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A Review of Techno-Economic Modeling Methodology for a Wood-to-Ethanol Process

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ABSTRACT

Techno-economic modeling has been a valuable tool in directing and assessing the research and development efforts for biomass-to-ethanol processes. In developing a techno-economic model of a "generic" wood-to-ethanol process, we decided to follow a three-pronged design approach. This initially consisted of a detailed review of the current definition and technical maturity of the process, which concluded that the process remains complex and immature. More recently, we have critically assessed/compared two inherited models, and examined the historical and current trends in modeling design. We confirmed that process complexity and immaturity, in association with the capabilities of the available modeling tools and the ease with which they can be used, influenced the design and implementation of past models. We have discussed these influences with reference to our own model development decisions. For example, on review of two inherited techno-economic models, we decided that our new model would require a greater degree of flexibility in its structure and user interface.

Index Entries: Techno-economic modeling; biomass-to-ethanol process; lignocellulose-to-ethanol process; spreadsheet models; flowsheet simulators.

INTRODUCTION

Past techno-economic modeling work has been used for a variety of reasons. Although many groups have used this approach to estimate the likely cost of producing ethanol from various lignocellulosic substrates,

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past models have tended to be most useful in establishing the level of maturity of each of the component steps. For example, we have used our past techno-economic model *(1)* to assess various biomass-to-ethanol options, and found that the front-end (pretreatment, fractionation, enzymatic hydrolysis) steps were both technically immature and represented a large component of the total product cost. Consequently, our more recent work has looked at various process options (SO_2 pretreatment, alkali and peroxide-enhanced fractionation, and enzyme recycle hydrolysis) in an attempt to provide a more defined overall process and reduce the proportion of the total product costs attributed to the front-end steps. We have previously described both the technical results of our recent research efforts and our current process development philosophy *(2–4)*. These process options along with our previous modeling experience suggested that modification or development of a new model must address the need for greater flexibility, ease of development, or modification and ease of use.

HISTORICAL BIOMASS-TO-ETHANOL MODELING

Process modeling of the biomass-to-ethanol process has been ongoing since the early 1980s, with most earlier efforts *(5,6)* concentrating on the enzymatic hydrolysis portion of the process and with the overall economics based on the price of producing glucose. At this time, most computationally intensive tasks, such as techno-economic modeling, were restricted to large, expensive mainframe computers. Microcomputers were only beginning to enter the market, and the process modeling tools were restricted to high-level programming languages and procedural structuring. This often meant that this type of modeling was viewed as being too complex and expensive. Spreadsheets were severely limited in their computational and storage capabilities, and flowsheet simulators were not yet available. At this time, modeling efforts did not simulate the entire process. Consequently, they did not imitate the complex interrelated nature of the biomass-to-ethanol process steps, or provide the means to determine the influence of both the individual and combined process steps on the production cost of ethanol. Thus, these models effectively represented the mathematical equivalent of a nonintegrated physical model, such as a lab-scale process development unit (PDU) or a small pilot plant.

Integrated biomass-to-ethanol process models *(7,8)* began to appear around the mid-1980s, and continued, along with most engineering and computationally intensive applications, to utilize high-level programming languages and procedural structuring for their development. The graphical user interface and object-oriented programming concepts were only beginning to influence the microcomputer market for personal and business applications. Although the complexity of the biomass-to-ethanol process had always been recognized, it was only with the development of integrated models that the relative importance of the various process steps

or parameters and the influence of byproduct production could be readily determined through sensitivity or parametric analysis. These models represented the mathematical equivalent of an integrated physical model, such as a development- or commercial-scale plant, and they provided, for example, scale-up influences on both the technology and economics of the overall process being evaluated. Although linear programming *(9)* was also attempted, it was found to be an inappropriate modeling method, since much of the bioconversion process is not linear, thus requiring linear approximations and the determination of a large number of coefficients that may be difficult to measure or estimate. A representative example of the models that were developed over this period is the SERI-Chem Systems-Lawrence Berkeley Laboratories Study *(7)*. This model used a modular structure, was written in a high-level programming language (APL), and accessed the ICARUS equipment capital cost data base. It was based on an aspen feedstock and contained the following subprocesses: steam-exploded pretreatment, fed-batch enzyme production using RUT C30 strain of *Trichoderma viride*, separate enzyme hydrolysis and fermentation, and vapor reuse (benzene) distillation. An enzyme recycle option using the Lawrence Berkeley Laboratories countercurrent adsorption research was also included. Although the simulation program modeled the back end of the process (fermentation, distillation, waste treatment, and heat generation), there was little detail provided. It was also proposed by researchers, and later shown by these models, that the immaturity of the process front end (pretreatment, enzyme production, and hydrolysis) resulted in a major contribution of this component to the overall cost of producing ethanol. A comprehensive kinetic model to describe cellulose conversion for various pretreatments, feedstocks, and hydrolysis conditions was not available, and consequently, the parametric analysis did not account for these interactions.

