Rapid Evaluation of Research Proposals Using Aspen Plus

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Abstract

An Aspen Plus model of our entire process (biomass to ethanol) is coupled with capital cost scaling and economic evaluation in MS Excel to rapidly evaluate new research proposals. The research ideas and expected results are incorporated into our base Aspen Plus model. Information from the Aspen simulation is linked to MS Excel to scale all equipment costs. The new capital and operating costs are used in a discounted cash flow analysis to determine the product (ethanol) cost. The impact on the product cost of each proposed research project is used as a major criteria in determining whether or not to fund the research. This methodology allows for rapid evaluation of many proposals and ensures that the impact of the proposed work on all areas of the plant is addressed.

Our base case costs, complete vendor quotes and other calculations supporting the design are stored in an MS Access database which is queried into MS Excel when changes are made.

I. Introduction

The National Renewable Energy Laboratory (NREL) is operated by a consortium of Midwest Research, Battelle and Bechtal for the U.S. Department of Energy (DOE). The laboratory is responsible for the execution of several research programs in energy efficiency and renewable energy for the DOE. These programs include such diverse technologies as photovoltaics, wind power, geothermal, biomass power, hydrogen and biofuels as well as others.

This paper discusses process design and economic evaluation for the Biofuels program. The Office of Fuels Development at DOE has funded research on the development of renewable, domestically produced fuels for transportation for many years. The government's interest in this area is related to issues of, national security, rural economic development, climate change, and air pollution. Over the years the program has supported a variety of fuel products. Today, the focus of this Biofuels program is to develop the technology necessary to allow industry to commercialize the production of fuel ethanol from lignocellulosic biomass. Lignocellulosic feedstocks, such as trees, grasses, agricultural waste as well as other wastes are rich in cellulose and hemicellulose. These biopolymers can be broken down into sugars and fermented to ethanol.

In managing the Biofuels Program for DOE, NREL funds research that has the most potential to meet the goals of commercializing this technology. Sponsored research is conducted at NREL as well as at universities and private industry. The principal question that begs answering is, which projects should be funded? This can be answered using the "Stage-Gate" process (Cooper, 1993).

II. Stage-Gate Evaluation Process

The Stage-Gate process, as put forward by Cooper (1993) focuses on the development of new products. We already know our product, its ethanol, so we have modified the process somewhat to look at process technologies, as our product. The steps to the Stage-Gate are shown in figure 1, starting with an Idea (Concept Development) and finishing with Commercialization. Because the government will not actually commercialize the technology, we are most interested in the stages through Confirming Feasibility. We expect to have industrial partners involved in the concluding steps of that stage. These industrial partners would then be satisfied to move the technology to the Development Stage.

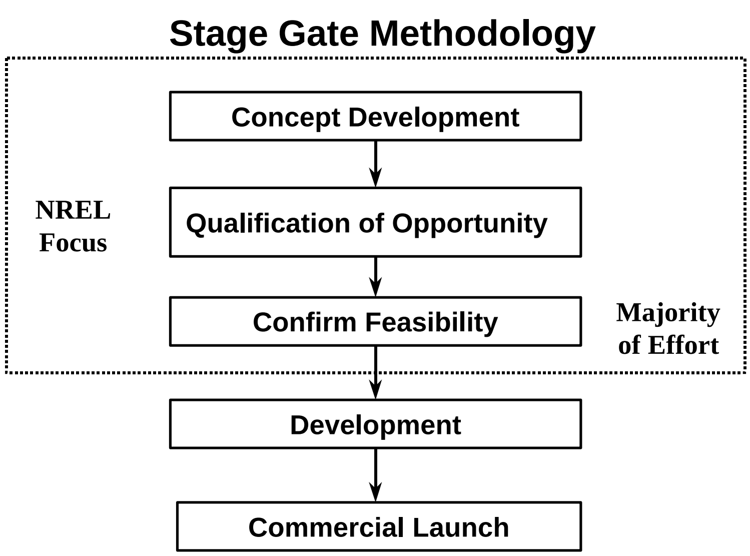


Figure 1.

The initial, Idea, stage is just that. Someone has an idea for a new process or improvement to an existing process. That Idea is captured by the program and reviewed by team leaders and managers (both technical and business development (marketing)) to insure that it meets some minimum criteria. These criteria include, does it fit with our strategic plan, does it appear feasible, and will there be a market for the technology? This first stage involves the original investigator explaining and illustrating how their idea meets the requirements of the first Gate to the Gate-Keepers (reviewers). If that can be done the Idea is ready to move through the Gate on to the Qualification of Opportunity Stage.

