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Integration of Feedstock Assembly System and Cellulosic Ethanol Conversion Models to Analyze Bioenergy System Performance

Multidisciplinary Analysis and Optimization

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Research barriers continue to exist in all phases of the emerging cellulosic ethanol biorefining industry. These barriers include the development of sustainable and abundant biomass feedstock, the assembly of viable assembly systems formatting the feedstock and moving it from the field (e.g., the forest) to the biorefinery, and improving conversion technologies. Each of these phases of cellulosic ethanol production are fundamentally connected, but computational tools used to support and inform analysis within each phase remain largely disparate. This paper discusses the integration of a feedstock assembly system modeling toolkit and an Aspen Plus® conversion process model. Many important biomass feedstock characteristics, such as composition, moisture, particle size and distribution, ash content, etc. are most effectively managed within the assembly system, but generally come at an economic cost. The integration of the assembly system and the conversion process modeling tools will facilitate a seamless investigation of the assembly system conversion process interface. Through the integrated framework, the user can design the assembly system for a particular biorefinery by specifying location, feedstock, equipment, and unit operation specifications. The assembly system modeling toolkit then provides economic valuation, and detailed biomass feedstock composition and formatting information. This data is seamlessly and dynamically used to run the Aspen Plus® conversion process model. The model can then be used to investigate the design of systems for cellulosic ethanol production from field to final product.

I. Introduction

Cellulosic biomass conversion processes are receiving increasing interest as a candidate technology for the production of ethanol. The biomass feedstock assembly system plays a critical role in establishing the fundamental attributes of biomass delivered to the biorefinery. These attributes include a number of characteristics that impact the operational requirements of the ethanol conversion process such as particle size, density, and moisture content. Due to its variable nature, biomass is generally a difficult material to work with, and large-scale implementation of biomass conversion process technologies is dependent on the development of systems robust enough to handle this variability in an economical manner.

One of the largest challenges facing the biorefinery industry is managing the logistics of the unit operations within the feedstock assembly system, which includes biomass production, harvest and collection, storage and

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queuing, preprocessing, and transportation and handling. Previous analyses have found that these operations can account for as much as 40 – 60% of the total ethanol production cost.[1] Making the production of cellulosic ethanol viable and profitable to biomass producers requires the unit operations within the assembly system to be less than 30% of the total ethanol production cost.[2]

The challenges of reaching these goals lie in improving current technologies for gathering and processing biomass and improving the logistics of how the biomass feedstock is transported and stored. The feedstock assembly system model toolkit addresses these challenges through enabling investigation of various equipment and configurations to attain these goals. The feedstock assembly system model is an economic model that encompasses the operations from biomass production through delivery to the biorefinery. The conversion model performs the analysis of converting the biomass feedstock to ethanol and provides an economical analysis of the process. The overall cost of taking the biomass from the field through the ethanol conversion process is dependent upon the efficiency with which these resources can be gathered, formatted, delivered, and converted.

While the feedstock assembly system model toolkit performs a cost assessment of the operations involved in getting the biomass to the biorefinery in a usable format, it does not include the cost analysis for the conversion process. Biomass properties and formatting information obtained from the feedstock assembly system analysis are necessary to complete the conversion process simulation and cost analysis, but due to the disparate nature of the models, data usually does not seamlessly and dynamically pass between the models. The ability to investigate the unit operations and their impact on the entire system requires a robust framework that facilitates the integration of the feedstock assembly system model and process simulation model. Through an integrated framework, users can design specific biorefineries based on location, feedstock, equipment, and unit operation specifications. This paper discusses the development and implementation of the framework necessary to perform this integration, as well as coupling the models within the framework to perform economical cost analyses for user-specified design scenarios.

