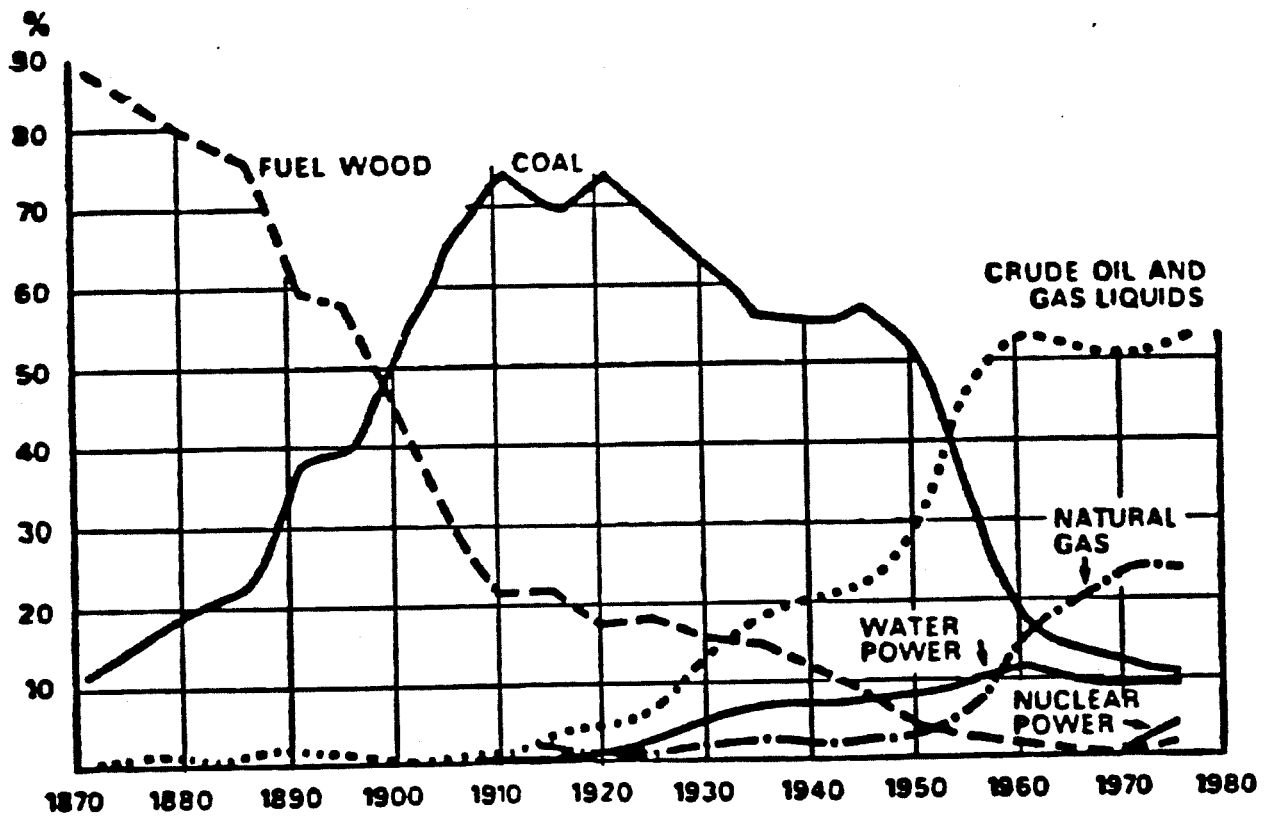
#### Forest Nation:

Environment Canada statistics show that forest accounts for 4,364,000 sq km, or 47%, of Canada's total land areas. Of that amount, 2,640,000 sq km is suitable for production (Canadian Forestry Service 1984). Together, paper and allied products and wood are Canada's leading industries according to Statistics Canada 1982, and Canadian Forestry Statistics, Statistics Canada 1983, confirm this. In 1983, the above industries had 216,273 employees, paid wages and salaries of \$5,767,228,000, and had an

added value to their products of \$9,933,027,000. This is illustrated in Table 1.1. Of the ten leading manufacturing industries in 1982, in Table 1.2, pulp and paper mills, and saw and planing mills (lumber), taken together, are the most important industries in terms of wages and salaries, total employment and value added. They employ 31.6% of all employees in these industries, and pay out 32.9% of wages and salaries. They rank second in terms of selling value of factory shipments.

Pre-eminence in the export market is even more striking with regard to pulp and paper, and lumber exports. They accounted for 12.58% of all Canadian exports in 1984, producing \$14,154,924,000 in export sales. (See Table 1.3)

It can be seen that from earliest days to the present, the forest has played an important part in Canada's development. As an alternative to petroleum and petroleum-based products, forest biomass conversion will broaden the significant contribution of the forest industries to manufacturing.



Source: A. Dolenko and S. Pnevmaticos, *Energy, Mines and Resources*, 1984.

**Figure 1.1: The Primary Energy Mix in Canada Since 1871**

	Manufacturing Activity						Total Activity				
	Number of establishments	Production & Related Workers		Cost of Fuel and Electricity (\$'000)	Cost of Materials & Supplies (\$'000)	Value of Shipments of Goods of Own Manufacture (\$'000)	Employees		Value Added (\$'000)		
		Number	Thousands of person-hours paid				Wages (\$'000)	Number		Salaries & Wages (\$'000)	
Wood	3 453	85 499	172 757	1 950 032	323 121	5 297 325	9 405 902	3 941 946	101 965	2 426 578	3 992 695
Paper & Allied	672	86 375	178 775	2 391 843	1 586 071	7 467 511	15 010 828	5 929 156	114 308	3 340 650	5 940 332

(1) Wood industries include: Sawmill, Planing Mill and Shingle Mills Products Industries, Veneer and Plywood Industries, Sash, Door and Other Millwork Industries, Wooden Box and Pallet Industry, Coffin and Casket Industry and Other Wood Industries

(2) Paper & Allied Products Industries include: Pulp and Paper Industries, Asphalt Roofing Industry, Paper Box and Bag Industries and Other Converted Paper Products Industries

**Table 1.1: Principal Statistics of the Canadian Forest Industry, 1983**

INDUSTRY	WAGES & SALARIES (\$'000,000)	RANK	TOTAL EMPLOYMENT	RANK	VALUE ADDED BY MANUFACTURE (\$'000,000)	RANK	SELLING VALUE OF FACTORY SHIPMENTS (\$'000,000)	RANK
PETROLEUM REFINING	734.0	8	20 155	9	2 119.3	5	21 370.0	1
MOTOR VEHICLE MFRS.	1 085.9	6	41 600	6	1 944.6	6	12 343.6	2
PULP & PAPER MILLS	2 436.4	1	82 892	1	4 512.8	1	10 650.1	3
SLAUGHT'G & MEAT PROD	757.5	7	34 390	7	1 214.6	8	7 927.0	4
IRON & STEEL MILLS	1 512.5	2	52 330	4	2 145.8	4	5 714.9	5
DAIRY PRODUCTS	561.9	9	25 796	8	1 098.2	9	5 364.1	6
MISC. MACH'Y & EQUIP.	1 444.1	3	62 382	2	2 562.5	2	5 123.7	7
MOT. VEH. PRTS. & ACCES	1 149.3	5	48 050	5	2 319.8	3	5 059.7	8
SAW. & PLANING MILLS	1 280.4	4	53 484	3	1 483.8	7	4 373.2	9
IND. ORGANIC CHEMS.	350.4	10	10 617	10	619.4	10	3 654.5	10

**Table 1.2: Ten Leading Manufacturing Industries, 1982**

Source: Canadian Pulp & Paper Association, Reference Tables, 1985.

<u>COMMODITY</u>	<u>1984</u> (\$'000 000)	<u>% OF TOTAL</u>	<u>1983</u> (\$'000 000)	<u>% OF TOTAL</u>
PULP & PAPER	9 901.1	8.80	8 038.6	8.84
NEWSPRINT	(4 783.6)	(4.25)	(4 005.1)	(4.40)
WOOD PULP	(3 908.0)	(3.47)	(3 057.6)	(3.37)
OTHER PAPER & BOARD	(1 209.5)	(1.08)	(975.9)	(1.07)
LUMBER	4 253.8	3.78	3 969.1	4.36
PASSENGER CARS & CHASSIS	13 889.6	12.35	9 573.0	10.52
MOTOR VEHICLE PARTS & ACCS	9 758.0	8.67	7 301.9	8.03
TRUCKS, TRUCK TRACTORS & TRAILERS	5 405.5	4.81	4 227.6	4.65
WHEAT	4 709.7	4.19	4 647.7	5.11
PETROLEUM	4 390.5	3.90	3 456.9	3.80
NATURAL GAS	3 886.4	3.45	3 958.2	4.35
ALUMINUM & ALLOYS, REFINED	1 900.0	1.69	1 744.2	1.92
GOLD & ALLOYS, REFINED	1 873.5	1.67	1 310.9	1.44
COAL	1 820.5	1.62	1 232.3	1.35
AIRCRAFT AND PARTS	1 781.3	1.58	1 519.9	1.67
OTHERS	48 925.5	43.49	39 983.7	43.96
<b>ALL EXPORTS</b>	<b>112 495.4</b>	<b>100.00</b>	<b>90 964.0</b>	<b>100.00</b>

**Table 1.3: Value of Principal Canadian Exports, 1982**

## 2.0 ALTERNATIVE SOURCES OF PETROLEUM & PETROLEUM PRODUCTS

Alternative sources of fuels and chemicals have been pursued in the past years, due to increases in the cost and interruptions in the supply of oil. A potential alternative is lignocellulosic material. This may be found in various forms, such as municipal solid waste (MSW), forest product waste (pulp mill waste, PMW), and some agricultural residuals (AR). These materials represent a largely untapped reservoir of chemicals and fuels. The key to using them is the conversion of cellulose to glucose, which can then be fermented to produce a variety of chemicals and fuels. This conversion process, hydrolyzing the cellulosic portion of wood to sugars, has long been known. In World War I, wood was commercially hydrolyzed to produce sugar for fermentation to alcohol. The early processes were relatively simple, but yields were so poor that they proved to be economically justifiable only under emergency conditions.

