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Methodology for Evaluating the Economics of Biologically Producing Chemicals and Materials from Alternative Feedstocks

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ABSTRACT

A wide range of chemicals and materials can be produced from renewable feedstocks through bioconversions. An iterative, progressively detailed technology screening approach was developed to identify the most promising candidates. Initially, candidates are selected into a portfolio based on their future potential as large-volume industrial chemicals or materials. Second, the candidates are ranked with respect to a simple economic criterion based on the market value, the price of the starting material, and the product yield. Simple comparisons are then made, where possible, between producing the product via the most competitive conventional route and via the proposed bioprocessing route. Next, qualitative information is gathered from industrial experts on the advantages and disadvantages of each product with respect to energy impacts, environmental quality, and economic competitiveness. Finally, engineering and economic evaluations are performed for the most promising candidates to assess the profitability of the bioprocessing route and to identify the research and development opportunities that have the greatest impact on energy savings, environmental quality, and economics. Forty chemicals and materials that could potentially be produced from renewable feedstocks were initially selected for evaluation by this methodology. From this, succinic acid was chosen for the first more detailed evaluation based on the initial screening results. The approach described in this article

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could be used by potential industrial producers to complement their forecasting of the technical and economic feasibility of producing chemicals and materials from renewable resources, and by researchers to identify opportunities for focused research and development.

Index Entries: Bioprocessing; process evaluation; economic analysis; biomass feedstocks; industrial chemicals.

INTRODUCTION

A number of commodity chemicals were once produced from renewable resources through fermentation processes; however, many of these processes were not able to compete with processes developed during the petrochemical revolution. Once again there is considerable interest in producing chemicals from renewable resources to reduce petroleum imports, bolster the domestic economy, and improve the environment. This renewed interest is justified by the many technological advances that could make these processes economically competitive, but numerous technical improvements will be necessary to realize the potential global benefits of biobased processes fully. Successful industrial commercialization of near-term products will go a long way toward establishing the needed infrastructure and, thus, will further catalyze the growing momentum in this vital field. Amid all the hopes for this technology lies a great deal of uncertainty. Careful attention to the sources of these uncertainties is vital to any process that attempts to sort out opportunities.

An efficient method to classify products and processes as to their potential for near-term (0–5 yr), midterm (5–10 yr), or long-term (10+ yr) application is necessary to aid in identification of promising opportunities for commercialization, research, and development from the large number of choices.

Accordingly, the methodology described in this article builds on methods and approaches previously developed and used by other investigators doing similar analyses (*1,2*) to help identify promising targets. It will describe an approach to sort through a number of alternatives rapidly to identify those that appear promising. Then, successively detailed analyses will be applied to determine the economic potential of those selected from the first round and identify opportunities to apply the technology commercially.

METHODS

This forecasting methodology consists of five phases: portfolio selection, initial economic screening, comparative analysis, qualitative analysis, and detailed economic analysis. An important aspect of this methodology is its successively more detailed, iterative approach.

Phase One: Portfolio Selection

The initial function of the first phase was to develop the portfolio of candidates on which the remaining analyses would be performed. A set of criteria was defined to select products to be included in the portfolio. Candidates were evaluated, somewhat subjectively, against the following criteria to decide on their inclusion in the portfolio. No single criterion was the most important for selecting candidates into the portfolio.

Selection Criteria

- High theoretical product yields from substrate: Only theoretical product yields were considered in the selection criteria. Many technologies exist to manipulate the metabolism of microorganisms. Metabolic alterations can remove competitive pathways and/or enhance the activity of rate-limiting enzymes. A long-term forecast should consider the potential that yields at industrial scale could closely approach theoretical yields.
- Market interest in the product as an end product or as an industrially important intermediate: The need for market interest is obvious. Here two classes of products can be considered. The first class includes existing commodity chemicals not currently produced from biomass. Examples include acetaldehyde, butanol, and isopropanol. The advantage to such products is that the market is already established and less effort is required to sell these products. On the other hand, competition will be strictly based on price because no product performance advantages are possible for products derived through biotechnology over those produced from petroleum. The second class of products is new materials that can be derived through, and are unique to, biotechnology. Examples include new adhesives, biodegradable plastics, biocompatible solvents, degradable surfactants, and enzymes for a variety of applications. For such products, initial competition would probably be based on performance, and the advantages of the bioproducts might provide unique niches for introduction into the marketplace. Therefore, less price pressure is possible initially for such new products. Ultimately, widespread use could be achieved by lowering price.
- High production volume (current or potential): One of the initial goals of this study was to identify products that could be produced from renewable feedstocks in large enough quantities to reduce raw material (e.g., petroleum) imports significantly.
- Nonfood use: Although many fermented foods could be made from renewable biomass resources, including single-cell protein and single-cell oil, the initial emphasis of this study is placed on chemicals and materials for nonfood applications.