The Qualification of Opportunity Stage is relatively short as well, but this is where the first economic evaluations of the technology are performed. With a minimal effort, the original investigator must further investigate the idea using existing resources. There should be no experimental work in this stage. The investigation should be focused around existing literature with extrapolations based on scientific knowledge and judgement. The original investigator must relate all of the background information, and process knowledge from related processes and literature to the process engineer for incorporation in to a process and economic model. To be able to pass Gate 2 the original investigator will have to demonstrate, with process engineering help, that the technology fits the strategy of the base process, continues to appear feasible and is economical attractive. In addition, the result of a Gate 2 review will require that goals and Show-Stopper Objectives be established as well as the time frame and resources required for meeting these objectives. If all of this is agreed to by the review team, which now includes DOE and outside reviewers, the project moves to Stage 3, Confirmation of Feasibility.

While there is considerable subjective information that must be considered to make a Go/No Go decision at these early stages, the process economics provides some objective information. Because of its objective nature, multiple projects can be prioritized as to their economical potential. This is of considerable help when trying to make funding decisions with a limited budget and lots of ideas for projects.

III. Process & Economic Modeling

Fundamentally all of the process modeling that we do at NREL results in the cost of ethanol produced (our product). However, there are two distinctively different uses for the information. One use requires the absolute cost of ethanol. This requires that all of the equipment and operating cost estimates be accurate and that items like feedstock cost, equipment installation and project contingencies be accurate as well. This is more difficult for us, as we are generally not dealing with a specific site, but are trying to do the analyses in a generalized fashion for any location in the US. The absolute cost of ethanol is extremely useful to the DOE for market penetration studies where it must be compared with the costs of gasoline and gasoline additives (octane enhancers and oxygenates). These competing fuels and additives have current and projected market values established by the market place and experienced forecasters. The absolute cost of ethanol is also required for site specific studies. However, as stated above, the development of absolute costs for site specific analyses is made easier by site information.

The second use of the cost of ethanol is as an incremental cost due to a process modification. When we look at a potential research improvement to a process, that improvement can be view as an incremental to the base cost. When viewed in this light, the specifics of feedstock costs, financing, contingencies and location are held constant and tend to have little influence on the incremental cost. For the purposes of comparing the relative merits of several projects, all with various “ancillary” inputs held constant, the comparison of incremental costs will be quite reliable.

III.1 Model Development

As mentioned above, the focus of our analysis is on the incremental improvements due to the research proposal. To best implement this analysis we first developed a base-case. This base-case is summarized in Table 1.

Table 1.
Lignocellulosic Ethanol Base-Case

Feed – Woodchips or Agricultural Waste
Feedrate – 2000 dry ton/day
Product – Fuel Grade Ethanol
Product Capacity – Approximately 70 MM gallons/year

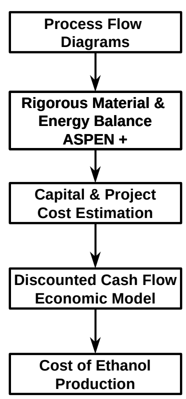
The process model encompasses the entire process which consists of nine process areas, see Table 2 and Figure 6, and is described by 23 process flow diagrams (PFD) and 181 costed pieces of equipment (Wooley, et al., 1999a, 1999b). These references give a more complete description of the process as well as the development of the base design and costs.

Table 2
Process Areas Include in Bioethanol Model

1. Feedhandling and Preparation
2. Prehydrolysis and Conditioning
3. Enzyme Production
4. Simultaneous Saccharification and Fermentation
5. Product Recovery
6. Waste WaterTreatment
7. Lignin Combustion and Power Generation
8. Storage
9. Utilities

We go through several major steps to developing the base model cost of our process and the product ethanol. These steps are illustrated in figure 2.

Figure 2
NREL's Approach to Process Design and Economic Modeling



The first step is to develop the preliminary PFD. We do not work alone in this activity. Routinely, we engage the services of engineering companies to help us with the process configuration. We rely on them to keep us informed of similar processes currently in industry. For those portions of the process which are based on new technology, we rely on the research that has been completed and any development efforts that have been accomplished to date. The engineering firms help us conform to standard engineering practices.