The conversion process has a complexity, due to the intractable nature of the substrate. Many approaches to this problem have been devised, all involving chemicals or biological systems to catalyze cellulose hydrolysis.

Technologies developed by the Biotechnology Department of Forintek Canada Corporation (FCC) involve the biological system approach, to exploit one of these untapped reservoirs of chemicals and fuels. In particular, the carbohydrate content of lignocellulosics of wood suggests the production of ethanol, butanol and butanediol. Compared to the starch or sugar crops

presently being used for ethanol production, lignocellulosics offer the advantages of lower costs, wider availability, and no competing uses as food or feed.

The potential products from lignocellulosic materials are summarized in Figure 2.1. The one which has received the most attention, for its as yet unrealized potential, is ethanol. As a solvent, it is second only to water, and its fastest growing use as such is in cleaning preparations and liquid detergents. It is a key material in the manufacture of drugs, plastics, lacquers, polishes, plasticizers, perfumes, and cosmetics. Ethanol has been used extensively in Canada as an antifreeze. Because of its transportability and combustibility, it has potential in the car fuel sector. It can be blended up to 10% with gasoline without modification in engine design, and can assist Environment Canada's program for the removal of lead from gasoline. Several tropical countries, notably Brazil, regard ethanol as an attractive petrochemical alternative. The sources and uses of ethanol are summarized in Figure 2.2. Thus, ethanol is identified as an end product with outstanding potential, and there has been a concentration on the research and development for its realization.

As may be seen from the process scheme in Figure 2.3, there are numerous possible products (ethanol, butanol, butanediol, enzymes or lignin) in the process. Which ones that should be produced in the future will depend on market conditions.

The current demand for ethanol is rather static, possibly because ethanol produced from biomass competes with the established ethanol of petrochemicals for the existing markets

rather than creating new ones. An important question for this investigation is whether, by process development, ethanol of biomass is producible in sufficiently cheap and large quantities for economic advantage. There will be assistance if the technological applications of ethanol widen its existing markets. But potential users would be unlikely to develop new applications without a cost reduction. On the other hand, incentive to improve processes needs a large market. This circle could be broken by political intervention, but such a policy requires a basis in the technology. The selection of ethanol production not only depends on market conditions for ethanol and its substitutes (crude oil, natural gas and coal derivatives), but may so be influenced by broadly based policy decisions.

A second major end product besides ethanol, is butanol. It can be readily converted to other chemicals such as butadiene which is used in the manufacture of synthetic rubber, and to butyl acetate, an important industrial solvent. The major coproduct from producing butanol is acetone which can also be used as an industrial solvent (eg. in the explosive industries). The residues from butanol production can be used as animal feed supplements.

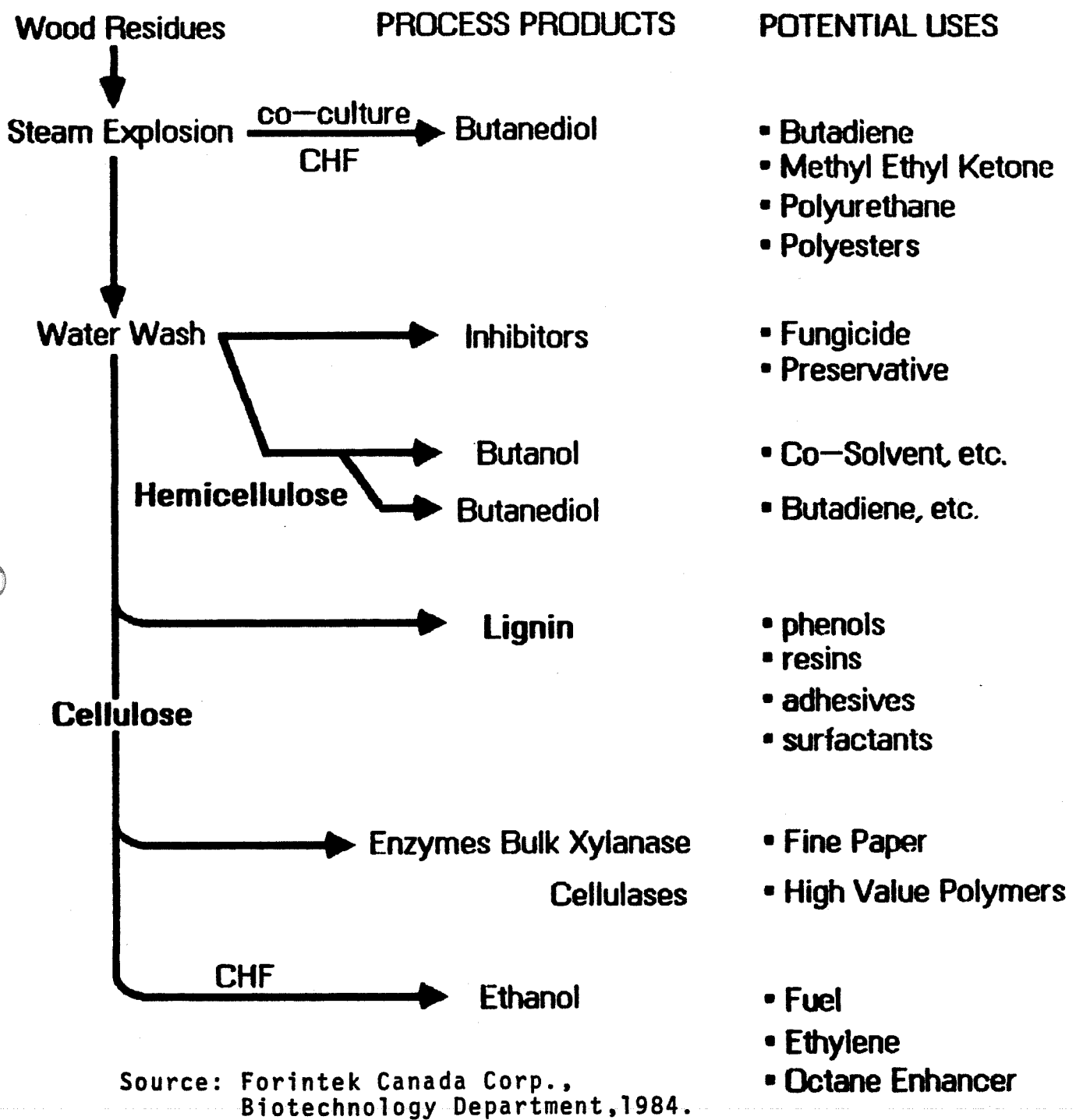
The other major end product that can be produced from the bioconversion process is 2,3-butanediol. Since most commercial glycols are synthetically manufactured from petroleum, there exists no market for 2,3-butanediol as an intermediate organic feedstock. However, 2,3-butanediol can be further processed to produce various chemicals which have great potential markets. Butanediol derivatives are utilized as solvents and as an ingredient in the

manufacture of vinyl fabrics, adhesives and synthetic rubber. Therefore, the production of 2,3-butanediol depends on its derivatives market conditions as well as on its substitutes.