- Ability to be biologically synthesized from the common sugars derived from various forms of biomass: Glucose and xylose are representatives of the hexoses and pentoses produced from renewable biomass feedstocks by pretreatment and hydrolysis operations. The initial products were chosen only if they could be produced by a microorganism using one of these types of substrates. In the future, consideration will be given to products that can be produced from feedstocks not containing polysaccharides. Examples here include biotransformation products of fatty acids from oilseed crops and materials produced by organisms that utilize carbon dioxide.

The initial portfolio size was limited to 40 products to allow for a focused study. Thus, successful comparison against the selection criteria did not assure a candidate's inclusion in the portfolio. The initial selection strategy was to develop a portfolio that was well balanced in terms of the processes and product families represented.

With a base portfolio established and the initial analyses performed, the current function of the product-selection phase is to add products to the portfolio on an ongoing basis. The selection criteria can be relaxed or varied according to the needs of the portfolio; again, the general objective is to maintain a portfolio containing a broad spectrum of technologies that will become applicable over a wide time frame.

Phase Two: Initial Economic Screening

The purpose of the second phase of the methodology is to help determine the order in which more time-consuming detailed analyses are performed on each product. The products are ranked and classified based on a simple economic criterion, termed the Fraction of Revenue for Feedstock (FRF). Simply stated, the FRF is the ratio of the cost of the feedstock to the value of the products derived from that feedstock. For multiple products, all of the revenue must be included for each of the coproducts, as in Eq. (1). The FRF must be less than unity for a process to be economically feasible; i.e., the value of the products obtained must be greater than the cost of the feedstock. The lower the FRF, the more promising the feedstock-product combination initially looks for further study.

$$\text{Fraction of revenue for feedstock} = [(\text{Cost of feedstock} / \text{Value of products})] = (C_f / \sum x_i \beta_i y_i \alpha_i V_i) \quad (1)$$

where i = number of feedstock components considered, C_f = unit cost of the feedstock, x_i = fraction of component i in the feedstock, β_i = hydrolysis weight-gain conversion factor (if applicable), y_i = theoretical yield of product derived from component i, α_i = percent of theoretical yield of product derived from component i, and V_i = value of the product derived from component i.

FRF calculations were performed for a number of scenarios representing both current conditions and future possibilities. These calculations were performed for each product using a variety of starch and lignocellulosic feedstocks. Sensitivity studies were performed varying feedstock costs, product values, and product yields. The entirety of those results is too extensive to be included in this article. Instead, results will be reported in a condensed form based on the following rationale.

All the feedstocks evaluated in the analysis thus far will yield glucose after some pretreatment and hydrolysis operation. The cost of this glucose will depend on the feedstock used and the method employed to carry out the hydrolysis. The value of any coproducts derived from nonglucose-yielding feedstock constituents can be taken as a credit against the cost of the delivered feedstock. Thus, the calculations and results can be simplified by using glucose syrup as the feedstock. Two cases are considered. The first case represents the current condition for which a $0.22/kg of glucose cost is assumed. This is a conservative estimate of the value of hydrolyzed corn starch if it were transferred from a corn wet-milling process to a fermentation section of the same plant. The second case represents a future situation where the cost of glucose is assumed to be $0.17/kg. In this case, the source of glucose could be hydrolyzed cellulose from a lignocellulose processing plant.

Like the feedstock costs, the value of the products and conversion yields are uncertain. The current selling prices of many of the products in the portfolio, obtained either directly from a manufacturer or from literature, such as the *Chemical Marketing Reporter*, are not accurate reflections of what the selling prices would be if those products were produced in larger quantities for a wide range of uses (e.g., as monomers for new polymers). No source of current product price information can be used without some subjective evaluation of whether that price is a good estimate of the value of the product in the future. For those cases where the product is already a large-volume commodity chemical, such as butanol, the current selling price is presumably a good estimate of the future value, neglecting inflation effects. In other cases, the future values of the products are estimated on a case-by-case basis giving careful consideration to the expected market applications and sales volumes in those markets. Estimating the future selling prices of the products is considered to provide a more accurate assessment of the FRF and, thus, more meaningful ranking results.

Finally, two cases can be considered for the conversion yields of products from feedstocks. The first case, representing the current state of the art, uses demonstrated yield data that were obtained as the result of an extensive literature search. To simplify matters, the highest reported yield of product on glucose was taken as the demonstrated yield. There is some uncertainty associated with using these values as representatives of expected yields in large-scale processes, where conditions are often less than optimum. The second case is based on a future scenario where metabolic engineering techniques have been applied to increase process yields to near the theoretical limits. This requires the calculation of the theoretical yield from glucose for each product in the portfolio. The maximum theoretical yield is taken to be the smallest of the maximum yields based on carbon availability, energy availability, and reducing potential (3).