Spreadsheet modeling *(10,11)* began to appear around the end of the 1980s. Microcomputers and spreadsheet software had become well established in the personal and business markets. The middle to late 1980s was a time period in which there were tremendous growth and development of both the hardware and software capabilities of microcomputers. Models and other computationally intensive applications that had previously required the computational and storage capabilities of a larger computer were now being developed or ported to these smaller stand-alone microcomputers. Spreadsheets became popular as a way to develop the calculational relationships rapidly between process variables, via cell addressing or cell naming conventions, without having to learn a programming language. Model development using spreadsheet software acquired many capabilities that previously had to be programmed, such as the ability to format and generate reports and/or charts, the ability to read, illustrate, and write the contents of storage files, and in a small way, internal error checking and debugging by showing intermediate results. The modeling also acquired

capabilities that were unique to spreadsheets, such as the easy incorporation of supplied spreadsheet functions (interest calculations, look-up tables, random number generators, and so forth), the ability to do sensitivity analysis rapidly by changing the value of one cell or variable and noting the change in the final ethanol price, development of simple flat-file data bases, and the ability to automate common tasks through the development of small programs using macro languages. The IOGEN study *(11)* is representative of the type of modeling carried out at this time. The model was built using Lotus 1-2-3 spreadsheet software and based on an aspen feedstock. Residual solids from the process were assumed to supply all the energy requirements for the plan, and surplus electricity was projected to be sold: Very high enzyme production yields from lactose were also assumed.

Although flowsheet simulators were available in the mid-1980s, they were only generally accepted as a means to model processes or unit operations, and were used on a regular basis by process and research engineers in the latter part of the 1980s and early 1990s. Flowsheet simulators, like spreadsheets, provided the user with commands to format and generate reports, plus read, illustrate, and write the contents of storage files. However, unlike spreadsheets, they were somewhat limited in their capability to produce charts. They utilized a graphical interface and ready-made unit processes and data bases/estimation routines for estimating flowstream component properties to build a model. However, because of their computationally intensive nature, flowsheet simulators often required long periods of time to provide modeling results. The latter feature often makes flowsheet simulators an inappropriate application for sensitivity analyses or Monte Carlo simulations. This type of software, owing in large part to its size and computational requirements, was at this time restricted to mainframe or minicomputers. The hardware constraint along with the cost of the software, lack of economics modeling, and steep learning curve (generally associated with the requirement to learn which of many options to select for the determination of thermodynamic and other chemical properties) tended to limit the use of flowsheet simulators for techno-economic modeling. Furthermore, the commercially available-simulators were developed primarily for the design and evaluation of physicochemical processes, and as a result, did not provide ready-made unit operations for biological processes or readily characterize biologically derived materials. Users were forced to develop modules in a high-level programming language for the biological processes, which were subsequently linked to the flowsheet simulator kernel and users were also forced to assign properties directly to the biologically derived materials. Even with these constraints, flowsheet simulators were primarily used for techno-economic modeling during this time.

Techno-economic modeling since the late 1980s has been carried out by a few groups using object-oriented high-level languages to build whole applications that include some of the features of flowsheet simulators *(12)*. However, most modeling has used flowsheet simulators *(13,14)* or

enhanced spreadsheets *(1,15)*. There has generally been a convergence of features within these three previously distinct modeling methods, primarily as a result of the proliferation of graphical user interfaces in microcomputers. The graphical user interface has spawned the use of graphical controls and dialog boxes, object-oriented programming, and dynamic linkage of applications and their files.

Object-oriented high-level languages, such as C++ and Visual Basic, have become popular over the period since the late 1980s primarily as a result of their recognized productivity gain for developing graphical user interfaces. At least one research group *(12)* interface and modular structuring similar to flowsheet simulators. However, it also includes economic evaluation, sensitivity, and Monte Carlo simulation features. Furthermore, because it is strictly limited to the biomass-to-ethanol processes, the training time should be significantly shorter than an equivalent commercial flowsheet simulator.

Flowsheet simulators since the late 1980s, as mentioned previously, have become a valuable design and assessment tool for process engineers. With the growing computational and storage capabilities of microcomputers, many of the previously developed commercially available simulators have been ported to the desktop. It has also been recognized by the developers that simpler, less-full-featured programs can reduce the training time and also the computer hardware demands. Some of the developers are also beginning to recognize the need for economic analysis modules, modules that model biological unit operations, and data base/calculational routines that estimate biological material properties. The basic principles associated with flowsheet simulators are generally recognized as being good for the rapid development of process scenarios, in that the user only has to select the required unit operations and specify the values for the required number of variables to define the solution fully. However, the current flowsheet simulators are not capable of providing a user who is both knowledgeable in modeling this particular type of process and reasonably computer-literate with the ability to produce lignocellulosic-to-ethanol process scenarios easily and assess their economic feasibility. An example of a flowsheet simulation over this time period is the University of Lund Study *(14)*, which compared three wood-to-ethanol processes (concentrated hydrochloric acid process [CHAP]; Canada, America, Sweden hydrolysis [CASH], a two-step weak acid hydrolysis; and an enzymatic process using a dilute sulfur dioxide pretreatment). The modeling was done using ASPEN PLUS (Aspen Tech Inc., Cambridge, MA), a commercial flowsheeting program that is normally used for thermochemical process design. All three processes used pine as a feedstock and were based on the same plant capacity. The main product was 95% ethanol (w/v) with the residual solids and methane used to produce process steam while the carbon dioxide was sold on the open market.