II. Background and Model Integration

As the largest source of renewable energy every year since 2000, biomass has become one of the nation's most important energy sources. Biomass provides the only renewable resource alternative to liquid transportation fuels.[3] The 30 x 30 goal established by the U.S. Department of Energy states that 30% of the gasoline consumption in 2004 can be replaced by biomass resources converted to transportation fuels by the year 2030.[4] Reaching this goal will require 60 billion gallons of ethanol to be generated, which equates to approximately 600 to 700 million dry matter tons of biomass annually.[4] The Billion Ton Vision study validates the possibility of achieving the 30 x 30 goal by identifying more than 1.3 billion tons of available biomass resource available on an annual basis for energy production.[5]

A. Feedstock Assembly System Model Toolkit

As noted earlier, the feedstock assembly system model represents all the operations necessary to move the biomass from standing in the field or forest to the reactor throat of the ethanol conversion process. The feedstock assembly system is responsible for formatting and preparing the biomass to meet the requirements and constraints necessary for the conversion process to operate at an efficient level as well as handling the logistics of transportation and storage of the biomass. The characteristics of biomass feedstocks under consideration vary widely, which impacts the performance of each unit operation within the feedstock assembly system. Much effort has been put into developing unit operation models within the feedstock assembly system to perform cost and performance analyses for each process.

The feedstock assembly system can be broken down into five unit operations:

- *Biomass production* represents the beginning of the feedstock assembly system and involves biomass crop selection, land use, and the agronomic practices that influence biomass yield, harvest, and collection operations.[6]
- *Harvest and collection operations* handle the cutting and gathering of the biomass in a sustainable manner as well as densification operations such as baling or bundling to better assist the handling, storage, and transportation of the biomass.[6]
- *Storage and queuing* encompasses the operations necessary to store the biomass until it is needed by the biorefinery. These operations must also address uncertainties that arise from seasonal harvest times and year-to-year yield variation.[6]
- *Preprocessing operations* change the format of the biomass to improve the feedstock properties before insertion into the conversion process. Improving the feedstock's physical characteristics such as density,

moisture level, and flowability allows for improved handling and higher efficiencies in the conversion process.[6]

- *Transportation and handling* occur throughout the feedstock assembly system, and thus the logistics for transporting and handling the biomass are tightly coupled to the other operations throughout the feedstock assembly system.[6]

The feedstock assembly system model toolkit (see Figure 1) captures and aggregates the economic impact of unit operations, providing an opportunity to explore various scenarios to improve logistics and deliver an ideal feedstock format for the conversion process that is cost-effective. The feedstock assembly system model toolkit used in this work was developed in Microsoft Excel™.