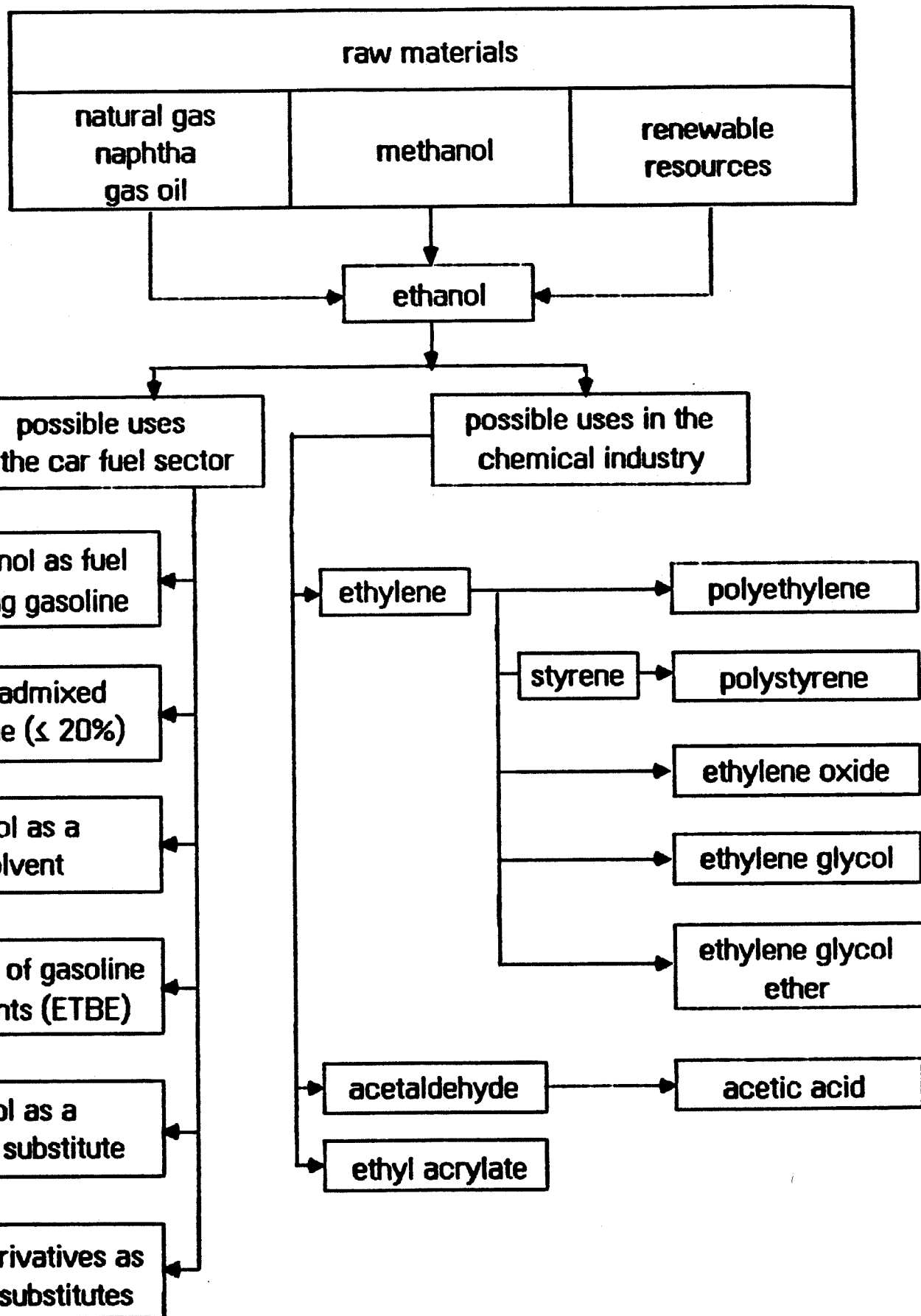
The process has lignin as one of the major coproducts, and this material can be converted to many medium and high value products. The opportunities that exist for a lignin based chemicals industry are vast. The areas that show potential include the enzymatic and chemical modifications of lignin. The end products from these include phenols, vanillins, resins, adhesives, and so forth. The production of lignin and its products is unique to the bioconversion process, and it is for this reason that the nature of the chemical industry will be changed by the research in this area.

As a spinoff from the research at FCC, a new process has been developed for the production of purified xylanase enzymes (the other major coproduct), which can be used in the manufacture of dissolving pulp.

Therefore, these end products of biomass conversion have great potential, but their major handicap at present appears to be their economic competitiveness to their petrochemical produced equivalents.



**Figure 2.1: Overview of Potential Products from Lignocellulosic Residues**



**Figure 2.2: Sources and Uses of Ethanol**

Source: Bremen & Schmoltzi "Economics & Politics of the Ethanol Market"  
Tibtech. Jan. 1986



### 3.0 STRUCTURE OF THE PROCESS

There are two major technological approaches to accomplish the conversion of cellulose to glucose: chemical (acid hydrolysis) and biological (enzymatic hydrolysis). Both methods catalyze the hydrolysis of cellulose to glucose; however in the case of acid hydrolysis, the reaction occurs under relatively extreme conditions of temperature and pH which necessitates the use of expensive equipment. Also, the reactions that take place during acid hydrolysis yield products other than glucose from side reactions, some of which can be deleterious to subsequent fermentations.

Enzymatic hydrolysis of cellulose occurs at or near ambient conditions of temperature, pressure, and pH. The reaction that takes place is relatively specific, with glucose being the major product. The overall rate of enzymatic conversion of cellulose to glucose occurs at a slower rate than acid hydrolysis; however, the consideration of specific product formation and decreased equipment costs favour the enzymatic approach in most cases.

At Forintek, the enzymatic hydrolysis has been the focus of research for the last several years.

### 3.1 BIOLOGICAL CONVERSION PROCESS

The process under consideration consists of three major components:

- (I) steam pretreatment of lignocellulosic residues, followed by
- (II) enzymatic hydrolysis of the carbohydrate polymers, and the subsequent
- (III) fermentation of the sugars.

After the steam pretreatment, the cellulose, hemicellulose and lignin components of wood, are separated. The carbohydrate polymers (cellulose and hemicellulose) are enzymatically hydrolyzed to their monomeric sugars. The monomeric sugars are then fermented to ethanol, butanol, or butanediol. The process requires the production of extracellular cellulase enzymes.

The process scheme under consideration is shown in Figure 3.1. The lignocellulosic feedstock is aspen wood chips. The FCC conversion process is based on enzymatic hydrolysis of the steamed aspen wood chips and this requires the production of enzymes.

Most of the incoming chips are steamed to the hydrolysis process, while some of them are steamed towards the enzyme production process. The chips needed for the enzyme production step are steam treated, and then water extracted. The treated material is used as the substrate for the growth of the fungus Trichoderma harzianum, which produces both cellulase and xylanase enzymes. These enzymes can be separated with a simple ultrafiltration step, and this novel approach allows the production of bulk purified xylanase enzymes.

The bulk of the woodchips are used for hydrolysis and are steamed treated with or without the addition of catalysts. The treated chips are water extracted, and this water extraction process effectively removes the hemicellulose sugars from the cellulose and lignin. The water soluble stream is then converted to butanol or butanediol (with coproducts acetone and ethanol) through the use of xylanase enzymes and fermentative microorganisms. The lignin material can be separated from the cellulose with a dilute alkali extraction. The lignin extracted in this manner can be used in other applications, such as enhanced oil recovery, adhesives, resins and phenols. The remaining insoluble is used for ethanol production.

An alternative process is the direct conversion of the steamed chips without fractionation. The hemicellulose and cellulose can be hydrolyzed to xylose and glucose and then fermented to butanol or butanediol and their coproducts with the help of the cellulase enzymes and fermentative microorganisms. This is the CHF1 process route in Figure 3.1.

Should this bioconversion process, of woodchips to chemicals and fuels, prove to be economically advantageous, the process can also be applied, with some modification, to the conversion of other alternative sources of lignocellulosics such as municipal solid wastes and agricultural residuals.

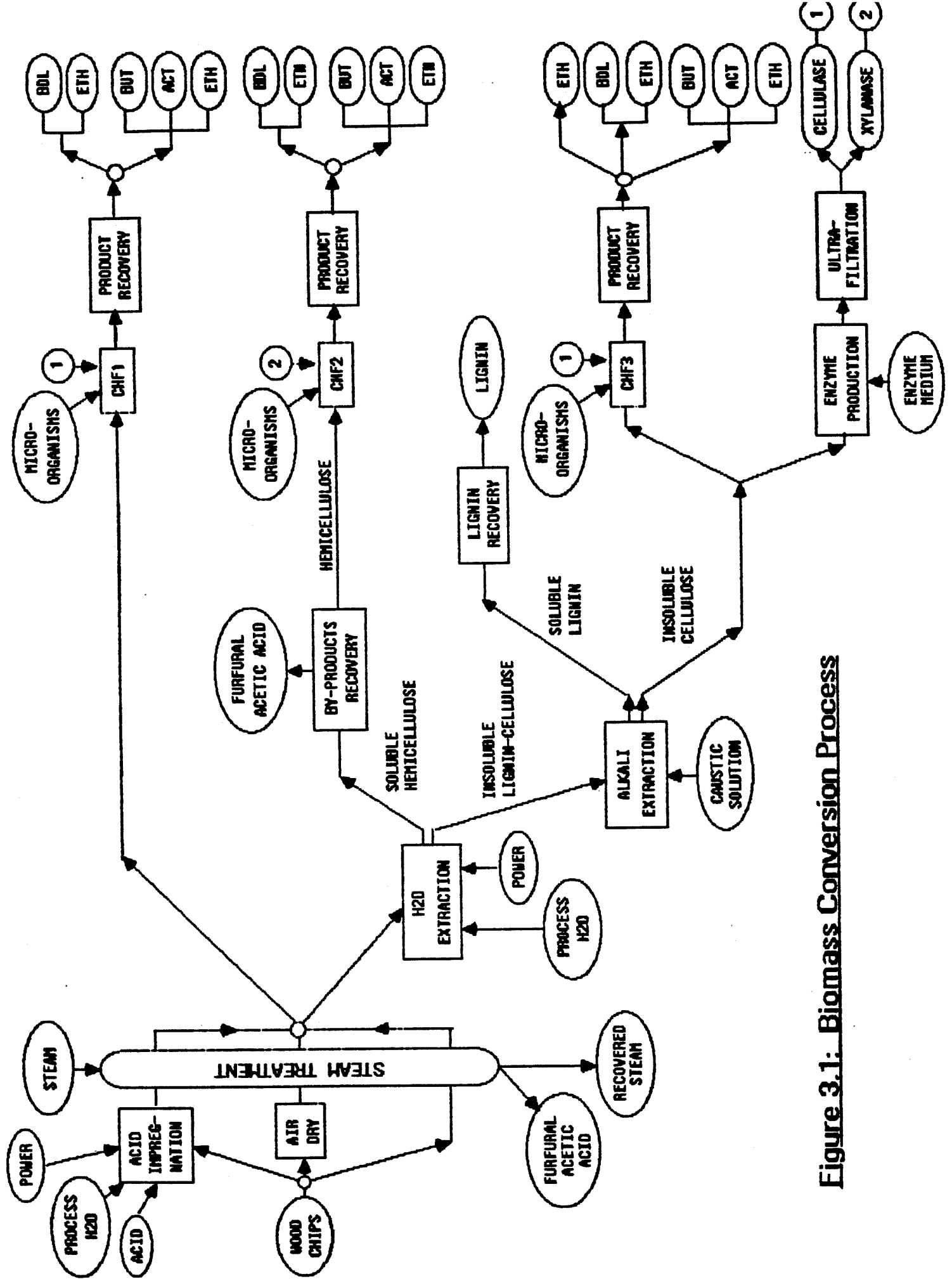


Figure 3.1: Biomass Conversion Process

#### 4.0 PROCESS DEVELOPMENT

The new forest chemical industry has similarities with the petrochemical industry, where there is a single primary input used to produce many outputs. Instead of crude oil, the primary input now is wood chips. There are basic activities or processes, whose inputs and outputs, and other characteristics, are known from process engineering.