Phase two results will be reported for two scenarios. The first scenario represents the present conditions, and the FRF results reflect the current estimated feedstock costs, the currently demonstrated product yields, and the estimated product values for large-scale production. The second scenario represents a potential future condition in which feedstock costs are lower because of the use of dedicated, low-cost lignocellulosic feedstock crops, the demonstrated yields are replaced with theoretical product yields, and product values are estimates of their value for large-scale production.

The products can be classified into near-, mid-, or long-term opportunity categories based on the FRF. An FRF cutoff value can be arbitrarily chosen and used to make the initial classification. Any product whose FRF is below the cutoff under the first scenario would be classified as a near-term opportunity. If the product's FRF is below the cutoff under the second scenario, it would be classified as a midterm opportunity. All others would be classified as long-term opportunities.

In using this approach, it must be remembered that key properties (e.g., relative volatility compared to water) can have significant impacts on processing costs (e.g., product recovery and purification). Thus, even though a product may rate low in the FRF analysis, it may still be economic because it is easy to process. As a result, some judgment is required in the interpretation of this approach.

Phase Three: Comparative Analysis

Comparative analyses of proposed bioprocessing routes with current routes were performed at an early stage of process evaluation to help decide the order in which candidates are investigated in more detail. The basis for this comparison was the estimated raw material costs for each of the processing routes (4). The raw material costs are a significant fraction, 50–90% or more, of the production cost for most commodity chemicals. A preliminary economic comparison can be made between the bioprocessing route and the current petrochemical route assuming the raw material costs are an approximately equal fraction of the total production costs of each route.

The parameter of interest here is the ratio of the raw materials costs, shown in Eq. (2). The ratio is modified by a risk factor of 1.3 to take into account possible problems, unknowns, and intangibles in a given bioprocess. One might also view this factor as accounting for the fact that in most situations, the capital required for the existing petrochemical-based process is either partially or completely paid off. Thus, any competitive process would have to have substantially lower production costs.

Raw material cost ratio = (Estimated cost of raw materials for petrochemical process / Estimated cost of raw materials for bioprocess) × (1 / Risk factor) (2)

If the raw material cost ratio (RMCR) is greater than unity, the proposed bioprocess shows potential, based on raw material costs alone, for being competitive with the existing petrochemical process. A ratio considerably less than unity suggests that the bioprocess could have difficulty competing with the current petrochemical route.

Similar to the FRF calculations, both a currently achievable bioprocess and a theoretically achievable bioprocess can be considered. The basis for determining the raw material costs for the currently achievable bioprocess part of this analysis is the demonstrated yield factor, based on glucose, multiplied by 0.5 to adjust for unaccounted raw materials and the uncertainty in translating bench- or pilot-scale yield data to production scale. For some cases, this adjustment factor overpenalizes the bioprocess because some yields have been demonstrated at the large scale, and/or additional raw material costs are negligible. Nevertheless, it has been used in all cases for consistency. The basis for determining the raw material costs for the theoretically achievable bioprocess part of this analysis is the theoretical yield factor, based on glucose, multiplied by 0.95. Now the adjustment factor is applied to account for the inability of a full-scale process to achieve 100% of the theoretical yield. No adjustment is made to account for additional raw materials since, in theory, processes could be developed in which they would no longer be required or would be negligible.

Only currently achievable petrochemical processes were considered. The assumption here is that these processes have already been virtually optimized and that opportunities for additional process improvements would not be substantial. The basis for determining the raw material costs for the petrochemical processes is the current demonstrated yield factor, based on the primary precursor. These data were obtained from the literature, mostly from the Stanford Research Institute's *Chemical Economics Handbook* (*5–13*). No adjustment factor was applied to the yield factor, because all raw material costs are assumed to be known and the yield is clearly demonstrated at full scale. The results have been summarized into a table that gives the RMCR for the currently achievable bioprocessing scenario and the theoretically achievable bioprocessing scenario, each with an estimated fixed glucose cost of \$0.22 and \$0.17/kg, respectively.

These comparative analyses should be viewed as a first attempt to compare the competitiveness of bioprocesses with the current petrochemical-based processes and will be used only to help identify the order in which more detailed engineering economic analyses will be performed. The comparison of more detailed engineering analyses will provide a better measure of the competitiveness of the bioprocessing route. These detailed engineering analyses will also be used to identify the key research opportunities for bridging the competitive gap between bioprocesses and petrochemical processes.

Phase Four: Qualitative Analysis

The quantitative evaluations were complemented by gathering opinions from a diverse group of informed professionals from the biotechnology and chemical processing industries. One objective was to seek out judgments as to the relative merits of the products with respect to the following three categories: energy impacts, environmental quality, and economic competitiveness. Another objective was to expose and explore the underlying assumptions leading to different judgments. The respondents were asked to identify the impact that adoption of the renewables-based technology would have on a variety of specific issues in the three categories mentioned above. In an attempt to avoid overanalysis, no effort was made to quantify the results. Instead, the results are peripherally considered when making decisions as to the order in which products are evaluated in more detail in the fifth phase of the analysis.