Since the late 1980s spreadsheets have become more graphically oriented with the incorporation of more drawing capabilities. For example,

three-dimensional spreadsheet capabilities can be accessed through tabbing of worksheets within a workbook; the inclusion of graphical controls (including buttons, check boxes, menus, drop-down list menuing, scroll bars, spinners, and dialog boxes) is possible, and more sophisticated macro languages or full programming languages that allow the development of graphical user interfaces similar to those in flowsheet simulators can be used. Spreadsheets have also become more flexible in that they now have the ability to link dynamically to various other entities (i.e., objects, dialogs, worksheets, workbooks, and applications). Two spreadsheet models (the Virginia Polytechnical Institute [VPI] Study *(15)* and the Forintek Study *(16)*) representative of this time period were inherited by our research group.

Although there have been a number of techno-economic models built over the last 10 years for a hardwood-to-ethanol process, most of the details associated with their calculational logic have not been published or made publicly available. This is not altogether unreasonable, since they require a considerable amount of time to develop and would require a sizable document to describe their logic fully. Furthermore, it is difficult to assess the effect of changes in one particular portion of the whole process without building a complete process model, because the individual subprocesses are strongly interdependent and the measure of progress in the development of the process is the production price of the final product. Consequently, it was recognized that although a full model would be required to provide a reasonable assessment of new developments in any of the subprocesses, the amount of time required to develop a completely new model would be substantial. Fortunately, we recently acquired the complete description of the two hardwood modeling efforts mentioned previously, a model of the whole hardwood-to-ethanol process from Forintek Canada completed in 1991 and a model of the steam pretreatment and fractionation subprocesses from VPI completed in 1994. Through a process of integration and refinement of these two models (discussed in more detail below), the time and effort required to build a complete hardwood-to-ethanol model were shortened. However, it must be recognized that these past models did not, for the most part, reflect the results of research completed since the early 1990s. Therefore, some new subprocess modules based on more recent data, particularly in the pretreatment and hydrolysis areas, had to be developed.

ASSESSMENT AND MODIFICATION OF INHERITED MODELS

Model Structure

The biomass-to-ethanol process, with its multiple components and processing steps, is complex. Furthermore, most of the front-end components of the process have not been tested in an integrated large-scale facility. A model of this process should therefore be capable of easily including

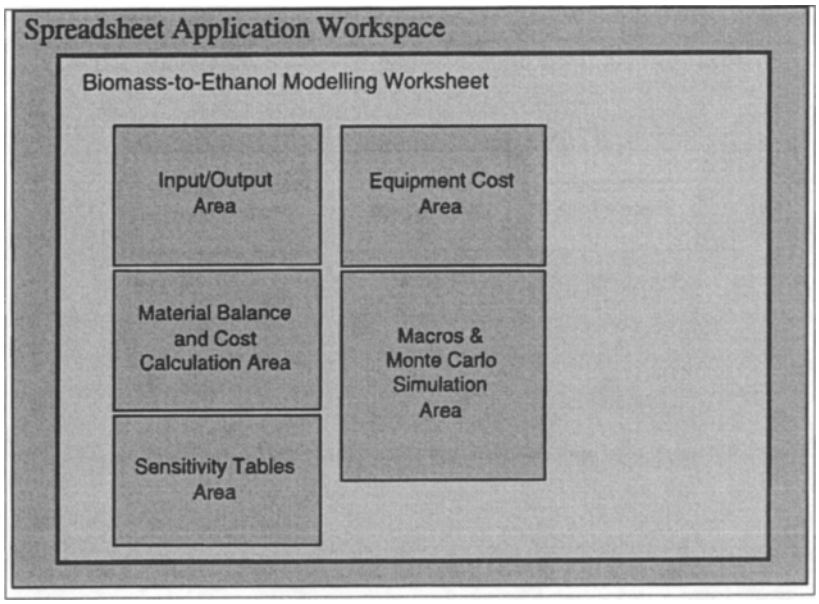

Fig. 1. Forintek model structure.

and evaluating a number of process and equipment options. Two structural concepts, modularization and encapsulation (discussed in more detail below), have been shown to enhance both software development in general and the ability to build on past techno-economic modeling efforts. The incorporation of these structural concepts should provide the framework for a flexible and long-lived model.

Modularization

A review of the Forintek model indicated that it was organized on the type of activity that was carried out (Fig. 1), i.e., Input/Output, Material Balance Calculation, Energy Balance Calculation, Capital Cost Estimation, Operating Cost Estimation, Sensitivity Analysis, and Monte Carlo Simulation. As a result, the subprocess input/output and calculational routines were intertwined. This structure did not allow the user to change the process or the process options rapidly, since the calculations for each process step were spatially dispersed over the spreadsheet area.