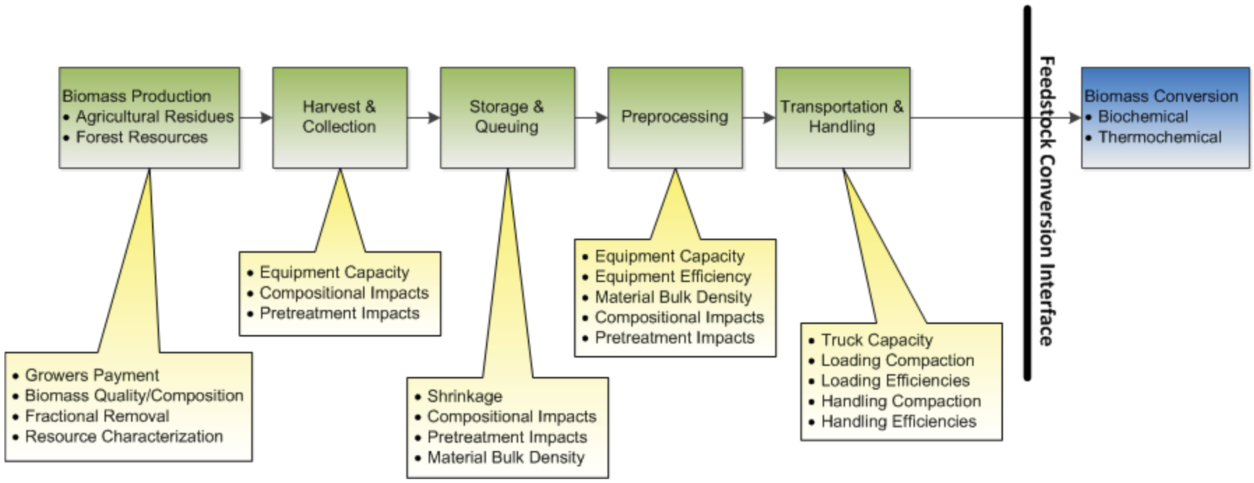

Figure 1. Supply system unit operations with parameters that drive cost

B. Conversion Process Models

Biomass conversion processes can be used to convert fractions of biomass into liquid transportation fuels. Two processes currently available to convert biomass into ethanol are biochemical and thermochemical conversion. Biochemical conversion utilizes enzymes or acid to break down the lignocellulosic biomass product intermediates such as fermentable sugars, which can then fermented to alcohols such as ethanol.[8] Thermochemical conversion technologies include processes such as gasification and pyrolysis, which heat biomass at restricted oxygen levels to produce product intermediates that can be converted into liquid fuels.[7] Thermochemical conversion can also compliment biochemical processes by converting non-fermentable biomass to ethanol. The work presented here utilizes a biochemical conversion model developed in Aspen Plus®, a modeling tool for conceptual design, optimization, and performance monitoring for various industrial applications.[9] The efficiency of the biochemical conversion process is dependent upon physical properties of the biomass such as composition, particle size, density, and moisture. The conversion process model uses feedstock compositional and moisture data to perform calculations necessary to find the cost of the biochemical conversion process for the specified feedstock.

C. Integration Framework

The feedstock assembly system and conversion processes are inherently connected, but the computational tools used to perform analyses for each model are largely disparate. Integrating these two models together requires a framework which allows the models to communicate and share data. Integrating analysis models requires modularizing the analytical tools of the feedstock assembly system model to enable information to be aggregated throughout the system and reported to a computational interface. The modularization of the feedstock assembly system model facilitates a greater flexibility in integrating and coupling resource assessment tools with the framework. Through this framework, the computational interface is tasked with receiving and managing user input and transmitting the wide array of data and information. The integrated models dynamically receive information and assess the impact on the individual unit operation and on the entire system. The framework utilized in this paper is the Virtual Engineering Suite (VE-Suite).[10]

1. VE-Suite

VE-Suite is a virtual engineering framework developed at the Ames Laboratory that provides a comprehensive decision-making environment that enables users to design, analyze, and modify complete systems. Through the VE-Open communication specification, integrated models within the framework utilize information and data distributed throughout the system.[11] Utilization of the VE-Suite framework simplifies information and data exchange between models by providing an environment for integration and coupling of models. By adhering to VE-Open specifications, the modularized unit operations of the feedstock assembly system model can be integrated and coupled along with the conversion process model into a comprehensive environment, allowing for interaction with the computational analysis tools on a model level as well as a system level through a computational interface.

VE-Suite is comprised of three components. It coordinates the engines of each using VE-Open:

- *VE-Conductor* is the graphical user interface that allows the user to interact with the model and datasets.
- *VE-Xplorer* is the graphical engine the displays the geometric model and datasets in the virtual environment.
- *VE-CE* is the computational engine that synchronizes the data being handled within various analysis and models.