Phase Five: Detailed Economic Analysis

The effort required to complete this stage of the analysis is significantly greater than that for the initial stages, and it is beyond the scope of this article to discuss the steps and tools used in any detail. To focus on the most promising options for this more time-consuming effort, the results from the initial stages are used to rank the order in which products undergo the more rigorous integrated product/process economic analysis. Again, the objective is to classify the products and associated process technologies into near-, mid-, or long-term opportunity categories. The classifications resulting from this fifth phase will be regarded as the most accurate because many more details are considered. The purpose of this phase is not to prepare extremely detailed process designs, which require considerable expense to carry out, but to provide a quantitative measurement that, when supplemented by a consensus of qualitative opinion, can be used to rank the projects relative to one another. Detailed designs and rigorous profitability analyses are future activities performed on projects whose manufacturing technology and product markets become ripe for commercialization.

Material and energy balances for the processes are performed using spreadsheet models that are supplemented, when necessary, with output from ASPEN-based simulations of particular unit operations. An equipment schedule is developed from the process flow sheet, and the equipment is sized according to the relevant material or energy flows to/from any particular piece of equipment. The cost of the equipment is determined by means of vendor quotes, historical data, and process equipment cost estimating software (*14*). The factoring method is used to estimate the total fixed capital investment and recurring capital-related costs, from the purchased equipment cost. The estimated uncertainty accompanying this capital investment estimate is assumed to be $\pm 30\%$. Raw material, utility, and operating labor costs are determined independently, and used to estimate working capital requirements and sales- and labor-related costs.

A discounted cash flow analysis is used to predict the required selling price of the product. The difference between the product's estimated market value and the product's predicted selling price is the criterion on which the projects are again ranked. This ranking, together with the qualitative opinion, will be used to classify the final options into near-, mid-, and long-term opportunities.

Further engineering economic analyses will be performed to guide research and development activities. Sensitivity studies will be performed to determine the parameters and variables that most strongly affect the overall economics and identify opportunities for technology improvement through research and development. These studies can also be used to synthesize process alternatives and to direct subsequent uncertainty analyses.

Summary of Methodology

The methodology developed is the result of an attempt to create an as-simple-as-possible methodology that will give meaningful results. It is important to point out that the screening methodology is an iterative process. Most of the parameters that affect the investment and manufacturing costs are subject to change, some much more rapidly than others, as a result of better information or technology improvements. For example, demonstrated new technology concepts may shift a process rank from a long-term opportunity to a mid- or near-term opportunity. Because of the potential for such changes, the periodic reevaluation of the projects is necessary at the various levels of analysis.

RESULTS

Examples of the kind of results from the initial phases are given below for the screening of a number of products/processes down to a few for more detailed study. In this case, succinic acid was identified as a possible promising near-term opportunity, both by the initial classification methods and by qualitative opinion. Some of the results of the initial detailed economic analysis of succinic acid are given to provide an example of the detail considered in the fifth phase of the analysis.

Phase One: The Current Product Portfolio

The portfolio is currently made up of the products in Table 1. Note that a few of the products are currently produced through fermentations or bioconversions, e.g., citric acid and dextran. Actual process information on these products is used to validate the tools and techniques developed to carry out this work.

Table 1
Product Portfolio

Acetaldehyde	Butanol	Isopropanol	Protease
Acetic acid	Butyraldehyde	Itaconic acid	Pullulan
Acetone	Butyric acid	Lactic acid	Rhamsan gum
Acrylic acid	Cellulase	Lysine	Scleroglucan
Adipic acid	Citric acid	Malic acid	Sorbitol
Alginate	Dextran	Oleic acid	Succinic acid
Ascorbic acid	Fumaric acid	Polyhydroxybutyric acid	Surfactin
Azelaic acid	Gluconic acid	1,3-Propanediol	Tartaric acid
Bacterial cellulose	Glycerol	Proprionic acid	Xanthan gum
2,3-Butanediol	Hyaluronic acid	Propylene glycol	Xylitol

Phase Two: Fraction of Revenue for Feedstock Results

Table 2 provides the results of the FRF calculations for two cases based on (1) current feedstock cost and demonstrated product yield, and (2) estimated future feedstock cost and theoretical product yield. Demonstrated yields have not yet been located in the literature for five of the products. Theoretical yields could not be calculated for the cellulase and protease enzyme complexes, or for the complicated surfactin molecule. The cost of the feedstock used, glucose syrup, was $0.22/kg for the current scenario and $0.17/kg for the future scenario. Current product prices were used in the FRF calculations for those products already being produced in large volumes (*15*). If the product is currently a small or intermediate volume product, an estimate of the product's value if it were to be produced in large quantities was used.