The VPI model was organized into modules (Fig. 2) that represented subprocess or unit operational options. This structuring allowed more rapid changes to the process by the modeler than was provided by the Forintek model, since the calculations for each subprocess or unit operation were located in the same general area on the spreadsheet. The modules appear to have been developed in one spreadsheet, and then the appropriate subprocesses for a particular process scenario were copied to another spreadsheet and linked. Although this structure is superior to the

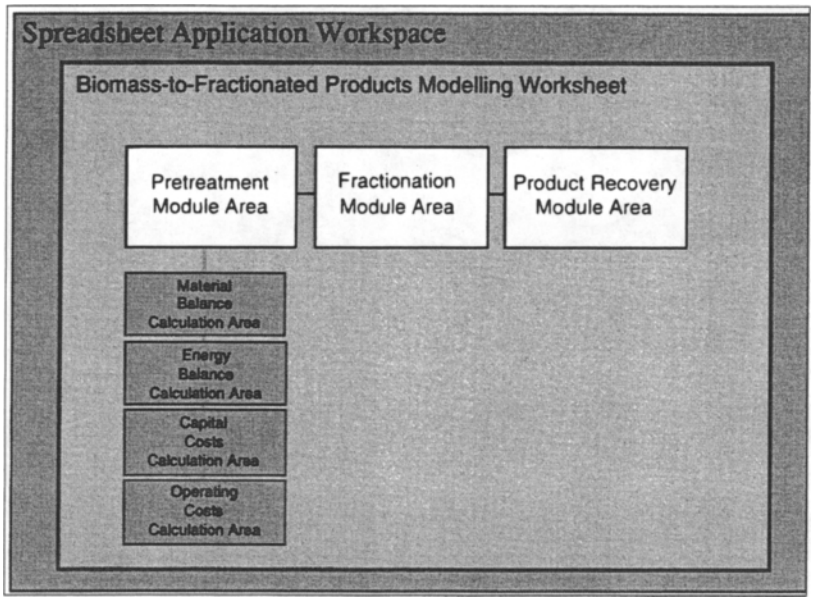

Fig. 2. Virginia Polytechnical Institute model structure.

Forintek model, it still lacks the potential for rapid process modification found in a flowsheet simulator-type of structure.

The latest version (5.0) of Microsoft Excel (used for the current STeam Explosion Assessment Model [STEAM]) provides the means to develop easily a modular structure that represents various subprocesses and types of calculations within each subprocess (Fig. 3). Each of the files is now referred to as a "workbook," since each layer of the three-dimensional file is now called a "worksheet" and can be accessed through a graphical tabbing system analogous to a physical filing cabinet or card file. The graphical structuring allows the designer to separate the various calculational or storage requirements easily, for a particular subprocess, into separate graphical layers. As in previous three-dimensional spreadsheets, the "worksheets" within the "workbooks" can be linked either through worksheet-row-cell referencing or through cell naming.

A further modular structuring feature of Excel is the ability to link various workbooks. This provides the developer with the ability to link the various subprocesses into a complete process scenario. Linkages can be fixed through methods, such as worksheet-row-cell referencing or worksheet-cell naming conventions. Alternatively, they can be more flexible and dynamic, through development of an "executive workbook" and/or an executive program. Consequently, there is a substantial level of flexibility now available to the model developer for designing and implementing a structure that is modularized, and reflects a structure similar to flowsheet simulators or previous high-level language models.

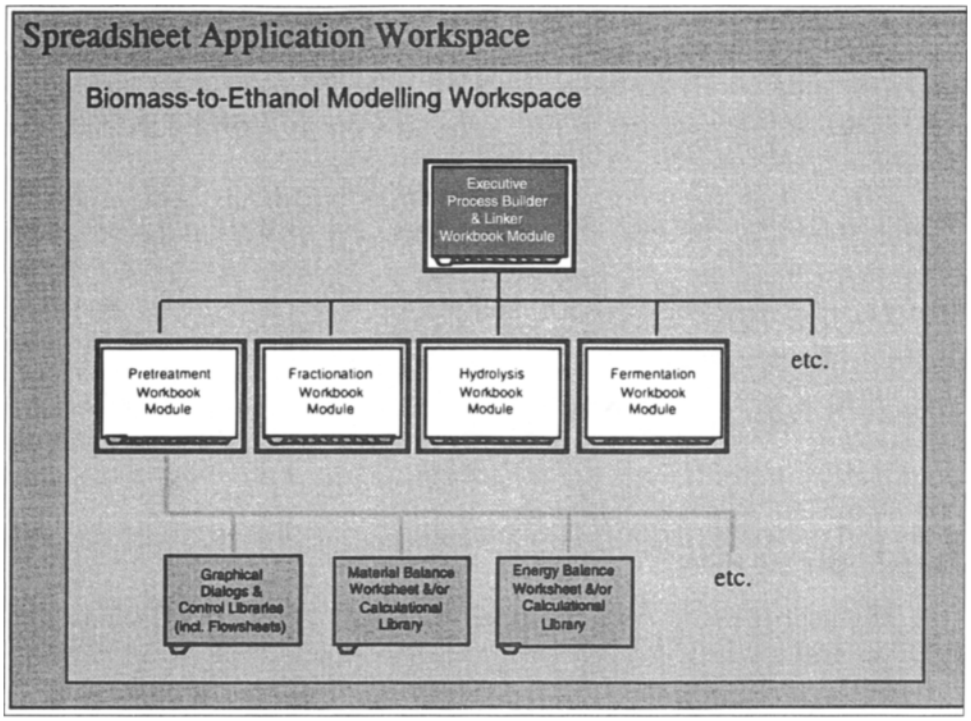

Fig. 3. Forest Products Biotechnology STEAM model structure.