The input for a process may be supplied from a limited source, such as plant capacity, which puts a constraint on its output; or inputs of several processes may share the same limited source, and thus their outputs have a joint constraint. They may be supplied by outputs of other processes, and demands must not exceed the supplies, so there are further constraints. These processes may be scaled, or given different intensities, with the effect of modifying levels while keeping them in the same proportion. This is a basic linearity which opens the way to Linear Programming models. By putting these processes together, with various intensities, and with the knowledge of process characteristics, an integrated process model is built from components.

The processes may involve parameters like a temperature or pressure, which need to be fixed if the system is to remain linear. Thus a full optimization will require an optimization also in respect to these parameters.

Process development and plant design are dedicated to producing an input-output technology with potential for profits under anticipated market conditions and trends. In the optimized

operation of the plant, the profit, or the difference between the cost of inputs and revenue of outputs, will be maximized.

In any case, this model can be utilized as a tool to analyze process technology on an economic level, addressing questions of sensitivity. This analysis provides important indicators, guiding research and development in the process technology and plant design.

A further discussion on activity analysis and a simplified example of a linear programming problem are included in Appendix A.

#### 4.1 DATA ORGANIZATION

The models and the data used here can be very complex, with many variables. Since it is ongoing R&D, changes have to be made, not just in variables but also in overall structure, including the introduction of new elements. It is helpful to have a clear view of the data as a whole.

The scheme that can be adopted here for models or any analysis, has a primary importance. It has to be lived with as an ongoing facility, by the many different persons who are in some way concerned with it. For usefulness, it could be a repository for a broader range of data than would be involved in any particular analysis, model or report, arranged so it can be accessed as needed, by individuals, or by computers.

It is suitable, in this case with the activity analysis approach, to construct a single matrix, gathering all the data, as illustrated in Table 4.1. The rows may be associated with variables, and the columns with activities. The matrix may contain information on processes, such as inputs and costs, outputs produced (intermediate and final), plant capacities, profits, shadow prices etc. A convenient modularity is achieved by partitioning this in a suitable fashion, by grouping together variables and activities that have some significant association. For example, the "Final Outputs" row of Table 4.1 will contain ethanol as one of the possible end products of the bioconversion process. Therefore all activities associated with ethanol production (ie. the inputs required to produce ethanol such as

wood chips, various PSIG of steam, acid, power etc., the production technology, and the amount of ethanol that can be sold or absorbed by its market) are grouped under the table headings:

Buying Inputs, Process Input-Output and Sell Outputs, respectively. The shadow prices and profits generated from selling any of these products (intermediate and/or final) will also be included in the data scheme. Blocks of data may again be partitioned, so we will have groups within groups. For example, coproducts such as furfural, lignin and cellulase enzymes that are produced from ethanol are grouped together. Following labels will lead to any element. Ideally, every data element should be accounted for its origin. Similarly, we could have other data schemes to represent the other possible end products, butanol and butanediol. We could also put together these three separate schemes into a single data scheme which contains all the three possible end products and their associated activities in the appropriate cells.

The data, provided in such a manner, should make a complete, easily understood document. Besides forming a basis for analytical study, it would be a ready source of information. The actual formulation of the data scheme into a working model is described in detail in Section 5.1.

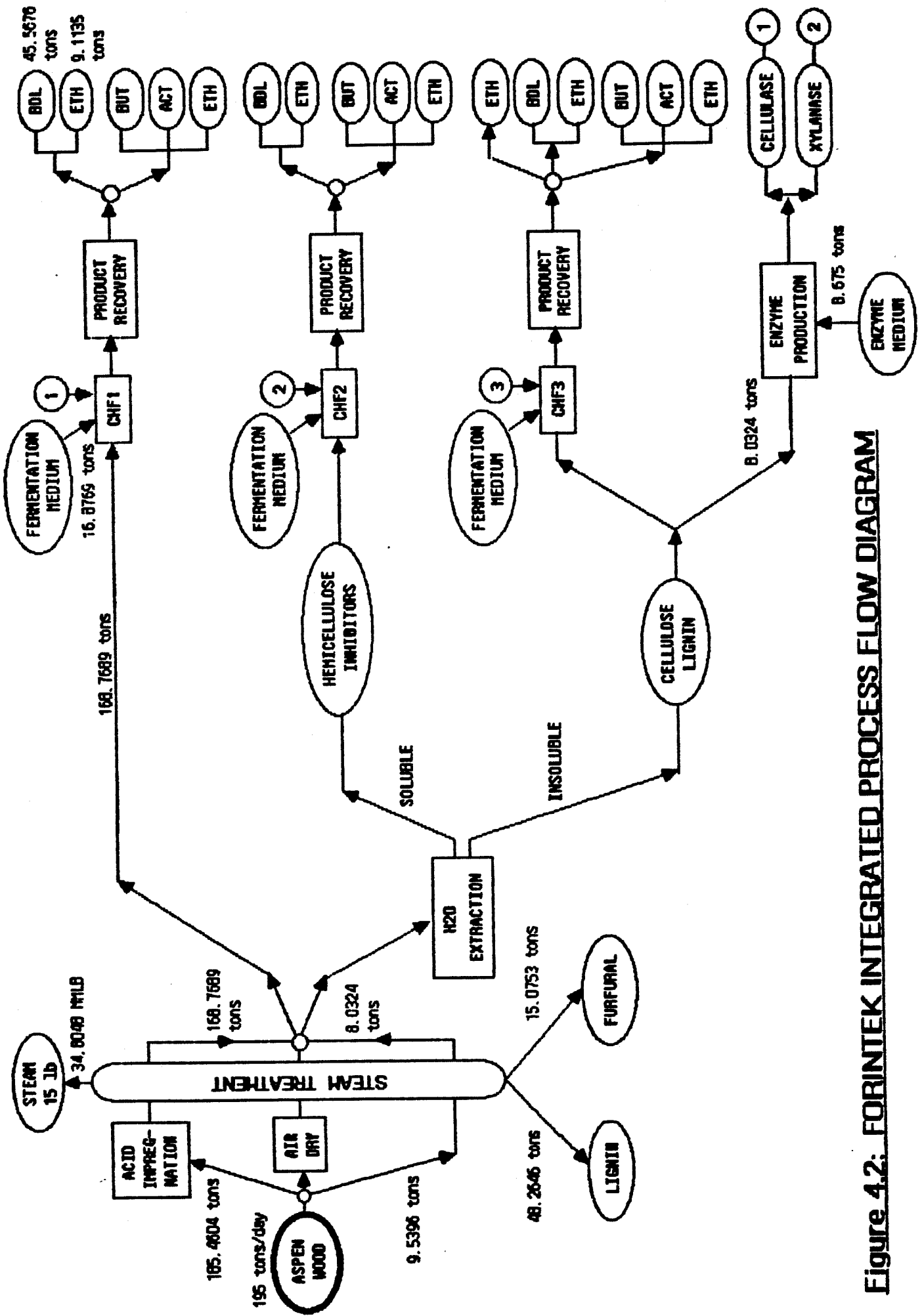
I/O VARIABLES	ACTIVITIES			SHADOW PRICES
	BUY INPUTS	PROCESS INPUT-OUTPUT	SELL OUTPUTS	
	AI	AS	AO	
LIMITED CAPACITIES (FIXED/VARIABLE)	VC			u1 u2 ...
INITIAL INPUTS	VI			
INTERMEDIATE	VS			
FINAL OUTPUTS	VD			
ACCOUNTS OBJECTIVES PROFIT	VM			
INTENSITIES	$x_1, x_2, \dots$	$t_1, t_2, \dots$	$y_1, y_2, \dots$	

**Table 4.1: Activity Analysis Data Scheme**

## 4.2 MODEL FORMULATION

Once the matrix of data has been constructed in a way suitable for the process being considered, one can then proceed with this information to build a model, particularly of linear programming form.

A preliminary integrated process model, based on the Biomass Conversion Process (Figure 3.1), has been formulated at Forintek (included in Appendix B). The model contains one objective function of maximizing profits, 62 constraints (two less than and equal to, 41 equalities and 19 greater than and equal to) and 165 variables. The flow diagram representation of this model is illustrated in Figure 4.2 to represent the various processes of converting wood residues into fuels and chemicals. By modelling the fundamental process information, as well as information on market size and prices, and production costs, the end-product mix that offers the best potential for commercial feasibility will be identified. The simulated model can be used to identify systems sensitivity to production costs; market prices and technical process parameters. In essence, the model can provide FCC (Forintek Canada Corporation) researchers with information needed to establish research priorities to achieve their objective of identifying a commercial application of wood residues via bioconversion technology.