The last column of the table gives the results of a classification into the near-, mid-, and long-term opportunities based on an FRF cutoff value of 0.30. Any product whose FRF was below 0.30 when using the current estimated feedstock cost and the demonstrated product yield was classified as a near-term opportunity; 14 of the 40 products would be classified as near-term opportunities under this scheme. Products were classified as a midterm opportunity if their FRF was below 0.30 when using the estimated future feedstock cost and the theoretical product yield; 16 of the 40 products were classified as midterm opportunities. The remaining 10 are classified as long-term opportunities.

Phase Three: Results of Comparative Analyses

Twelve of the 40 products in the portfolio have been evaluated thus far in this comparative-analysis phase. Many candidates in the portfolio can be readily produced only through bioprocessing routes, e.g., lysine or pullulan, and other products, such as citric acid, are currently produced

Table 2
Results of FRF Calculations and Initial Project Classification

Product	Expected product value, $/kg	Demonstrated yield, kg/kg	FRF, Current, –	Theoretical yield, kg/kg	FRF, Future, –	Classification
Acetaldehyde	1.01	N/A	N/A	0.59	0.28	M
Acetic acid	0.73	0.95	0.32	1.00	0.23	M
Acetone	0.75	0.12	2.44	0.48	0.47	L
Acrylic acid	1.52	N/A	N/A	0.80	0.14	M
Adipic acid	1.43	N/A	N/A	0.75	0.16	M
Alginate	2.20	0.52	0.19	0.90	0.09	N
Ascorbic acid	2.20	0.01	10.00	0.98	0.08	M
Azelaic acid	1.52	N/A	N/A	0.52	0.21	M
Bacterial cellulose	2.20	0.25	0.40	0.90	0.09	M
2,3-Butanediol	1.98	0.33	0.34	0.50	0.17	M
Butanol	0.90	0.25	0.98	0.41	0.46	L
Butyraldehyde	0.95	N/A	N/A	0.40	0.45	L
Butyric acid	1.06	0.38	0.55	0.49	0.33	L
Cellulase	2.20	0.27	0.37	N/A	N/A	M
Citric acid	1.81	0.87	0.14	1.07	0.09	N
Dextran	2.20	0.30	0.33	0.53	0.15	M
Fumaric acid	1.48	0.72	0.21	0.97	0.12	N
Gluconic acid	1.98	0.90	0.12	1.09	0.08	N
Glycerol	1.28	0.50	0.34	0.88	0.15	M
Hyaluronic acid	1.10	0.25	0.80	0.65	0.24	M
Isopropanol	0.79	0.12	2.32	0.33	0.65	L
Itaconic acid	2.20	0.65	0.15	0.72	0.11	N

(continued)

Table 2 (*continued*)

Product	Expected product value, $/kg	Demonstrated yield, kg/kg	FRF, Current, –	Theoretical yield, kg/kg	FRF, Future, –	Classification
Lactic acid	0.77	0.95	0.30	1.00	0.22	N
Lysine	1.65	0.50	0.27	0.70	0.15	N
Malic acid	1.79	0.56	0.22	1.12	0.08	N
Oleic acid	1.37	0.05	3.21	0.37	0.34	L
Polyhydroxybutyric acid	1.10	0.40	0.50	0.47	0.33	L
1,3-Propanediol	1.32	0.80	0.21	0.42	0.31	L
Propionic acid	0.90	0.46	0.53	0.55	0.34	L
Propylene glycol	1.28	0.27	0.64	0.42	0.32	L
Protease	2.20	0.10	1.00	N/A	N/A	N
Pullulan	2.20	0.43	0.23	0.90	0.09	N
Rhamsan gum	2.20	0.40	0.25	0.90	0.09	N
Scleroglucan	2.20	0.36	0.28	0.90	0.09	N
Sorbitol	0.79	0.36	0.77	0.93	0.23	M
Succinic acid	0.88	0.87	0.29	0.98	0.20	N
Surfactin	1.65	0.02	6.67	N/A	N/A	M
Tartaric acid	2.20	0.05	2.00	0.83	0.09	M
Xanthan gum	2.20	0.60	0.17	0.90	0.09	N
Xylitol	0.88	0.12	2.10	0.84	0.23	M