Object-Oriented Encapsulation (Flowsheet, Input/Output, Calculation)

Encapsulation is a term used in computing science to refer to the capability of combining routines that operate on a data structure together with the data structure itself. Spreadsheets such as those used for the Forintek and VPI models incorporate this concept by keeping together the data (cell values), data structure (array represented visually by the row-column addresses), and the routines that operate on the data structure (cell formulae). However, spreadsheets at the time that the Forintek and VPI models were built did not include the encapsulation of the flowsheet that was used to develop or design the overall data or process structure. Object-oriented programming (OOP), which has become popular since the introduction of graphical user interfaces for microcomputers, incorporates and extends the encapsulation concept through including both the calculational routines that operate on a data structure and methods or routines that draw a graphical representation of the object for the user. This extra graphical abstraction allows the user to manipulate the relationships between data structures more easily and/or to create rapidly new objects that inherit the characteristics of the parent. Flowsheet simulators, e.g., ASPEN Plus, are an example of a type of program that uses the extended graphical characteristics of OOP programming for the user interface. Flowsheet simulators

map a graphical representation of process objects (subprocesses and/or unit operations) and process interrelationships (flowstream) to the associated data structures and routines (calculational and graphical). This graphical flowsheeting feature is often recognized as being a key to the popularity and flexibility of flowsheet simulators.

Through the use of current spreadsheets, such as Excel, with its graphical objects (controls, dialogs, toolbars, and menus) and a programming language (Visual Basic), it is now possible to include the flowsheet, input/output, and calculational relationships of the various subprocesses and unit operations within a spreadsheet format. The graphical objects can now be mapped directly to the data structures and calculational routines associated with the subprocess and/or unit operations. This allows for rapid manipulation of the relationships between these operations, and the potential for graphical vs manual linkage of the subprocesses and unit operations to create new scenarios.

Model User Interface

The user interface, in this study, refers to both the interface used to develop and evaluate various process scenarios, as well as the interface for editing the input variables, calculational routines and accessing, or reporting the output variables. To develop techno-economic models, the first step is generally the development of a series of flowsheets for the overall process and for each of the process steps. This flowsheeting process, as mentioned previously, is an integral part of flowsheet simulators, and this feature is often recognized as being a key to their popularity and flexibility.

The model user interface of the two inherited models was essentially a standard spreadsheet interface (Fig. 4) with the user entering the values and formulae for the various variables via the formulae entry bar in spreadsheet row/column format. Both models did not include a specific error checking routine or formulae security. However, there was a slight difference in the overall interface of the two models. The Forintek designers expected the user or developer to find the appropriate areas for input/output and modification of the existing calculational routines, whereas the VPI model provided, through a structuring that emphasized process steps rather than calculational types, an easier environment to modify.

In both the inherited models, the user was forced to refer to process flowsheets that were not part of the modeling application in order to understand the process details, e.g., flowstream numbering. The process flowsheets were either hand-drawn (Forintek model) or computer-drawn (VPI model) in another computer application.

Current spreadsheet capabilities now allow the model developer to include features previously found only in flowsheet simulator user interfaces. Within the STEAM model, each process/subprocess is built from