2. VE-PSI

In this work, Aspen Plus® is utilized for the biochemical analysis of ethanol conversion for biomass feedstocks under consideration. The integration of the Aspen Plus® model requires a robust interface to interact with the software's system-level operations and to the model-level decision-making operations. The Virtual Engineering Process Simulator Interface (VE-PSI) provides such functionality.[12] VE-PSI is a computational interface within the VE-Suite framework that adheres to the VE-Open specification.[10] VE-PSI provides access to basic system-level operations such as opening and closing Aspen Plus®, running simulations, and saving results. VE-PSI also enables interaction on a per-model basis by providing access to individual components within Aspen Plus® models. This allows users to alter operational parameters such as temperatures, pressures, and feed rates of components to optimize process simulations, as shown in Figure 2. The generalized nature of VE-PSI allows for integration of any Aspen Plus® model into the VE-Suite framework, providing an intuitive environment for users unfamiliar with the Aspen Plus® interface to design and optimize systems.

Figure 2. The software flowchart for the use of VE-PSI with Aspen Plus®

III. Case Study

The case study for this work focused on a select set of technologies for harvesting corn stover. During corn grain harvest, the stalk is engaged by the header below the ear and the material other than grain (mog) either is pushed to the ground or is processed through the combine and is spread out at the rear of the machine. This results in biomass residue consisting of stubble, chaff, and cobs remaining in the field. The compositional differences between the residue components impact the ethanol conversion efficiency. Therefore, identifying harvest equipment capable of proficiently gathering the most compositional rich residue can greatly improve ethanol conversion and ultimately reduce the cost to produce ethanol.

Figure 3. Windrowing treatments options

This study examines four pieces of windrowing equipment utilized during the harvest and collection operations: wheel rake, self-propelled windrower, bar rake, and flail shredder (see Figure 3). Table 1 shows the overall collection efficiency of each piece of equipment along with the residue collection efficiency based on the amount of residue left on the field. It can be seen based on residue collection efficiency that bale composition will vary based on the equipment that gathered the residue. As a result the bales will have different ethanol conversion efficiencies. The total collection efficiency also plays an important role in economic evaluation of the overall supply system. The less efficient a machine can gather the residue, the more acres the system requires to gather the biomass required to meet the needs of the biorefinery. Expanding the number of acres required to support a biorefinery greatly impacts the overall cost of supplying the biomass to the biorefinery. Biomass moisture content plays a significant role throughout the operations in the supply system. Table 1 also includes moisture content ranges at the time of harvesting which affects the efficiency of the harvest equipment and overall operation.

Windrowing Treatment	Collection Efficiency (%)				Bale Composition (%)			Moisture
	Chaff	Stubble	Cobs	Total	Chaff	Stubble	Cobs	(% w.b.)
Wheel Rake	37	0	18	24	67	0	33	12-18
SP Windrower	27	62	2	30	30	68	2	11-31
Bar Rake	71	0	0	52	100	0	0	11-20
Flail Shredder	57	47	1	44	54	45	1	9-13

Table 1. Windrowing treatment experimental data

IV. Results and Discussion

This work focused on the integration of the modularized unit operations of the feedstock assembly system model and a conversion process model within a dynamic framework to perform an overall cost analysis for a specified feedstock from biomass production through ethanol conversion. To validate the initial integration and coupling of unit operations, a harvest scenario involving four windrowing treatments was chosen. The model is initialized through user inputs for each unit operation. The unit operations occurring up to and after the windrowing treatment are kept constant to isolate the economic impact the treatments have on the system. Figure 4 demonstrates preparation of the network of operations by equipment selection and process model initialization through the computational interface.