Table 3
Raw Material Cost Ratio (RMCR) Results of the Comparative Analyses

Product	Current scenario	Theoretical scenario
Acetic acid	0.48	1.24
Acetone	0.06	0.59
2,3-Butanediol	0.45	1.69
Butanol	0.31	1.26
Butyric acid	0.31	1.00
Glycerol	0.68	2.94
Isopropanol	0.05	0.33
Malic acid	0.58	2.50
Polyhydroxybutyric acid	0.52	1.51
Propionic acid	0.35	1.04
Propylene glycol	0.30	1.13
Succinic acid	0.90	2.50

through bioprocessing, even though a petrochemical route is available. Although it is theoretically possible to produce some products, such as acetaldehyde and butyraldehyde, through bioprocesses, no bioprocessing options have been proposed, and thus yields and raw material costs for these processes cannot be determined. Table 3 gives the results of the comparative analysis for two scenarios—currently achievable bioprocesses and theoretically achievable future bioprocesses—in which demonstrated product yields were used in the current case and the theoretical product yields were used in the future case. The costs of the glucose feedstock used for these two cases were $0.22 and $0.17/kg, respectively. The costs of the petrochemical feedstocks and the product yields from the petrochemicals were the same for both comparisons. Recall that an RMCR greater than unity indicates that the proposed bioprocessing route shows a potential economic advantage, based on raw material costs alone, compared to the existing petrochemical process.

The current scenario RMCR for all 12 products is below unity, meaning that the conventional petrochemical process is more competitive than the bioprocess based on the raw material costs alone for existing bioprocessing yields and high glucose costs. However, note that there appears to be the potential that many of the bioprocesses could become competitive if various process and biocatalyst improvements enhance the product yield and lower cost feedstocks are employed. Although the theoretical scenario represents an optimistic case, it should be remembered that raw material costs are only part of the overall economic picture of any process; more detailed engineering and economic analyses are required to assess the competitiveness of bioprocess alternatives accurately compared to conventional processes.

Phase Five: Manufacturing Cost Summary for a Biobased Succinic Acid Process

Succinic acid was identified as a possible near-term opportunity by the initial classification analysis because it has the best RMCR of those evaluated for the current scenario, one of the best RMCRs for the future scenario, a desirable FRF for existing and future technology, and is representative of a broad group of products (organic acids) with favorable FRFs. This choice was also judged to be reasonable by a number of industrial experts. Succinic acid can be used as an intermediate in the chemical synthesis of 1,4-butanediol, tetrahydrofuran, and adipic acid with a large market potential. However, large-scale use requires that succinic acid be produced less expensively than through its current petrochemical route, and a research and development program must be directed at opportunities to lower its cost of production. This may be possible through a bioprocessing route using a renewable resource.

The base-case model for the succinic acid process used in this analysis is described in a recent patent (*16*), and is depicted in the simplified process flow diagram of Fig. 1. As discussed previously, material and energy balances were developed for this process, and operating and capital costs were estimated. A condensed manufacturing cost summary for the base-case succinic acid process is given in Fig. 2. Numerous case studies and sensitivity analyses have been performed with a spreadsheet model to help direct a research and development effort to explore further the possible energy savings that might result from large-scale production of succinic acid from renewable resources.

The initial engineering economic analysis identified a number of areas where process improvements are necessary to be economically competitive. One of these areas is the product recovery operation. The base-case process would produce large quantities of calcium sulfate as a byproduct. This solid byproduct would most likely need to be disposed of in landfills, an environmentally undesirable and costly scenario. Advanced processing concepts exist that would reduce, or eliminate altogether, this waste-disposal problem. This is one example of how engineering economic analysis can be used to direct research and development efforts. Process performance parameters resulting from such efforts are used to update the economic analyses, which in turn further refine process development directions. In the future, this approach will be applied to other products/processes that pass the initial screening methodology to identify the most promising projects for directed research and development.

CONCLUSIONS

Caution must be used in interpreting the results of these evaluations, because they are approximations subject to varying degrees of uncertainty

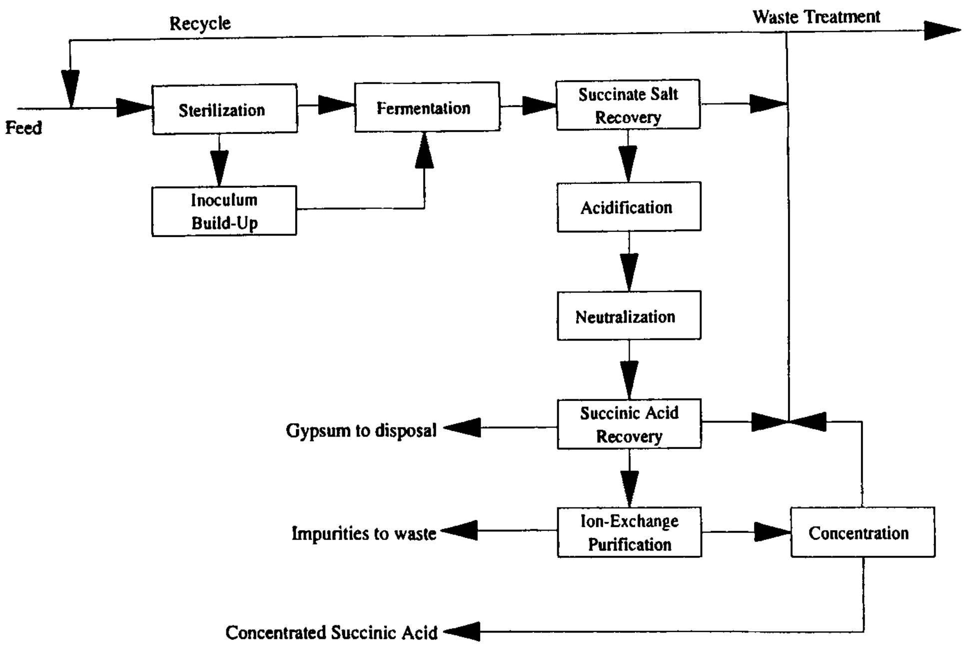

Fig. 1. Process concept for bioproduction of succinic acid.