Forintek Model

	A	B	C	D	E	F	G	H	I	J	K
1	Input	500	OD tonnes aspen/day			(Range= 100 to 1000 OD tonnes/day)					
2											
3	Output	5.5E+07	L ethanol/year		Total capital cost		5.3E+07	dollars			
4		158504	L ethanol/day				0.97677	$/L			
5		317.008	L ethanol/OD tonne wood			PEtOH =	0.86717	TOTOC =			
6											
7		PROCESS PARAMETERS									
8											
9	Feedstock Handling	Wood	20833.3	Throughput of wood chips, dry kg/hr							
10	Steam Pretreatment	MC	50	Moisture content of wood chips, wt% (wet basis)							
11	Steam Pretreatment	WD	433	Density of wood, kg/m3							
12	Steam Pretreatment	BDW	112	Bulk density of wood chips, kg/m3 of reactor volume							
13	Steam Pretreatment	TEMP	240	Temperature of high pressure steam, deg C							
14	Steam Pretreatment	TWOOD	20	Temperature of input wood chips, deg C							
15	Steam Pretreatment	SHW	0.5	Specific heat of wood, cal/g.deg C							
16		MCLCI	0.4	Moisture content of wet lignin cake, wt fraction							
17	Enzyme Production	cEP	0.1	Substrate consistency in enzyme production fermentors, w/v fraction							
18	Enzymatic Hydrolysis	cCH	0.1	Substrate consistency in cellulose hydrolysis fermentors, w/v fraction							
19	Pentose Fermentation	cXH	0.1	Dissolved solid concentration in xylose-to-ethanol fermentors, w/v fraction							
20	Fractionation - Water Wash	cSX	0.08	Dissolved solid concentration in hemicellulose extract, w/v fraction							
21	Fractionation - Alkali Wash	cLX	0.04	Lignin concentration in lignin extract, w/v fraction							
22	Fractionation - Alkali Wash	cNaOH	0.004	Concentration of NaOH in caustic solution feed to lignin extractors, w/v fraction							
23	Enzymatic Hydrolysis	eCL	12.5601	Cellulase loading in cellulose hydrolysis fermentors, FPU/g substrate							
24	Pentose Fermentation	eXL	0	Xylanase loading in xylan hydrolysis fermentors, IU/g substrate							
25	Fractionation - Alkali Wash	fNaOHr	0	Caustic recovery, fraction of NaOH input							
26	Fractionation - Water Wash	fC5WS	0.75	Fermentable sugars in water solubles, wt fraction of total dissolved solids							
27	Fractionation - Alkali Wash	fRH	0.888	Fraction of caustic insolubles (SEW-WIA) digested in cellulose hydrolysis fermentors							
28											
29											

Fig. 4. Spreadsheet input/output interface of Forintek model.

graphical objects representing the various unit processes/major pieces of equipment and their associated flowstreams. Both the graphical elements representing the unit processes/pieces of equipment and the flowstreams have associated properties that are now accessed through input/output dialog boxes (Fig. 5). In this case, the chemical, physical, process-related and economic attributes of the feedstock flowstream are shown. Each graphical object is linked to the next lower level of detail through simply "clicking" with the mouse on the graphical representation or icon of the object. For example, "clicking on" the pretreatment subprocess icon in the current process (Fig. 6) will expose or bring up the pretreatment subprocess flowsheet (Fig. 7). Each unit process/piece of equipment within a subprocess has associated properties, including calculational routines. For example, details for the steam reactor (object with steam shown entering) contained within the steam-pretreatment subprocess (Fig. 7), can be accessed through clicking on the icon of the reactor. This brings up the equipment option dialogs (Fig. 8) with the currently calculated values for the balances (material and energy) and cost estimations (operating and capital) for this particular piece of equipment. This dialog also provides access to the programming modules associated with the various calculations (Fig. 9) through clicking on the appropriate button within the Calculation Libraries area of the dialog.

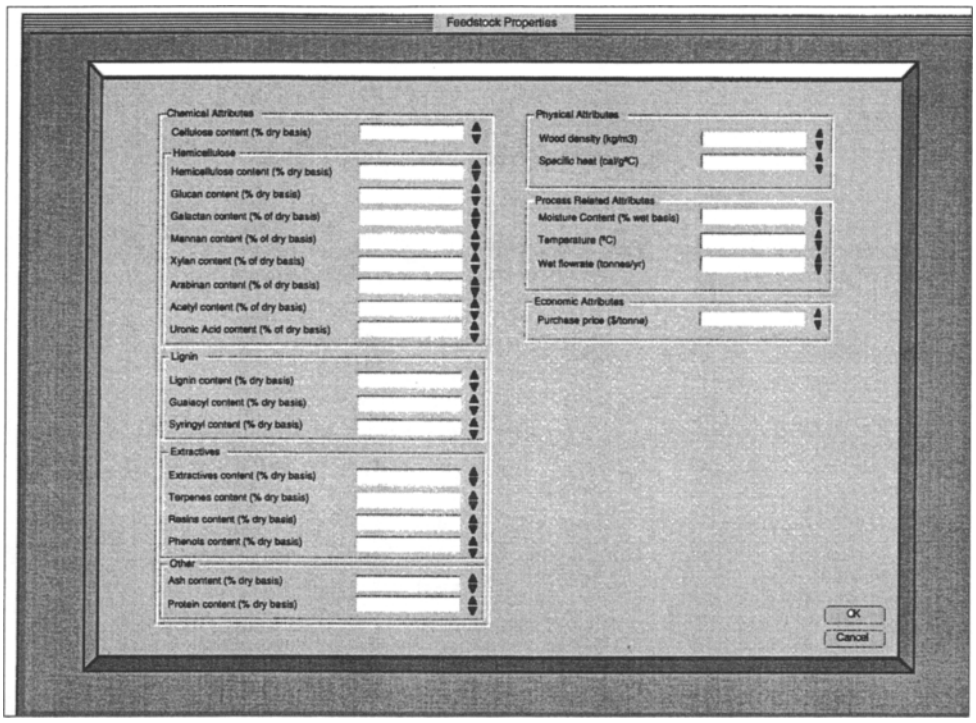

Fig. 5. An example of an input/output dialog box from the STEAM model.