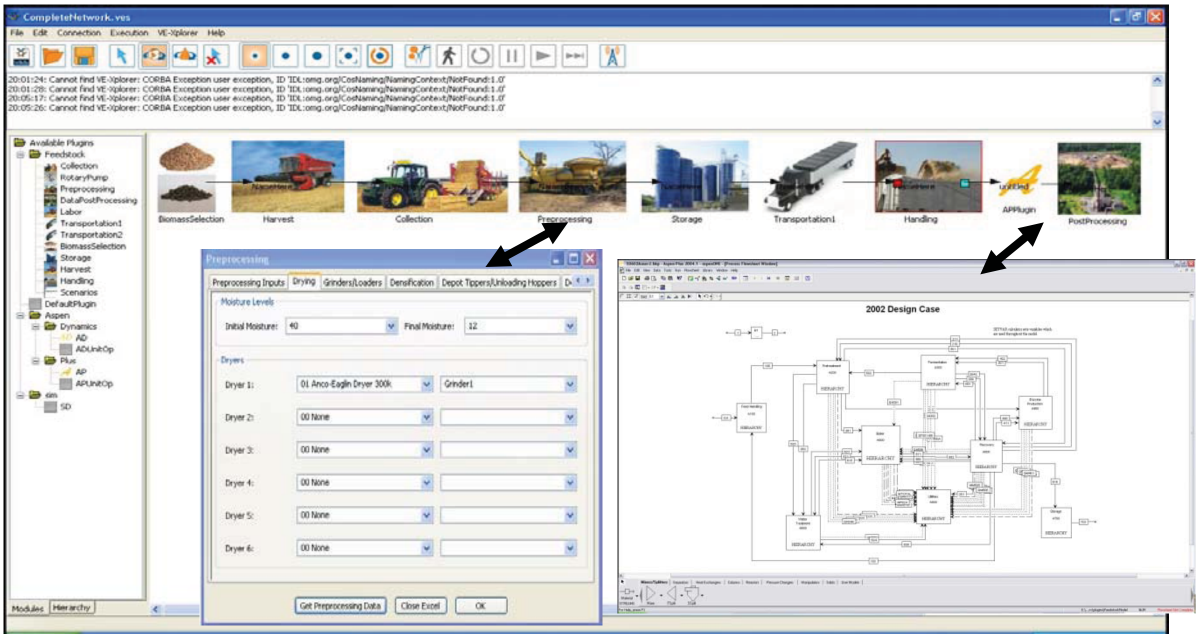

Figure 4. Computational interface for interacting with unit operations and the process model

Through the VE-PSI interface, Aspen Plus® system-level functionality is exposed to the user as well as model-level functionality. It is assumed that operational parameters of the biochemical process have been validated and thus only interfacing with system-level operations of Aspen Plus® will be utilized in this work. Through VE-PSI, the Aspen Plus® model is opened and displayed within the VE-Suite framework, which includes hierarchy blocks of the model and a layout of the biochemical process similar to how it is displayed within Aspen Plus®. Through the dynamic framework and utilizing VE-PSI functionality, system-level operations are exposed and utilized for reinitializing the model, running the simulation, and saving the results without user intervention. Experimental data provides the compositional and moisture data necessary to complete the biochemical process simulation. This information is accessed based on the windrowing treatment selection and is passed through the network to the Aspen Plus® model.

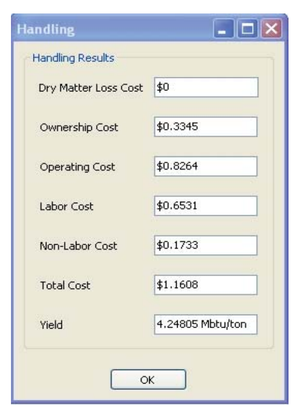

Figure 5. Individual unit operation cost analysis

Once equipment parameters for each unit operation are set and the process model is reinitialized the simulation can be initiated. Through the dynamic framework, unit operations are processed while their results are passed to the next operation in the supply system network. Cost calculations for harvesting and collection, storage and queuing, preprocessing, and transportation and handling are performed based on process intermediates delivered from the prior operation. The process intermediate physical parameters and operation equipment selection impact the individual unit operation cost. As shown in Figure 5, individual supply system unit operation economical analysis can be obtained through the computational interface.

Upon completion of the supply system, VE-PSI receives the compositional input data and the Aspen Plus® simulation is dynamically initiated. Upon completion of the simulation the results are saved, and the cost calculations for the ethanol conversion process can be calculated. Through the framework, Excel™ spreadsheets that accompany the biochemical process model are opened and macros are called to extract energy data from the biochemical process model and place the data into the Excel spreadsheets for cost analysis. Using the energy data from the populated spreadsheets along with the aggregated supply system unit operation costs, calculations are performed to find the final Minimal Ethanol Selling Price (MESP).