**Figure 4.2: FORINTEK INTEGRATED PROCESS FLOW DIAGRAM**

## 5.0 FORINTEK INTEGRATED PROCESS MODEL

During the past ten months of employment with FCC, I have been involved with the economic analysis of the conversion process of wood residues to various chemicals and fuels. A simulation model was developed and a solution was generated using a computer package called LP83. This package utilized the simplex algorithm of solving LP problems. This model and a detailed description of its format is included in Appendix B. My responsibilities were to refine and update this model to accurately represent the particular processes presently being investigated by the Biotechnology Department.

In the course of my work, it was found that the model formulation in its present format was difficult to follow by those not familiar with the particular computer program used. It was decided to put the model into a spreadsheet format consistent with the data scheme presented in Section 4.1. A recently developed LP computer program permitted interfacing with a spreadsheet, to read a problem from it and write back the results.

## 5.1 INTEGRATED PROCESS MODEL - Spreadsheets Version

The actual data scheme formulation of the Forintek Integrated Model is represented below in a Lotus spreadsheet format.

From left to right, the spreadsheet is divided into four main sections. The first section under the heading, Buy, contains ten activity inputs: ASPPURCH, H2SO4PUR, POWERPUR, CWPURCH, PWPURCH, STM15PUR, STM200PU, STM600PU, ENMEDIUM and FERMED. They represent aspen purchased, sulfuric acid purchased, power purchased, cooling water purchased, process water purchased; 15 PSIG steam, 200 PSIG steam, 600 PSIG steam purchased, enzyme medium purchased and fermentation medium purchased, respectively.

The second section is divided into eight input-output processes, each of which is further subdivided. Each of these subdivisions contains a number of process activities. The first input-output process, 'steam treatment', consists of three subdivisions. The first, 'green chips', contains six activities: SEEC4FGN, SEEE4FGN, SEEG4FGN, SEEI4FGN, SEEJ4FGN, SEEK4FGN\*. The second subdivision, 'air dried chips', contains five activities: SEEB4FAN, SEED4FAN, SEEF4FAN, SEEH4FAN and SEEI4FAN. The last of these three subdivisions, 'acid impregnated chips', contains four activities: SEEA3FG2, SEEC3FG2, SEEE3FG2 and SEEG3FG2. The second input-output process, 'to combined hydrolysis and fermentation', consists of the same three subdivisions and their respective activities as for the steam treatment process. The third input-

\* The explanation of these short forms is included in Appendix B under the heading Forintek LP - Symbols.

output process, 'CHF1' (combined hydrolysis and fermentation process one), is divided into two production units. The first unit, production of butanediol and its co-product, consists of eight activities: H1D52N3B, H1D12N3B, H1D55N3B, H1D15N3B, H1D52N5B, H1D12N5B, H1D55N5B and H1D15N5B. The second production unit, butanol and its co-products, also consists of eight activities: H1B52N3B, H1B12N3B, H1B55N3B, H1B15N3B, H1B52N5B, H1B12N5B, H1B55N5B and H1B15N5B. The fourth input-output process, 'water washing', is divided into two subdivisions, 5 litres/kg of water consumption and 10 litres/kg of water consumption. Each of these consists of the same three subdivisions and their respective activities as for the steam treatment process, as well as the activities in the 'to combined hydrolysis and fermentation' process. The fifth input-output process, 'enzyme production', consists of ten activities: EPA4SBSS, EPB4SBSS, EPC4SBSS, EPD4SBSS, EPE4SBSS, EPF4SBSS, EPG4SBSS, EPH4SBSS, EPI4SBSS and EPJ4SBSS. The sixth input-output process, 'CHF2', is divided into two subdivisions. The first, production of butanediol and its co-product, consists of eight activities: H2D12N3B, H2D22N3B, H2D15N3B, H2D25N3B, H2D12N5B, H2D22N5B, H2D15N5B and H2D25N5B. The second production unit, butanol and its co-products, also consists of eight activities: H2B12N3B, H2B22N3B, H2B15N3B, H2B25N3B, H2B12N5B, H2B22N5B, H2B15N5B and H2B25N5B. The seventh input-output process, 'CHF3', is divided into three subdivisions. The first, production of butanediol and its co-product, consists of eight activities: H3D52N3B, H3D12N3B, H3D55N3B, H3D15N3B, H3D52N5B, H3D12N5B, H3D55N5B and H3D15N5B. The second production

unit, butanol and its co-products, consists of eight activities: H3B52N3B, H3B12N3B, H3B55N3B, H3B15N3B, H3B52N5B, H3B12N5B, H3B55N5B and H3B15N5B. The third production unit, ethanol, consists of twenty-four activities: H3E55N2B, H3E55N4B, H3E15N2B, H3E15N4B, H3E35N2B, H3E35N4B, H3E25N2B, H3E25N4B, H3E51N2B, H3E51N4B, H3E11N2B, H3E11N4B, H3E31N2B, H3E31N4B, H3E21N2B, H3E21N4B, H3E50N2B, H3E50N4B, H3E10N2B, H3E10N4B, H3E30N2B, H3E30N4B, H3E20N2B, and H3E20N4B. The activity SEATOTAL represents the total amount of steam exploded aspen under various conditions. The last input-output process, 'products (and co-products) recovery', consists of six activities: FURRECOV, ETHRECOV, BDLRECOV, BUTRECOV, ACTRECOV and LIGRECOV.

The third section, sales, contains six chemicals and fuel products and co-products: FURSALE, ETHSALE, BDLSALE, BUTSALE, ACTSALE and LIGFUEL.

The final section is divided into four subsections: type of constraints ( $\geq$ ,  $\leq$ ), RHS (right-hand side values), slacks/surplus and the shadow prices. For additional information regarding the shadow prices, see Section 5.3.2 Marginal Analysis.

From top to bottom, the spreadsheet is divided into six partitions: objective, capacity, inputs, balance, limits and sales, and optimum and reduced costs.

The first partition, 'objective', contains the objective function (to maximize profit) of the LP problem.

The second partition, 'capacity', consists of eight capacity constraints: SEACAPAC, H2S04CAP, DRYCAPAC, WWCAPACT, ENPRDCAP, CHF1CAPC, CHF2CAPC and CHF3CAPC.

The third partition, 'inputs', consists of ten input constraints: ASPAVAIL, H2SO4REQ, POWERREQ, COWATREQ, PRWATREQ, STM15REQ, ST200REQ, ST600REQ, ENMEDREQ and FERMEDRQ.

The fourth partition, 'balance', consists of thirty-three balance constraints: ASPENBAL, SEA1BALN, SEA2BALN, SEA3BALN, SEA4BALN, SEA5BALN, SEA6BALN, SEA7BALN, SEA8BALN, SEA9BALN, SEA10BAL, SEA11BAL, SEA12BAL, SEA13BAL, SEA14BAL, SEA15BAL, SEATOTAL, PETROBAL, WSREMBAL, WIPENTBA, WIHEXOBA, HEXPENBA, XYASEBAL, CLASEBAL, FURBALAN, BDIOLBAL, BUTANBAL, ACTONBAL, ETNOLBAL, LIGNINBA, CHF1INHB, CHF1BALN and CHF2INHB.

The fifth partition, 'limits and sales', consists of five and six constraints respectively: FURLIMIT, BDLLIMIT, BUTLIMIT, ACTLIMIT and ETHLIMIT; FURSALES, ENOLSALE, BTDL SALE, BTOLSALE, ACTNSALE and LIGNSALE.

The final partition, 'optimum and reduced costs', contains the optimum activities values and their respective reduced cost values. For additional information regarding reduced costs, see Section 5.3.1 Cost Analysis.

It should be noted that the activity and constraint names are chosen for documentation purposes only.





efficient \*\* initiated by Adam Ferrie, continued by Ratanak Ung under the supervision and guidance of  
to combined hydrolysis and fermentation (CHF) ...

	impregnated chips			green chips				air dried chips				
	SEEC3F62	SEEE3F62	SEEG3F62	SEC4FGNT	SEE4FGNT	SE64FGNT	SEI4FGNT	SEJ4FGNT	SEK4FGNT	SEB4FANT	SED4FANT	SEF4FANT
(maximize profit)	-3.68	-3.68	-3.68									
SEACAPAC	1	1	1									
H2SO4CAP	1	1	1									
DRYCAPAC												
WVCAPACT												
ENPRDCAP												
CHF1CAPC												
CHF2CAPC												
CHF3CAPC												
ASPAVAL												
H2SO4REQ	0.012	0.012	0.012									
POWERREQ	1.41	1.41	1.41									
COMATREQ												
PRWATREQ												
STM15REQ	-0.38	-0.38	-0.38									
ST200REQ												
ST600REQ	0.38	0.38	0.38									
ENMEDREQ												
FERNEDREQ												
ASPENBAL	-1	-1	-1									
SEA1BALN				-1								
SEA2BALN					-1							
SEA3BALN						-1						
SEA4BALN							-1					
SEA5BALN								-1				
SEA6BALN									-1			
SEA7BALN										-1		
SEA8BALN											-1	
SEA9BALN												-1
SEA10BALN												
SEA11BALN												
SEA12BALN												
SEA13BALN	0.881											
SEA14BALN		0.855										
SEA15BALN			0.91									
SEATOTAL				1	1	1	1	1	1	1	1	1
PETROBAL												
WSREMBAL												
WIPENTBA												
WIHEXOBA												
HEXPENBA												
XYASEBAL												
CLASEBAL												
FURBALAN	0.034	0.05	0.08									
BDIOLBAL												
BUTANBAL												
ACTONBAL												
ETNOLBAL												
LIGNINBA	0.194	0.212	0.248									
CHF1INH8												
CHF1BALN												
CHF2INH8												
FURLIMIT												
BDLLIMIT												
BUTLIMIT												
ACTLIMIT												
ETHLIMIT												
FURSALES												
ENDLSALE												
BDLSALE												
BDLSALE												
ACTNSALE												
LIGNSALE												