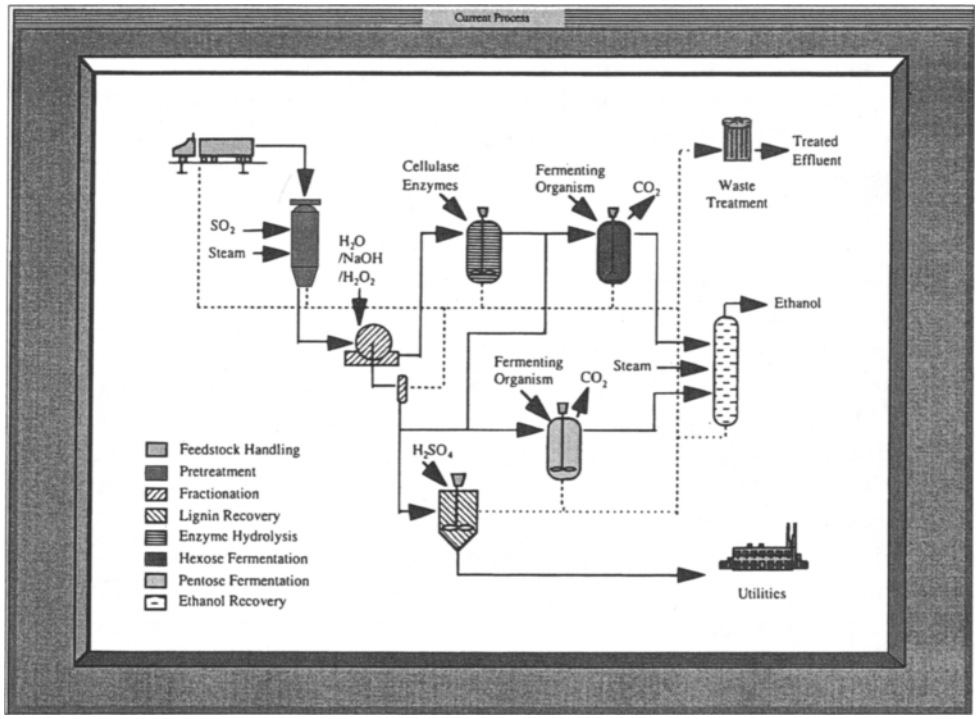

Fig. 6. STEAM model generic wood-to-ethanol process flowsheet.

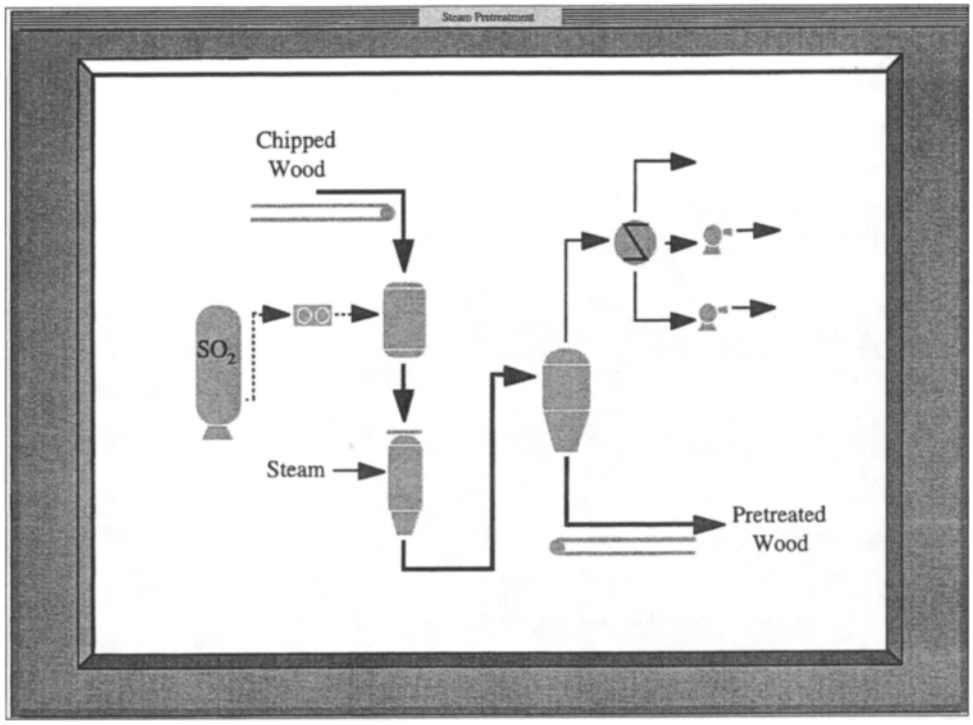

Fig. 7. STEAM model pretreatment subprocess flowsheet.