and, consequently, to a wide range of subjective judgments. The analyses are intended simply to identify those products and processes that warrant more detailed investigation, but the conclusions drawn depend on an individual firm's business environment. This would include, but is not limited to, careful consideration of the required research and development strategy and the firm's technical and marketing acumen. The methodology presented here is a simple model that can provide truly meaningful results only when it is applied within the proper context.

The screening methodology has several features that make it particularly useful for evaluations. First, it is performed in stages that are successively more detailed, each stage presumably providing more accurate results than its predecessor. The initial stages of the methodology allow for rapid screening of many projects to identify those that warrant greater study. This is done by focusing initially on the feedstock cost and the product yield, because feedstock or raw material costs, typically the largest fraction of total production costs, are relatively easy to estimate. Thus, they lend themselves well to a preliminary ranking analysis scheme. Furthermore, if reasonable product yields are not obtainable, the product cannot be economically viable and does not merit further scrutiny. The FRF ratio provides a simple criterion on which to rank, and partially eliminate, the products for more detailed analyses, but the FRF should not be used by itself to identify a product/process as an absolute success.

The application of the RMCR ratio to the methodology provides an early evaluation of the potential competitiveness of the biobased processes

Succinic Acid Production from Glucose Syrup

Location	Midwest	Annual Capacity	71,940,000 kgs succinic acid
Effective Date to Which Estimate Applies	Oct-91	Cost Index Type	CE Plant Index
Predicted Selling Price, $/kg:	**$0.930**	Cost Index Value	357.7
Fixed Capital	$30,780,000		
Working Capital	$6,970,000	Total Capital Investment	$37,750,000

Assumptions

Plant Life	10 years	Investment Tax Credit, First Year	0.0%
DCF Rate-of Return	15.00%	Working Capital, (determined independently)	N/A
Equivalent Return on Investment	27.13%	Assumed Inflation Rate	3.5%
Equipment Service Life, MACRS Depreciation	5 years	Percent of Total Fixed Capital Investment Spent in Year -3	30.0%
Building Service Life, Straight-Line Depreciation	30 years	Percent of Total Fixed Capital Investment Spent in Year -2	50.0%
Combined Federal and State Tax Rate	37.0%	Percent of Total Fixed Capital Investment Spent in Year -1	20.0%
Equipment Salvage Value	0.0%	Percent of Start-Up Costs Spent in Year -1	30.0%

Production Cost

	$ per yr	$ per kg product
Raw Materials	$37,930,000	$0.527
By-Product Credits	$0	$0.000
Utilities	$10,690,000	$0.149
Ion Exchange Resins	$560,000	$0.008
Operating Labor	$1,180,000	$0.016
Labor Related Costs	$800,000	$0.011
Capital Related Costs	$2,430,000	$0.034
Sales Related Costs	$1,340,000	$0.019
Total Expense at 100% Capacity, proof year: 5	**$54,930,000**	**$0.764**

Revenue

	$ per yr	$ per kg product
Revenue from Sales	$66,900,000	$0.930
Net Annual Profit	$12,530,000	$0.174
Annual Income after Taxes	**$8,920,000**	**$0.124**

Raw Material Costs

			$ per kg raw material
Glucose Syrup	95 DE	ANL, NREL Estimate	$0.220
Corn Steep Liquor	50 % Solids	ANL, NREL Estimate	$0.055
Calcium Hydroxide		CMR, 12/25/92	$0.057
Sulfuric Acid	100%	CMR, 12/25/92	$0.095
Carbon Dioxide	liquid, 99.5% purity	Air Products	$0.088
Tryptophan		ANL Estimate	$24.031
Cysteine HCl		NREL Estimate	$7.055
Sodium Hydroxide		CMR, 1/7/91	$0.527
Hydrochloric Acid		CMR, 1/7/91	$0.061
Sodium Carbonate		CMR, 1/7/91	$0.432
Cation Resin	Dowex 50 WX 8, Dow Chemical	Dow Chemical	$67.021
Anion Resin	Amberlite IRA-94, Rohm & Haas	NREL Estimate	$66.139

Fig. 2. Manufacturing cost summary for succinic acid.

with existing processes. Like the FRF, the RMCR analysis is simple enough to make case studies and sensitivity analyses uncomplicated. This is desirable because it is very important to assess the future potential of the bio-based processes in selecting products/processes to emphasize. In many cases, the process economics can be significantly improved by potential, realistically achievable process improvements that these ratios help define.