III.1.1 Aspen Plus Model Development

Once the process flow diagrams are sketched out we can begin the development of a process model. To this audience it may be obvious why we would use a process simulator, specifically ASPEN Plus, but to many others it is not. Many would like to use a spreadsheet only. We are opposed to that for several reasons. A simulator such as ASPEN Plus has thermodynamic models, and rigorous unit operation models built-in, so there is no need for us to program them. The simulator can easily handle complex processes with solids, such as we have. Even with all of the built-in capabilities, ASPEN Plus is still easily customizable when necessary. Very importantly, a simulator is self-documenting and is easily understood by anyone knowledgeable in the software. Finally, it is commercially supported and widely accepted by the process industries.

Development of the ASPEN Plus model involves using all information available. This information again comes from engineering firms (primarily for conventional technologies, e.g., waste water treatment, lignin burner, power generation, etc.), DOE sponsored research (both at NREL and elsewhere) and from outside meetings and consultations. All of this information has been put together into a complete model of the bioethanol process (Wooley et al., 1999a). The magnitude of the model is summarized in Table 3.

Table 3
ASPEN Plus Model for Bioethanol Production

147 Unit Operation Blocks
59 Chemical Components
217 Material Streams
211 Heat and Work Streams
60 Control Blocks (Design-Spec & Fortran)

While the ASPEN Plus model is completely rigorous in its mass and energy balance calculations, it is not completely predictive. We sometimes do more detailed modeling in either stand-alone ASPEN Plus models or other platforms (e.g., MatLab, ASPEN/SP, Scientist, Excel, etc.) and translate the information to the complete ASPEN Plus model via a simpler, generally empirical form. We do this for several reasons, first it allows us to work more easily with a detailed model if it is of a smaller area of the plant (complex recycles do not get in the way), secondly this allows us to use any model platform, not just ASPEN Plus. Finally, it allows the complete model to execute and converge in a more reasonable timeframe. The downside of this separate approach is that we have to deal with the effect of recycles in a discontinuous fashion, moving plant model recycle information to the detailed model, checking for an impact and adjusting the full plant model. Also, we are limited in how many unit-unit interactions we can assess. We use this approach for complex kinetic models, agitator power models and some distillation optimization.

III.1.2 Base Equipment Costs Database

Once the mass and energy balance model is complete, the process equipment must be costed. For the base-case, we generally size each piece of equipment using spreadsheets, sometimes ASPEN Plus or other software. Sometimes we are able to get equipment vendor to size and supply a cost estimate. This is critical for some of the unusual equipment in the process. We also make use of our engineering company contacts to get cost estimates from our designs or an engineering company's design. If we have no other source of a cost estimate we use the Icarus Corporation estimation software.

We are developing this detailed information for a base case only. Therefore, we need to scale the equipment costs for other alternatives being evaluated. To do this we have made a MS Access database of the detailed size and cost information for each piece of equipment, see Table 4.

Table 4
MS Access Equipment Cost Database, Fields

SYS_KEY	Unique Identification Number, Used only to make records Unique
EQUIPMENT_NUM	Equipment Number, e.g., D-501, T-101, etc.
DESIGN_DATE	Date of Original Entry of Information
ASSOCIATED_PFD	Drawing Number Associated with the Piece of Equipment, e.g., PFD-P100-A201
EQUIPMENT_NAME	Descriptive Name of the Equipment
EQUIPMENT_DESCRIPTION	Short description of the equipment, size, type, etc.
EQUIPMENT_CATEGORY	Coded Field.
EQUIPMENT_TYPE	Coded Field.
NUM_REQUIRED	Number of duplicate pieces required.
NUM_SPARES	Number of Spares.
BASE_COST	Cost of the single unit.
COST_YEAR	Year the cost is referenced to.
COST_BASIS	Coded Field. Source of the cost information.
INSTALLATION_FACTOR	Multiplier on base cost to account for installation.
INSTALLATION_FACTOR_BASIS	Coded Field. Source of installation factor information.
SCALE_FACTOR_EXP	Exponent used in the standard scaling of the base cost field and the Base for scaling.
SCALE_FACTOR_BASIS	Coded Field. Source of scaling exponent information
BASE_FOR_SCALING	Flowrate of size that is used for scaling. Not necessarily the actual design basis used for sizing.
BASE_TYPE	Coded Field. Description of what the Base for Scaling is, e.g., flow, size, duty
BASE_UNITS	Units of the Base for Scaling
PROCESS_STREAM_FOR_SCALING	Actually the ASPEN variable name of the Base for Scaling, could be a stream or other variable.
OBSOLETE	Generally N for No.
NOTES	General notes about the sizing or costing.
UTILITY_TYPE	Coded Field. What types of utilities are used this piece of equipment.
UTILITY_STREAM	What ASPEN stream contains the utility information for this piece of equipment.
UTILITY_CALC	Coded Field. The method ASPEN uses for these utility calcuation
MATERIAL_CONST	Material of Construction used for costing.
MODIFY_DATE	Date it was last modified
MODIFY_UID	User that last modified the database record.
DOCUMENT	Linked Adobe Acrobat pdf file containing details of sizing and costing calculations and vendor quotes.