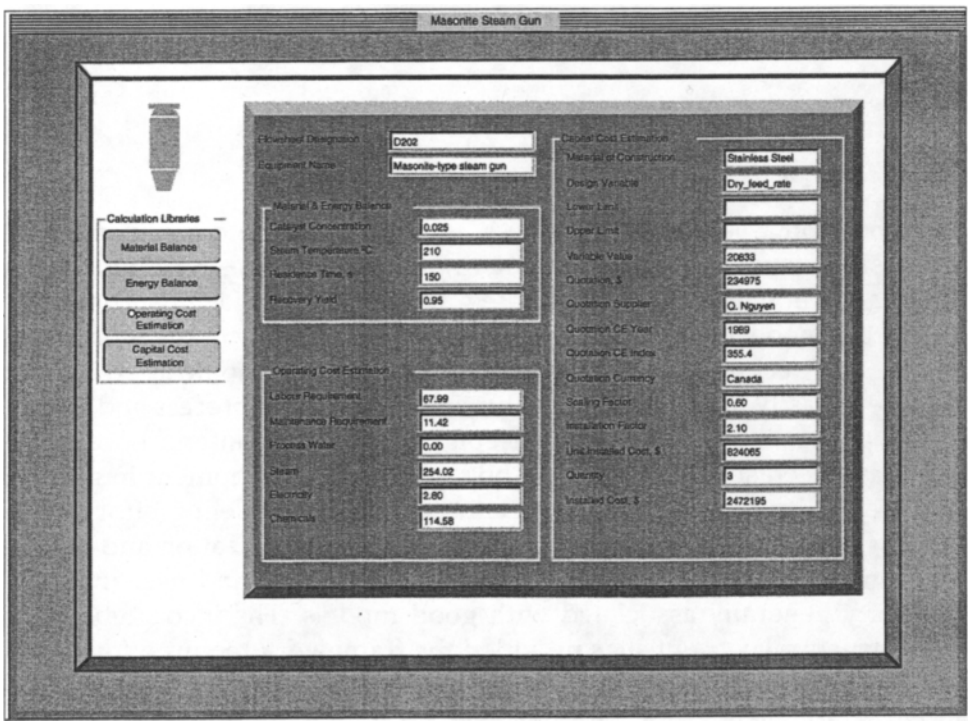

Fig. 8. STEAM model equipment option and calculational routine access.

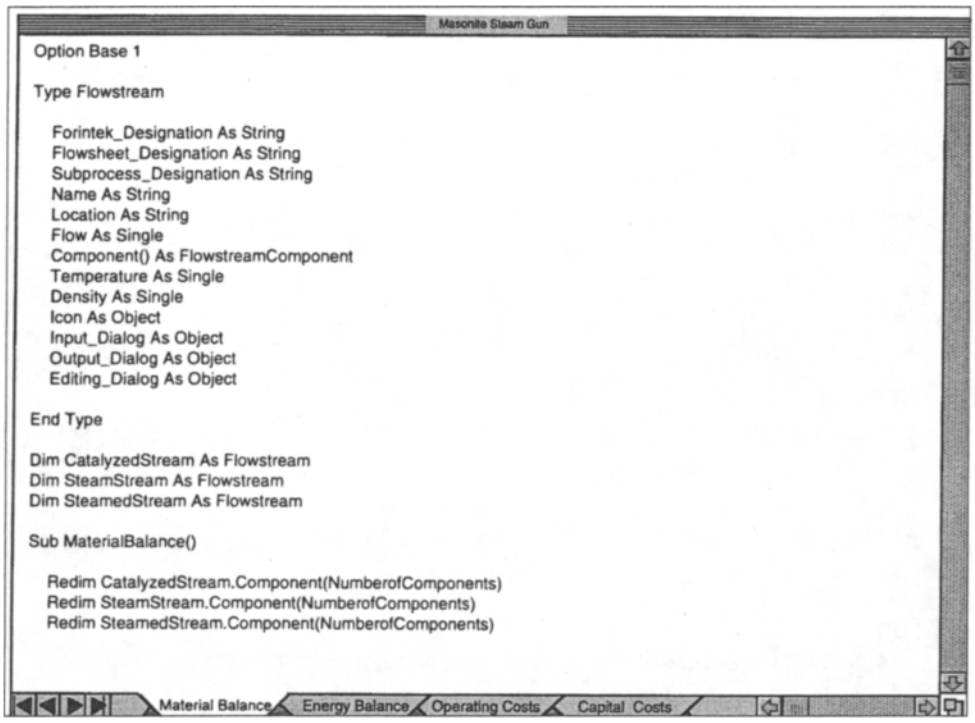

Fig. 9. An example of a STEAM model calculational routine.

CONCLUSIONS

The biomass-to-ethanol process, with its multiple components and processing steps, is complex. Furthermore, most of the front end of the process has not been tested in an integrated large-scale facility. The structure of the model dictates to a large extent the flexibility of the model as a whole. Any techno-economic model of this process should therefore be capable of easily including and evaluating a number of process and equipment options. Two structural concepts, modularization and encapsulation, have been shown to enhance both software development in general and the ability to build on past techno-economic modeling efforts. The STEAM model structure includes elements of modularization and encapsulation to ensure the adequate calculational routine and user interface flexibility generally associated with good models. The incorporation of these structural concepts has provided the framework required for a flexible and long-lived model that currently forms the basis for regular interaction among the International Energy Agency (IEA) network on bioconversion.

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