Table 2 provides the final results of the simulations for the specified windrowing treatments. To obtain a conservative MESP the highest moisture content from the range provided from Table 1 was used during the simulations for the respective windrowing treatment. Final cost also includes a grower payment which is assessed on a per ton basis. Two grower payment options were also explored. In Table 2, the impact of a single suboperation within the supply system can be observed. It can be seen from Table 1 that the bar rake has the highest collection efficiency and in Table 2 that it has the lowest MESP providing a direct correlation between collection efficiency and the MESP (see Figure 6). It should also be noted that although the SP windrower has a greater collection efficiency than the wheel rake, its use results in a higher MESP. This is due to the considerably higher moisture content during the windrowing treatment of the SP windrower than the wheel rake, proving that moisture content during the harvest operation plays a significant role in supply system cost. This can also be seen in the cost differences between "as received" and "per dry ton". Windrowing treatments that produce biomass with significantly higher moisture content require additional drying before it can be delivered to the biorefinery.

Windrowing Treatment	$30 grower payment				$20 grower payment			
	Moisture	As Received	Per Dry Ton	MESP	Moisture	As Received	Per Dry Ton	MESP
Wheel Rake	18%	$80.87	$98.62	$1.85	18%	$72.24	$88.10	$1.74
SP Windrower	31%	$74.97	$108.66	$2.02	31%	$67.71	$98.13	$1.90
Bar Rake	20%	$66.16	$82.70	$1.70	20%	$57.74	$72.17	$1.58
Flail Shredder	13%	$78.84	$90.62	$1.80	13%	$69.68	$80.10	$1.68

Table 2. Cost analysis of supply system and biochemical conversion with varying windrowing treatments