It is very important to note that the database contains information about scaling the costs. This information includes the scaling exponent for the equation below.

$$New\ Cost = Original\ Cost \left(\frac{New\ Size*}{Original\ Size*} \right)^{\exp}$$

* or characteristic linearly related to the size

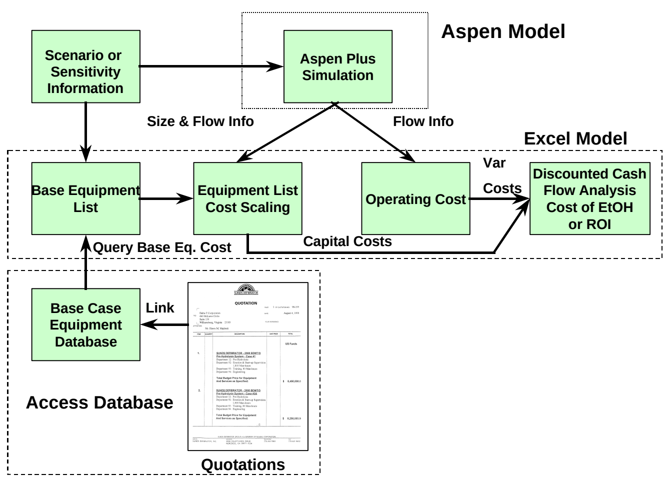
The database also contains an identification of the scaling item that will come from the ASPEN Plus simulation. This is not always the size of the unit, but could be the feedrate, or heat duty. The key is that what ever value is used to scale the cost that it be linearly related to the size. When the size must be used, it is generally calculated in a Fortran block in ASPEN Plus, so we can minimize the number of variables that are retrieved from ASPEN Plus.

In addition to all of the numeric field data contained in the cost database, we've also include a document of varying lengths (2 to 100 pages) that describes in complete detail the design and cost calculations that were preformed for that piece of equipment. If a vendor cost quotation exists, it is included. If the calculation was preformed in another software package, the results from that program are included. Everything we would ever need to understand the design and cost of that piece of equipment is stored there.

This database has been populated for the base-case. We expect that the research alternatives that we will be analyzing require only slight modifications to this list. Generally, most of the costs for the alternatives will be calculated by scaling the existing original equipment. For the special, new or significantly different uses, new designs and cost estimates are generated and stored in the database for that case.

III.1.3 Discounted Cash Flow Model – Putting it all together!

With the ASPEN Plus model and MS Access database in place we wrote a discounted cash flow rate of return (DCFROR) model in MS Excel. This MS Excel spreadsheet and its inputs are outlined in figure 3.



Complete Economic Analysis Model

Figure 3.

The DCFROR model uses inputs from the costs database for the base equipment costs. Material and energy flows and some equipment size information from the ASPEN Plus simulation are used to scale equipment costs and to determine the costs of feedstocks and other supplies for each alternative. Using the product flow from Aspen Plus the final cost of ethanol production per gallon can be calculated.

It is very important that we not have to design and cost all equipment for each alternative. By retrieving information from the cost database on the base cost, base variable (size, flow, etc.) and the base size (e.g., might be ft^2 if it is size or kg/hr if it is flow) the DCFROR model in MS Excel can scale the costs to the new process. As stated earlier, only when the base-equipment is inappropriate or quite dissimilar in size does an new specific equipment design and cost need to be completed and added to the database.

The information needed from Aspen Plus is accumulated in a sensitivity block where it can be sent to the MS Excel model via a paste link or using a Visual Basic interface to the Aspen Plus Summary File Toolkit, developed by M. Jarvis (1999) of Aspen Technology, Inc.

To better illustrate the process of "Putting it all together", Figure 4 shows a typical query of data from the MS Access database directly into the MS Excel spreadsheet. This is preformed on the process number (embedded in the PFD number). In this case the query would be Associated PFD like 'PFD-P100*'. If a new piece of equipment was added to the database for a particular alternative, it could be given its own equipment number or a modification of the number it is replacing (e.g., T-101a might replace T-101). Results of the query become an MS Excel look-up table to be used by the Equipment Cost Scaling sheet, also in MS Excel. Therefore old and new equipment can be queried from MS Access, but then not specified in the Equipment Cost Scaling sheet.