Optimum 185.4603

Reduced costs 93.66528 23.43640 92.76884 89.75931 98.11359 89.89357 89.46311 93.18808



butanol and its co-products

Water washing ...  
5 litres/kg of wat  
with green chips  
W5EC4FGN W5EE4FGN

H1D55N5B H1D15N5B H1B52N3B H1B12N3B H1B55N3B H1B15N3B H1B52N5B H1B12N5B H1B55N5B H1B15N5B

(maximize  
profit)

	H1D55N5B	H1D15N5B	H1B52N3B	H1B12N3B	H1B55N3B	H1B15N3B	H1B52N5B	H1B12N5B	H1B55N5B	H1B15N5B	W5EC4FGN	W5EE4FGN
SEACAPAC											1	1
H2S04CAP												
DRYCAPAC												
MWCAPACT												
ENPRDCAP												
CHF1CAPC	5	5	3	3	3	3	5	5	5	5		
CHF2CAPC												
CHF3CAPC												
ASPAVAIL												
H2S04REG												
POWERREG	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9		
COMATREG	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53		
PRWATREG	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.001	0.001
STM15REG	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19		
ST200REG												
ST600REG												
ENMEDREG												
FERMEDRB	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1		
ASPENBAL												
SEA1BALN											-1	
SEA2BALN												-1
SEA3BALN												
SEA4BALN												
SEA5BALN												
SEA6BALN												
SEA7BALN												
SEA8BALN												
SEA9BALN												
SEA10BAL												
SEA11BAL												
SEA12BAL												
SEA13BAL												
SEA14BAL												
SEA15BAL												
SEATOTAL												
PETROBAL											0.081	0.09
WSREMBAL											0.106	0.103
WIPENTBA											0.058	0.036
WIHEXOBA											0.474	0.489
HEXPENBA											0.532	0.525
XYASEBAL												
CLASEBAL	4.5	9	4.5	9	4.5	9	4.5	9	4.5	9		
FURBALAN												
BDIOLBAL	0.12	0.13										
BUTANBAL			0.12	0.16	0.07	0.09	0.15	0.19	0.09	0.12		
ACTONBAL			0.06	0.08	0.04	0.05	0.08	0.1	0.05	0.06		
ETNOLBAL	0.024	0.026	0.02	0.03	0.01	0.02	0.03	0.03	0.02	0.02		
LIGNINBA												
CHF1INH8												
CHF1BALN	1	1	1	1	1	1	1	1	1	1		
CHF2INH8												
FURLIMIT												
BDLLIMIT												
BUTLIMIT												
ACTLIMIT												
ETHLIMIT												
FURSALES												
ENOLSALE												
BTOLSALE												
ACTNSALE												
LIGNSALE												

Optimum

Reduced costs 113.1417 113.9080 84.23902 49.31331 134.8143 119.3293 47.15756 17.17876 110.4266 93.14169 72.19603 1.663150

er consumption

with air dried chips

with acid impregnated chips

W5E64FGN W5E14FGN W5EJ4FGN W5EK4FGN W5EB4FAN W5ED4FAN W5EF4FAN W5EH4FAN W5E14FAN W5EA3FG2 W5EC3FG2 W5EE3FG2

(maximize

profit)

SEACAPAC

H2SO4CAP

DRYCAPAC

WNCAPACT

ENPRDCAP

CHF1CAPC

CHF2CAPC

CHF3CAPC

ASPAVAIL

H2SO4REQ

POWERREQ

COMATREQ

PRWATREQ

STM15REQ

ST200REQ

ST600REQ

ENMEDREQ

FERNEDRQ

ASPENBAL

SEA1BALN

SEA2BALN

SEA3BALN

SEA4BALN

SEA5BALN

SEA6BALN

SEA7BALN

SEA8BALN

SEA9BALN

SEA10BAL

SEA11BAL

SEA12BAL

SEA13BAL

SEA14BAL

SEA15BAL

SEATOTAL

PETROBAL

WSREMBAL

WIPENTBA

WIEXDBA

HEXPENBA

XYASEBAL

CLASEBAL

FURBALAN

BDIOLBAL

BUTANBAL

ACTONBAL

ETNOLBAL

LIGNINBA

CHF1INHBB

CHF1BALN

CHF2INHBB

FURLIMIT

BDLLIMIT

BUTLIMIT

ACTLIMIT

ETHLIMIT

FURSALES

ENDLSALE

BTDLSALE

BTDSALE

ACTNSALE

LIGNSALE

	1	1	1	1	1	1	1	1	1	1	1	1
PRWATREQ	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001	0.001
SEA3BALN	-1											
SEA4BALN		-1										
SEA5BALN			-1									
SEA6BALN				-1								
SEA7BALN					-1							
SEA8BALN						-1						
SEA9BALN							-1					
SEA10BAL								-1				
SEA11BAL									-1			
SEA12BAL										-1		
SEA13BAL											-1	
SEA14BAL												-1
PETROBAL	0.088	0.075	0.046	0.034	0.079	0.094	0.108	0.097	0.08	0.117	0.124	0.12
WSREMBAL	0.098	0.119	0.122	0.124	0.078	0.088	0.101	0.098	0.126	0.134	0.148	0.175
WIPENTBA	0.019	0.014	0.008	0.007	0.061	0.037	0.017	0.014	0.007	0.01	0.006	0.004
WIEXDBA	0.487	0.488	0.464	0.428	0.496	0.493	0.474	0.437	0.438	0.442	0.42	0.337
HEXPENBA	0.506	0.502	0.472	0.435	0.557	0.53	0.491	0.451	0.445	0.452	0.426	0.381

Optimum

Reduced costs 75.66689 76.25690 97.36144 10.03030 63.24112 65.73812 75.28613 79.02262 68.19571 96.00640 64.24763 60.23446



Enzyme production ...

with acid impregnated chips

W1EA3F62 W1EC3F62 W1EE3F62 W1EG3F62 EPA4SBSS EPB4SBSS EPC4SBSS EPD4SBSS EPE4SBSS EPF4SBSS EP64SBSS EPH4SBSS

(maximize

profit)

SEACAPAC

H2S04CAP

DRYCAPAC

WNCAPACT

ENPRDCAP

CHF1CAPC

CHF2CAPC

CHF3CAPC

ASPAVAIL

H2S04REQ

POWERREQ

COWATREQ

PRWATREQ

STM15REQ

ST200REQ

ST600REQ

ENHEDREQ

FERNEDREQ

ASPENBAL

SEA1BALN

SEA2BALN

SEA3BALN

SEA4BALN

SEA5BALN

SEA6BALN

SEA7BALN

SEA8BALN

SEA9BALN

SEA10BAL

SEA11BAL

SEA12BAL

SEA13BAL

SEA14BAL

SEA15BAL

SEATOTAL

PETROBAL

WSREMBAL

WIPENTBA

WIHEX0BA

HEXPENBA

XYASEBAL

CLASEBAL

FURBALAN

BDIOLBAL

BUTANBAL

ACTONBAL

ETNOLBAL

LIGNINBA

CHF1INHB

CHF1BALN

CHF2INHB

FURLIMIT

BDLLIMIT

BUTLIMIT

ACTLIMIT

ETHLIMIT

FURSALES

ENOLSALE

BTOLSALE

BTOLSALE

ACTNSALE

LIGNSALE

	1	1	1	1	4	4	4	4	4	4	4	4
H2S04REQ					549	549	549	549	549	549	549	549
POWERREQ					4.05	4.05	4.05	4.05	4.05	4.05	4.05	4.05
COWATREQ					53	53	53	53	53	53	53	53
PRWATREQ	0.002	0.002	0.002	0.002	0.9	0.9	0.9	0.9	0.9	0.9	0.9	0.9
ST200REQ					1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.08
ENHEDREQ					1.08	1.08	1.08	1.08	1.08	1.08	1.08	1.08
ASPENBAL					-1							
SEA1BALN						-1						
SEA2BALN							-1					
SEA3BALN								-1				
SEA4BALN									-1			
SEA5BALN										-1		
SEA6BALN											-1	
SEA7BALN												-1
SEA8BALN												
SEA9BALN												
SEA10BAL												
SEA11BAL												-1
SEA12BAL	-1											
SEA13BAL		-1										
SEA14BAL			-1									
SEA15BAL				-1								
SEATOTAL												
PETROBAL	0.128	0.135	0.131	0.107								
WSREMBAL	0.134	0.148	0.175	0.167								
WIPENTBA	0.01	0.006	0.004	0.003								
WIHEX0BA	0.442	0.42	0.337	0.409								
HEXPENBA	0.452	0.426	0.381	0.412								
XYASEBAL					16.6	25.9	46.4	44.7	56.7	39.8	20.2	13.6
CLASEBAL					-55.4	-86.3	-154.5	-149.1	-189.1	-132.7	-67.3	-45.5