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APPENDIX

Sample FRF and RMCR Calculations

Two example sources of glucose that could be used as a substrate for fermentative production of chemicals and materials are corn and hybrid poplar. Sample FRF calculations are given below for each. Fractionation of starch and other valuable coproducts from corn can be achieved through a wet-milling process. Approximate recoveries and values of the constituents are given in Table A-1. Using the data from Table A-1, and assuming a corn cost of \$0.10/kg, the currently achievable FRF for succinic acid, using corn as the feedstock, is:

$$\text{FRF} = [\$0.10 \,/\, (0.676)(1.11)(0.98)(0.90)(\$0.88) + (0.037)(1)(1)(\$0.29) + (0.245)(1)(1)(\$0.12) + (0.042)(1)(1)(\$0.33)] = 0.157 \quad (3)$$

Now consider the production of succinic acid from hybrid poplar. Assume the cost of the feedstock is \$0.07/kg. The fractionation of cellulose and other valuable coproducts might be achieved through an acid or enzymatic hydrolysis plant. Approximate recoveries and values of the constitutuents are given in Table A-2. Using the data from Table A-2, a theoretically achievable FRF for succinic acid, using hybrid poplar as the feedstock, is:

$$\text{FRF} = [\$0.07 \,/\, (0.486)(1.11)(0.98)(1)(\$0.88) + (0.168)(1.13)(0.51)(1)(\$0.20) + (0.242)(1)(1)(\$0.04)] = 0.142 \quad (4)$$

Note that this FRF could be improved if higher value products were to be derived from the hemicellulose and lignin fractions. Thus, in a sense, this is a worst-case scenario of a theoretically achievable FRF for succinic acid from hybrid poplar.

The RMCR for succinic acid can be determined for two cases: the currently achievable bioprocess and the theoretically achievable bioprocess. Assume the costs of glucose for these cases are \$0.22 and \$0.17/kg, respectively. The current yield achievable is 0.87 kg of succinic acid/kg of glucose. The theoretically achievable yield is 0.98. In the petrochemical-based process, maleic anhydride is hydrated to maleic acid, and in a second step, the double bond is hydrogenated to yield succinic acid. The overall yield of succinic acid from maleic anhydride is approx 95%. With maleic anhydride valued at \$0.57/kg, the raw material cost for the petrochemical-based process is \$0.60/kg succinic acid. The raw material cost for the currently achievable bioprocess is:

$$\text{RMC} = [(\$0.22/\text{kg glucose}) \,/\, (0.87\ \text{kg succinic acid} / \text{kg glucose})(0.5)] = \$0.51/\text{kg} \quad (5)$$

Then, the RMCR for the currently achievable bioprocess, including the 30% risk factor, is:

$$\text{RMCR} = [\$0.60 \,/\, (\$0.51)(1.3)] = 0.90 \quad (6)$$

Table A-1
Data Used to Calculate the FRF for Succinic Acid from Wet-Milled Corn

Constituent i	Weight percent x_i	Product	Product value $/kg V_i	Theoretical yield y_i	% of Theoretical yield achieved α_i	Hydrolysis conversion factor β_i
Starch	67.62	Succinic acid	0.88	0.98	90%	1.11
Corn oil	3.70	Corn oil	0.29	1	100%	n/a
Gluten feed	24.47	Gluten feed	0.12	1	100%	n/a
Gluten meal	4.21	Gluten meal	0.33	1	100%	n/a

Table A-2
Data for Calculating the FRF for Succinic Acid from Hybrid Poplar

Constituent i	Weight percent x_i	Product	Product value $/kg V_i	Theoretical yield y_i	% of Theoretical yield achieved α_i	Hydrolysis conversion factor β_i
Cellulose	48.64	Succinic acid	0.88	0.98	100%	1.11
Hemicellulose	16.84	Ethanol	0.20	0.51	100%	1.13
Lignin	24.25	Boiler fuel	0.04	1	100%	n/a
Extractives	5.49	Extractives	0.00	1	100%	n/a
Ash, proteins	4.78	Ash, proteins	0.00	1	100%	n/a

The raw material cost for the theoretically achievable bioprocess is:

$$RMC = [(\$0.17/\text{kg glucose}) / (0.98 \text{ kg succinic acid} / \text{kg glucose})(0.95)] = \$0.18/\text{kg} \quad (7)$$

Then, the RMCR for the theoretically achievable bioprocess, again including the 30% risk factor, is:

$$RMCR = [\$0.60 / (\$0.18)(1.3)] = 2.56 \quad (8)$$