Extract Information from MS Access Database
Where PFD Like 'PFD-P100*'

ASSOCIATED PFD	EQUIP NUM	NUM REQ.	NUM SPAR E	NUM REQUIRED VAR	PROCESS ITEM FOR SCALING	BASE FOR SCALING	BASE COST	SCAL E EXP
PFD-P100-A30	A-300		0	INUMSSFA			19676	
PFD-P100-A30	A-301	1	0		STRM030	41777	12551	0.51
PFD-P100-A30	A-304	2	0		STRM030	41777	11700	0.51
PFD-P100-A30	A-305	2	0		STRM030	41777	10340	0.51
PFD-P100-A30	A-306	1	0		STRM050	381700	10100	0.51
PFD-P100-A30	H-302	3	0		AREA030	3765	25409	0.78
PFD-P100-A30	H-304	1	0		QSDF030	38339	3300	0.83

Figure 4.

Information from ASPEN Plus is then extracted from the Summary File (we use the input language, not the GUI for the large complete plant model) or the GUI. Figure 5 shows the information as it appears in the Aspen Look-Up table in MS Excel. Note, there are a mixture of values calculated from Fortran Blocks, heat work and material stream variables as well as unit operation block variables.

ASPEN Plus Simulation Information Transferred to Excel

Variable Names are in Alphabetical Order for Excel "Look-up" Table

Variable Name	Value	Units
AREA0302	3,700	
DIAMD501	3.89	METER
INUMSSFA	34	
NUMRCENT	3	
QRFD0502	986,470	CAL/SEC
QSDF0301	35,069	CAL/SEC
STRM0303	35,086	KG/HR
STRM0304	37,997	KG/HR
STRM0502	380,206	KG/HR
WRKWTOTL	-41,651	KW
Total Number of Items Retrieved: 154		

Calculated in FORTRAN in ASPEN

Unit Operation Variable

Heat Stream Duty

Material Stream Flow

Work Stream Power

Figure 5.

Once the information is on hand from the database and ASPEN Plus, we code the Equipment Cost Scaling sheet with the equipment number. From these inputs MS Excel will look-up the other necessary information from the ASPEN Plus Results page (look-up table) and the Equipment Cost Database Query Results Page (look-up table). Finally, the spreadsheet will determine the total equipment costs calculate the installed costs. We have another spreadsheet page that performs a similar operation for operating costs.

Finally, by specifying various financial information (held constant for all alternatives), the DCFROR calculation is preformed by MS Excel and the cost of ethanol is determined.

For each research alternative, the following steps are preformed, modify flowsheet, modify Aspen Plus model, execute Aspen Plus, retrieve Aspen information, retrieve cost DB information, and perform DCFROR calculation. Equipment cost modifications (other than scaling) are only necessary for new equipment.

IV. Example Analysis

For a typical review process we can have as many as 50 to 100 alternatives to access for each of 3 base-processes. This adds up to over 200 alternatives. In addition it is important to look at a high and low expectation of each possible research outcome, doubling again the number of alternatives.

To understand an illustrative example it is necessary to see the overall process flow. Figure 6 illustrates the overall process flow for producing ethanol from lignocellulosics via an enzyme based process. Feed is brought into the plant and stored, moved and sized (<u>Feed Handling</u>). From there it is conveyed to <u>Pretreatment</u> where it is treated with steam and dilute sulfuric acid to release the hemicellulosic sugars and prepare the cellulose for enzymatic hydrolysis. Before being processed further the hydrolyzate is neutralized and various toxic materials are removed in a <u>Conditioning</u> step. A portion of the hydrolyzate is used to grow cellulase enzymes in the <u>Enzyme Production</u>. These enzymes are then used in the <u>Simultaneous Saccarification and Fermentation</u> step where the remaining cellulose is converted to glucose by the enzymes just produced. As these sugars are produced they are immediately fermented to ethanol. The broth is then sent to <u>Product Recovery</u> where ethanol is recovered and the insoluble solids are separated from the sillage by centrifugation and soluble solids are concentrated by evaporation. The concentrated soluble solids and the insoluble solids are combusted to provide steam and power for the process in the <u>Burner/Boiler Turbogenerator</u>. Extra power is sold to the grid as available. Other areas are also included, such as Waste Water Treatment and Utilities (cooling water, chilled water, etc.), because process alternatives can impact these areas.