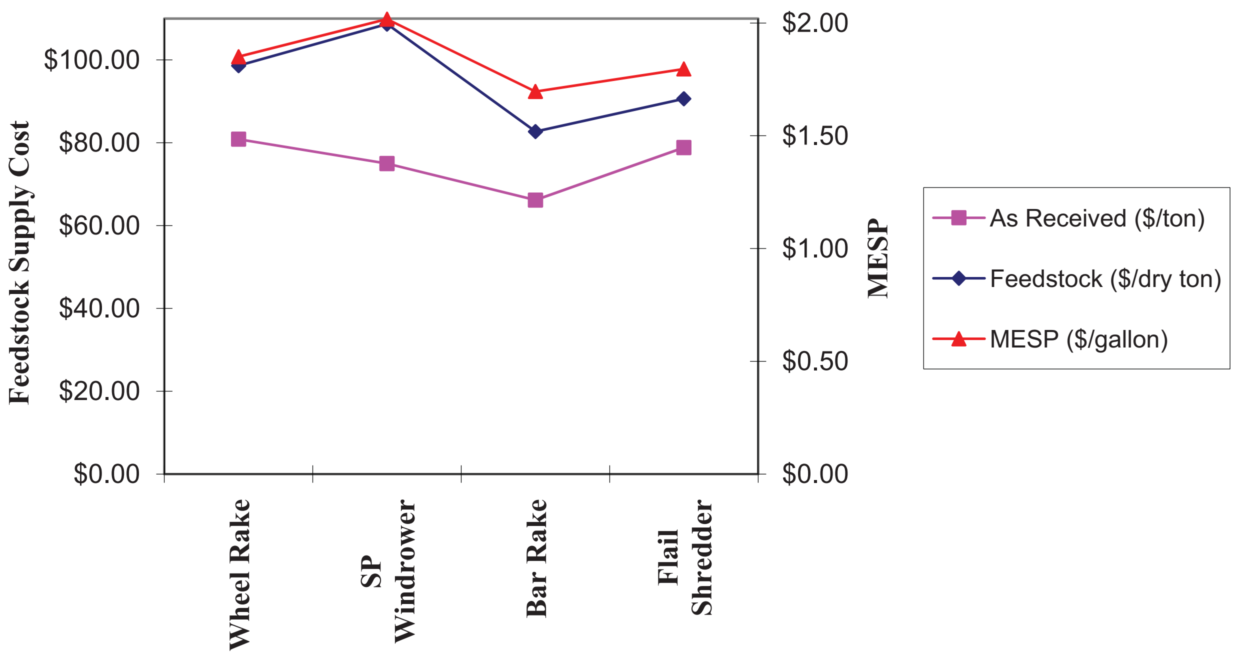

Figure 6. Comparison of supply system cost and MESP with different windrowing treatments

The integration of the Excel™-based feedstock assembly model and the Aspen Plus® process simulation model into the VE-Suite framework provides an opportunity to couple the disparate models and interact with them through an intuitive computational interface. Design parameters are exposed through the computational interface, allowing users unfamiliar with the models to design the overall system and perform analyses. The user can submit the design request and the analyses are performed behind the scenes. Unit operation results are distributed among the integrated models and system results are presented in a computational interface.

IV. Conclusion

Biomass is the largest source of renewable energy and the only one capable of being converted into transportation fuels. Reaching the 30 x 30 goal requires large-scale implementation of biomass conversion technologies and logistical improvements in moving biomass resources from the field to the biorefinery. Ethanol conversion process cost and efficiency is dependent upon the properties and format of the biomass feedstock after leaving the feedstock assembly system, but producing an optimal feedstock format for conversion may not be economically viable. Thus, this work focused on the integration of the feedstock assembly system model toolkit and the biochemical process model with the VE-Suite framework to provide a seamless and dynamic transfer of data and information between these disparate models. Through the integration framework, users design and analyze ethanol production systems based on location, feedstock, equipment, and unit operation specifications. Through modularization of the feedstock assembly system and VE-PSI, economic performance and feedstock characteristics can be determined per unit operation allowing users to identify limiting factors within the system design. Economic analysis is aggregated throughout the system providing a comprehensive cost assessment of the ethanol production system. Obtaining MESP is fully automated, allowing as little or as much user interaction with individual unit operations and overall system design parameters as necessary. The integration framework (see Figure 7) provides an intuitive interface for unfamiliar users to design and interact with complex models without having direct interaction with the analysis models.

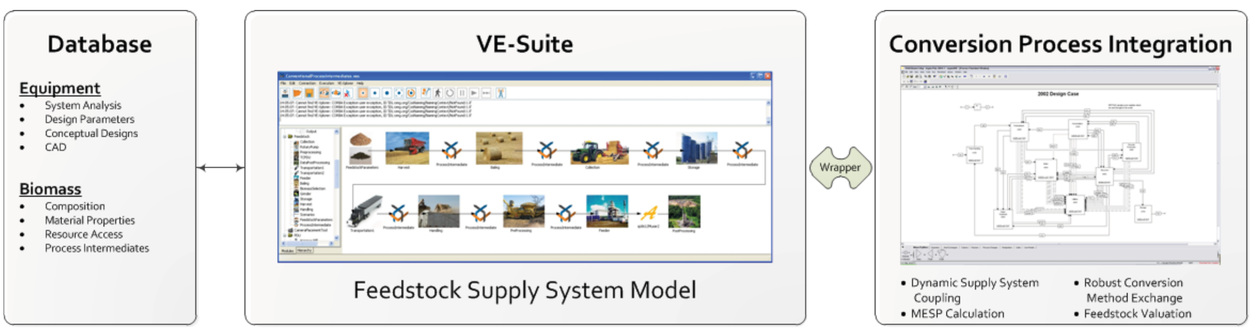

Figure 7. Integrated analysis environment

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