B.032366

Optimum

Reduced costs 93.71932 61.96055 57.94738

260.0596 128.6991 63.10682 70.78049

13.46643 249.8972 256.8996

CHF<sub>2</sub>  
production of butanediol and its co-product

butanol and its co

EPI45BSS EPJ45BSS H2D12N3B H2D22N3B H2D15N3B H2D25N3B H2D12N5B H2D22N5B H2D15N5B H2D25N5B H2B12N3B H2B22N3B

(maximize  
profit)

SEACAPAC												
H2S04CAP												
DRYCAPAC												
MWCAPACT												
ENPRDCAP	4	4										
CHF1CAPC												
CHF2CAPC			3	3	3	3	5	5	5	5	3	3
CHF3CAPC												
ASPAVAIL												
H2S04REQ												
POWERREQ	549	549	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9
COMATREQ	4.05	4.05	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53
PRMATREQ	53	53	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
STM15REQ	0.9	0.9	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19
ST200REQ												
ST600REQ												
ENMEDREQ	1.08	1.08										
FERMEDREQ			0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
ASPENBAL												
SEA1BALN												
SEA2BALN												
SEA3BALN												
SEA4BALN												
SEA5BALN												
SEA6BALN												
SEA7BALN												
SEA8BALN												
SEA9BALN												
SEA10BAL												
SEA11BAL												
SEA12BAL												
SEA13BAL												
SEA14BAL	-1											
SEA15BAL		-1										
SEATOTAL												
PETROBAL			-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
WSREMBAL												
WIPENTBA												
WIHEXOBA												
HEXPENBA												
XYASEBAL	19.6	15	-0.09	-0.18	-0.09	-0.18	-0.09	-0.18	-0.09	-0.18	-0.09	-0.18
CLASEBAL	-65.4	-50										
FURBALAN												
BDIOLBAL			0.17	0.23	0.1	0.13	0.2	0.26	0.12	0.15		
BUTANBAL											0.09	0.12
ACTONBAL											0.05	0.06
ETNOLBAL			0.034	0.046	0.02	0.026	0.04	0.052	0.024	0.03	0.015	0.01
LIGNINBA												
CHF1INH												
CHF1BALN												
CHF2INH												
FURLIMIT			1	1	1	1	1	1	1	1	1	1
BDLLIMIT												
BUTLIMIT												
ACTLIMIT												
ETHLIMIT												
FURSALES												
ENOLSALE												
BTOLSALE												
BTOLSALE												
ACTNSALE												
LIGNSALE												

Optimum

Reduced costs 202.6065 177.0775 73.22663 24.40887 130.1806 105.7718 48.81775

113.9080 89.49921 113.6664 89.95230

-products

CHF3 ...  
production of butanediol and its co-product

H2B15N3B H2B25N3B H2B12N5B H2B22N5B H2B15N5B H2B25N5B H3D52N3B H3D12N3B H3D55N3B H3D15N3B H3D52N5B H3D12N5B

(maximize profit)  
 SEACAPAC  
 H2S04CAP  
 DRYCAPAC  
 WWCAPACT  
 ENPRDCAP  
 CHF1CAPC  
 CHF2CAPC  
 CHF3CAPC  
 ASPAVAIL  
 H2S04REQ  
 POWERREQ  
 COWATREQ  
 PRWATREQ  
 STM15REQ  
 ST200REQ  
 ST600REQ  
 ENMEDREQ  
 FERMEDREQ  
 ASPENBAL  
 SEA1BALN  
 SEA2BALN  
 SEA3BALN  
 SEA4BALN  
 SEA5BALN  
 SEA6BALN  
 SEA7BALN  
 SEA8BALN  
 SEA9BALN  
 SEA10BAL  
 SEA11BAL  
 SEA12BAL  
 SEA13BAL  
 SEA14BAL  
 SEA15BAL  
 SEATOTAL  
 PETROBAL  
 WSREMBAL  
 WIPENTBA  
 WIHEXOBA  
 HEXPENBA  
 XYASEBAL  
 CLASEBAL  
 FURBALAN  
 BDIDLBAL  
 BUTANBAL  
 ACTONBAL  
 ETNOLBAL  
 LIGNINBA  
 CHF1INH  
 CHF1BALN  
 CHF2INH  
 FURLIMIT  
 BDLLIMIT  
 BUTLIMIT  
 ACTLIMIT  
 ETHLIMIT  
 FURSALES  
 ENLSALE  
 BTDL SALE  
 BTOLSALE  
 ACTNSALE  
 LIGNSALE

	3	3	5	5	5	5		3	3	3	3	5	5
POWERREQ	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9
COWATREQ	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53
PRWATREQ	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
STM15REQ	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19
FERMEDREQ	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
PETROBAL	-1	-1	-1	-1	-1	-1							
XYASEBAL	-0.09	-0.18	-0.09	-0.18	-0.09	-0.18		-1	-1	-1	-1	-1	-1
CLASEBAL								4.5	9	4.5	9	4.5	9
BDIDLBAL								0.15	0.2	0.09	0.09	0.18	0.23
BUTANBAL	0.06	0.08	0.11	0.14	0.07	0.09							
ACTONBAL	0.03	0.04	0.06	0.07	0.04	0.05							
ETNOLBAL	0.01	0.013	0.055	0.07	0.035	0.045		0.03	0.04	0.018	0.018	0.036	0.046
CHF2INH	1	1	1	1	1	1							

Optimum

Reduced costs 148.2745 127.3496 74.43812 40.83011 123.2134 98.82576 114.3930 82.61427 163.2108 172.1134 89.98420 58.20539

butanol and its co-products

production of etha

H3D55N5B H3D15N5B H3B52N3B H3B12N3B H3B55N3B H3B15N3B H3B52N5B H3B12N5B H3B55N5B H3B15N5B H3E55N2B H3E55N4B

(maximize

profit)

SEACAPAC

H2S04CAP

DRYCAPAC

WNCAPACT

ENPRDCAP

CHF1CAPC

CHF2CAPC

CHF3CAPC

ASPAVAIL

H2S04REQ

POWERREQ

CONATREQ

PRWATREQ

STM15REQ

ST200REQ

ST600REQ

ENMEDREQ

FERMEDREQ

ASPENBAL

SEA1BALN

SEA2BALN

SEA3BALN

SEA4BALN

SEA5BALN

SEA6BALN

SEA7BALN

SEA8BALN

SEA9BALN

SEA10BALN

SEA11BALN

SEA12BALN

SEA13BALN

SEA14BALN

SEA15BALN

SEATOTAL

PETROBAL

WSREMBAL

WIPENTBA

WIHEXOBA

HEXPENBA

XYASEBAL

CLASEBAL

FURBALAN

BDIOLBAL

BUTANBAL

ACTONBAL

ETNOLBAL

LIGNINBA

CHF1INH

CHF1BALN

CHF2INH

FURLIMIT

BDLLIMIT

BUTLIMIT

ACTLIMIT

ETHLIMIT

FURSALES

ENOLSALE

BTOLSALE

ACTNSALE

LIGNSALE

	5	5	3	3	3	3	5	5	5	5	2	4
POWERREQ	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9
CONATREQ	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53
PRWATREQ	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
STM15REQ	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19
ENMEDREQ												
FERMEDREQ	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1		
HEXPENBA	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
XYASEBAL	4.5	9	4.5	9	4.5	9	4.5	9	4.5	9	4.5	4.5
BDIOLBAL	0.11	0.14										
BUTANBAL			0.15	0.2	0.09	0.09	0.18	0.23	0.11	0.14		
ACTONBAL			0.08	0.01	0.05	0.05	0.09	0.12	0.06	0.07		
ETNOLBAL	0.022	0.028	0.025	0.033	0.015	0.015	0.03	0.038	0.018	0.023	0.015	0.21

Optimum

Reduced costs 146.9382 131.4320 75.29124 88.13020 138.5603 147.4630 46.63015

117.6355 97.87711 229.0171 132.5523

no1

H3E15N2B H3E15N4B H3E35N2B H3E35N4B H3E25N2B H3E25N4B H3E51N2B H3E51N4B H3E11N2B H3E11N4B H3E31N2B H3E31N4B

(maximize profit)

SEACAPAC												
H2S04CAP												
DRYCAPAC												
WVCAPACT												
ENPRDCAP												
CHF1CAPC												
CHF2CAPC												
CHF3CAPC	2	4	2	4	2	4	2	4	2	4	2	4
ASPAVAIL												
H2S04REQ												
POWERREQ	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9
COWATREQ	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53
PRWATREQ	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33
STM15REQ	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19
ST200REQ												
ST600REQ												
ENMEDREQ												
FERMEDREQ												
ASPENBAL												
SEA1BALN												
SEA2BALN												
SEA3BALN												
SEA4BALN												
SEA5BALN												
SEA6BALN												
SEA7BALN												
SEA8BALN												
SEA9BALN												
SEA10BAL												
SEA11BAL												
SEA12BAL												
SEA13BAL												
SEA14BAL												
SEA15BAL												
SEATOTAL												
PETROBAL												
WSREMBAL												
WIPENTBA												
WIHEXOBA												
HEXPENBA	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1
XYASEBAL												
CLASEBAL	9	9	13.5	13.5	18	18	4.5	4.5	9	9	13.5	13.5
FURBALAN												
BD10LBAL												
BUTANBAL												
ACTONBAL												
ETNOLBAL	0.2	0.27	0.25	0.28	0.26	0.3	0.18	0.24	0.24	0.31	0.29	0.32
LIGNINBA												
CHF1INHB												
CHF1BALN												
CHF2INHB												
FURLIMIT												
BDLLIMIT												
BUTLIMIT												
ACTLIMIT												
ETHLIMIT												
FURSALES												
ENOLSALE												
BTOLSALE												
BTOLSALE												
ACTNSALE												
LIGNSALE												