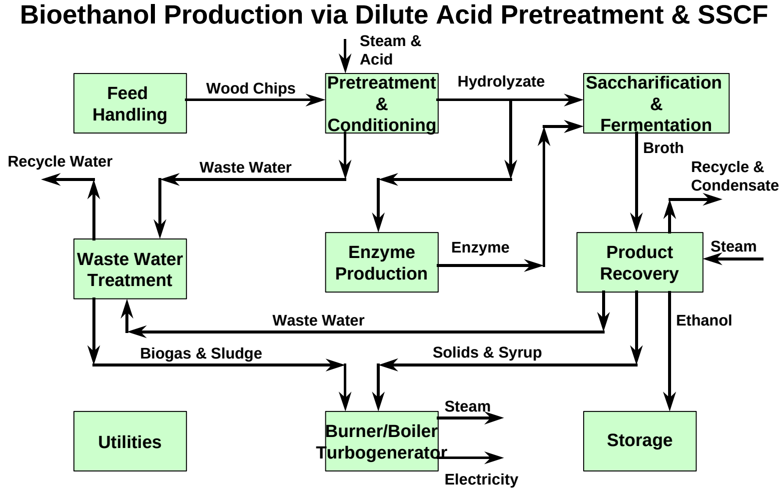


Figure 6.

As an example we look at several process alternative offered for the Pretreatment and Conditioning step and Enzyme Production. Table 6. Lists some example alternatives.

Table 5.

Example Process Alternatives

Process Area	Process Parameter
Pretreatment	Xylan to Xylose Conversion
Pretreatment	Solids Concentration in Feed
Pretreatment	Reactor Material of Constructi
Pretreatment	Acetic Acid Removal
Pretreatment	Sugar Recovery in IX
Enzyme Producti	Enzyme Loading
Enzyme Producti	Enzyme Productivity
Enzyme Producti	Sterilization

These alternatives were evaluated according to the procedure outlined above. The result is a set of incremental costs given in Figure 7.

Incremental Economic Impact of Research Alternatives

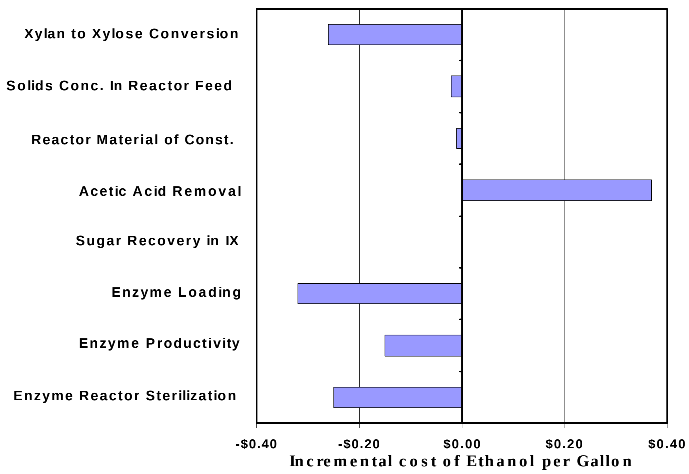


Figure 7.

The information provided in figure 7 clearly illustrates that some of these process alternatives are certainly worthy of further study, while others are inconsequential (solids concentration, sugar recovery and materials of construction) or even detrimental (removal of acetic acid)

V. Conclusion

We have illustrated a viable method for the rapid and rigorous evaluation of multiple process alternatives on a complete process cost analysis. The method makes use of an Aspen Plus simulation for the determination of the material and energy balance and some equipment sizing. Equipment design and costing is preformed once in a very rigorous fashion for a base-case. All information (numeric and anecdotal) generated during the base case equipment design and costing is stored for later retrieval in an MS Access database. The final cost calculations are then preformed in a MS Excel spreadsheet using a DCFROR type of calculation. Information from the Aspen Plus simulation is pulled into the spreadsheet via a Visual Basic interface to the Summary File Toolkit to form a look-up table of process information. The equipment cost information is queried out of the MS Access database directly into MS Excel to form a look-up table of process cost information. Equipment and operating scaling tables in MS Excel then look-up the necessary information from the process and cost tables and perform the DCFROR calculation. The result is a cost of ethanol that can be compared to other process alternatives.

This information is used at NREL to help evaluate the worth of funding or continuing to support research in the conversion of lignocellulosic biomass to ethanol.

VI. References

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