Optimum

Reduced costs 146.4019 111.7735 130.5700 115.7292 134.5257 114.7381 147.3930 117.7116 126.6142 91.98590 110.7823 95.94165

Products

H3E21N2B H3E21N4B H3E50N2B H3E50N4B H3E10N2B H3E10N4B H3E30N2B H3E30N4B H3E20N2B H3E20N4B SEATOTAL FURRECOV

(maximize profit)

	2	4	2	4	2	4	2	4	2	4	
SEACAPAC											
H2S04CAP											
DRYCAPAC											
WWCAPACT											
ENPRDCAP											
CHF1CAPC											
CHF2CAPC											
CHF3CAPC											
ASPAVAIL											
H2S04REQ											
POWERREQ	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	68.9	4.24
COWATREQ	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	2.53	20.3
PRWATREQ	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	0.33	
STM15REQ	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	0.19	
ST200REQ											9.09
ST600REQ											
ENMEDREQ											
FERMEDRO											
ASPENBAL											
SEA1BALN											
SEA2BALN											
SEA3BALN											
SEA4BALN											
SEA5BALN											
SEA6BALN											
SEA7BALN											
SEA8BALN											
SEA9BALN											
SEA10BAL											
SEA11BAL											
SEA12BAL											
SEA13BAL											
SEA14BAL											
SEA15BAL											
SEATOTAL											-1
PETROBAL											
WSREMBAL											
WIPENTBA											
WIHEXOBA											
HEXPENBA	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	
XYASEBAL											
CLASEBAL	18	18	4.5	4.5	9	9	13.5	13.5	18	18	
FURBALAN											-1
BDIOLBAL											
BUTANBAL											
ACTONBAL											
ETNOLBAL	0.31	0.34	0.11	0.14	0.15	0.19	0.18	0.19	0.19	0.21	
LIGNINBA											
CHF1INH8											1
CHF1BALN											-1
CHF2INH8											
FURLIMIT											
BDLLIMIT											
BUTLIMIT											
ACTLIMIT											
ETHLIMIT											
FURSALES											1
ENOLSALE											
BTDLSALE											
BTOLSALE											
ACTNSALE											
LIGNSALE											

Optimum

168.7689 15.07532

Reduced costs 109.7912 94.95049 182.0214 167.1807 171.1364 151.3488 165.1984 160.2514 169.1541 159.2603



RHS           Slacks/  
                  Surplus           Shadow  
                                  prices

(maximize  
profit)

SEACAPAC	>=	0	195	
H2SO4CAP	>=	0	185.4603	
DRYCAPAC	>=	0		
MWCAPACT	>=	0		-83.7798
ENPRDCAP	>=	0	32.12946	
CHF1CAPC	>=	0	506.3068	
CHF2CAPC	>=	0		
CHF3CAPC	>=	0		
ASPAVAIL	=	195	195	252.4041
H2SO4REQ	=	0		52.34
POWERREQ	=	0		0.046
COWATREQ	=	0		0.073
PRWATREQ	=	0		0.65
STM15REQ	<=	0	-34.8047	
ST200REQ	=	0		4.8
ST600REQ	=	0		5
ENMEDREQ	=	0		16.38
FERMEDREQ	=	0		
ASPENBAL	=	0		-267.404
SEA1BALN	=	0		-198.306
SEA2BALN	=	0		-205.733
SEA3BALN	=	0		-291.074
SEA4BALN	=	0		-288.065
SEA5BALN	=	0		-296.419
SEA6BALN	=	0		-198.305
SEA7BALN	=	0		-288.199
SEA8BALN	=	0		-287.769
SEA9BALN	=	0		-291.494
SEA10BAL	=	0		-283.984
SEA11BAL	=	0		-268.277
SEA12BAL	=	0		-305.351
SEA13BAL	=	0		-269.225
SEA14BAL	=	0		-254.301
SEA15BAL	=	0		-198.305
SEATOTAL	=	0		-198.305
PETROBAL	=	0		-899.514
WSREMBAL	>=	0		
WIPENTBA	>=	0		
WIHEXOBA	>=	0		
HEXPENBA	=	0		-223.966
XYASEBAL	>=	0	455.4351	
CLASEBAL	<=	0		1.978369
FURBALAN	=	0		-1274.69
BDIOLBAL	=	0		-714.691
BUTANBAL	=	0		-674.691
ACTONBAL	=	0		-594.691
ETNOLBAL	=	0		-494.691
LIGNINBA	=	0		35.30894
CHF1INH	>=	0	168.7689	
CHF1BALN	=	0		198.3059
CHF2INH	>=	0		
FURLIMIT	>=	0	15.07532	
BDLLIMIT	>=	0	45.56761	
BUTLIMIT	>=	0		
ACTLIMIT	>=	0		
ETHLIMIT	>=	0	9.113522	
FURSALES	=	0		-1320
ENLSALE	=	0		-540
BTDLSALE	=	0		-760
BTDLSALE	=	0		-720
ACTNSALE	=	0		-640
LIGNSALE	=	0		-10

Profit  
49218.81

Optimum

Reduced costs

## 5.2 ACTIVITIES AND CONSTRAINTS ANALYSIS

This section contains the interpretation of the optimal solution to the simulated model when using an input of 195 tons of aspen wood per day. The solution print-out from the package, LP83, used to solve this model follows a fixed format which is divided into two parts, the 'solution' and the 'constraint'.

The solution part states the activity of each variable for a maximum profit and gives the value of the objective function. For the spreadsheet version of the model, its solution is included in the 'optimum' row, as mentioned in Section 5.1 above. A summary of these non-zero activities of the solution part is included in Table 5.1. A detailed print-out of the solution part is included in Appendix B.

The constraint part gives the activity of the constraints and their slack values. For the spreadsheet version of the model, the constraint activities are included in the 'slack/surplus' column. A summary of the non-zero constraint activities is included in Table 5.2. Table 5.3 contains the representations of a list of all the non-zero variables that appear in the optimal solution or in Table 5.1.

### Model Solution Interpretation:

Despite the bioconversion process having a non-linear parameter such as temperature, time, substrate concentration etc., we have succeeded in simulating it on the linear activity system model, and formulating the optimization as a linear programming

problem. Thus when solving the problem, a maximum profit for an input of 195 tons of aspen woods per day was obtained as well as an optimal setting of the parameters is determined.

The solution indicates that with an initial arbitrary input of 195 tons per day of aspen wood, a maximum profit of \$49,218.8148 per day can be attained (a breakdown of how this profit is generated is included in Table 5.1). This produces 45.5676 tons of butanediol and coproducts of 15.0753 tons of furfural, 48.2646 tons of lignin in the steam treatment process (although lignin is usually recovered in the alkali extraction step) and 9.1135 tons of ethanol in the product recovery process.

The model has selected the acid impregnation of green chips with 220 C steam for 80 seconds process to pretreat approximately 95% of the original input material. After steam treatment, the material with the addition of enzymes and the fermentation medium undergoes the CHF1 conversion process to produce butanediol and ethanol. The balance of the input material is steam treated with 240 C for 180 seconds and then undergoes various chemical processes to produce enzymes which are then utilized in the above mentioned CHF1 process. (These process paths can be found in Figure 4.2.)

In generating the above mentioned optimum solution, the model has determined by utilizing the Simplex Algorithm, which particular process paths result in maximum profits. In so doing, the less efficient process paths are exposed.

Table 5.1: Summary of Forintek Integrated Process Model Solution

Objective Function Value = \$49,218.81 per day					
<u>Variable</u>	<u>Activity</u>	<u>Cost per unit</u>	<u>Costs</u>	<u>Sale Price per ton</u>	<u>Revenue</u>
ASPPURCH	195.0000 tons	\$15.00	\$2,925.00		
SEEJ4F6N	9.5396 tons	\$3.68	\$35.11		
SEEG3F62	185.4604 tons	\$3.68	\$682.49		
SE63F62T	168.7689 tons	\$0.00			
H1D12N3B	168.7689 tons	\$0.00			
SEATOTAL	168.7689 tons	\$0.00			
EPE4SBSS	8.0300 tons	\$0.00			
BDLRECOV	45.5676 tons	\$0.00			
BDLSALE	45.5676 tons			\$760.00	\$34,631.38
ETHRECOV	9.1135 tons	\$0.00			
ETHSALE	9.1135 tons			\$540.00	\$4,921.29
LIGRECOV	48.2646 tons	\$0.00			
LIGFUEL	48.2646 tons			\$10.00	\$482.65
FURRECOV	15.0753 tons	\$0.00			
FURSALE	15.0753 tons			\$1,320.00	\$19,899.40
H2SD4PUR	2.2300 tons	\$52.34	\$116.72		
POWERPUR	16813.3083 kwh	4.6cents	\$773.41		
CWPURCH	2855.3440 mmgal	7.3cents	\$208.44		
PWPURCH	481.4092 mmgal	\$0.65	\$312.92		
STM200PU	1072.8114 mmlb	\$4.80	\$5,149.49		
STM600PU	74.1000 mmlb	\$5.00	\$370.50		
ENMEDIUM	8.6750 tons	\$16.38	\$142.10		
FERMED	16.8769 tons	\$0.00			