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Process Modeling of Comprehensive Integrated Forest Biorefinery—An Integrated Approach

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Abstract The key to expanding the energy supply, increasing energy security, and reducing the dependency on foreign oil is to develop advanced technologies to efficiently transform our renewable bioresources into domestically produced bioenergy and bio-products. Conventional biorefineries, i.e., forest products industry's pulp and paper mills with long history of sustainable utilization of lignocellulose (wood), offer a suitable platform for being expanded into future integrated forest biorefineries. Due to the pre-existing infrastructure in current forest products operations, this could present a very cost-effective approach to future biorefineries. In order to better understand the overall process, technical, economic, and environmental impacts, a detailed process modeling of the whole integrated forest biorefinery is presented here. This approach uses a combination of Aspen Plus®, WinGEMS®, and Microsoft Excel® to simulate the entire biorefinery in detail with sophisticated communication interface between the three simulations. Preliminary results for a simple case study of an integrated biorefinery show the feasibility of this approach. Further investigations, including additional details, more process options, and complete integration, are currently underway.

Keywords Process modeling · Biorefinery modeling · Integrated forest biorefinery · Pulping · Ethanol · Aspen Plus · WinGEMS

Introduction

There has been an increasing interest in the development of biorefineries for the production of renewable energy, including liquid transportation fuels such as bioethanol and biodiesel, power and process steam, and chemicals, due to the increasing global demand of energy and transportation fuels especially in developing countries such as China and India, increase in fuel costs, and also concomitant pressures to reduce greenhouse gas emissions, and the need for energy security and environmental sustainability.

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There are, in general, four kinds of biorefineries: (a) starch based biorefinery producing ethanol and co-products (e.g., distillers' dried grains) from corn and other cereals; (b) sugar-based biorefinery using sugarcane, as is commonly practiced in Brazil; (c) biorefinery producing biodiesel from vegetable or animal oils and fats, including soybean oil, canola oil, sunflower oil, and recycled cooking oils etc.; and lastly (d) lignocellulosic biorefinery producing ethanol, power and steam, and possibly a host of other chemicals from lignocellulosic biomass, including corn stover, rice straw, wood, and forest wastes, dedicated fast-growing energy crops such as hybrid poplar and switchgrass etc. Among these, biorefineries of starch to ethanol, sugarcane to ethanol, and biodiesel have already been commercially practiced, with the global production capacity of 33 million cubic meters (MCM) bioethanol and 3.9 MCM biodiesel per year in 2005 [1]. The global production capacity of bioethanol and biodiesel by these three groups of biorefineries are still increasing because a number of biorefineries are being constructed or will be built in the near future. The production costs (excluding any subsidies) of starch ethanol, sugarcane ethanol, and biodiesel (produced from animal and vegetable oil) are 600–800, 300–500, and 400–800 \$/cubic meter of gasoline equivalent (CMGE), respectively [1]. Of these, the production costs of starch (corn) ethanol have the potential to be reduced by 400–600 \$/CMGE in the future owing to further process improvements and optimization [1]. However, starch ethanol (mainly corn–ethanol) requires high input of fossil fuels (up to 60–80% of the final fuel energy produced) [1], thus contributing to only around 20% reduction in CO_2 emission [1, 2]. The biodiesel biorefinery brings about 40–60% CO_2 reduction. But, the feedstock availability for biodiesel is limited compared to starch ethanol [1]. Sugarcane bioethanol has the lowest production cost and also brings about 90% reduction in CO_2 emission. But, sugarcane can only be suitably grown in subtropical areas with warm, sunny, and frost-free weather and fertile, well-drained soil, e.g., in Brazil. In addition, the feedstocks of these three groups require arable croplands for planting, which are in competition with food production. Therefore, there has been an increasing interest in lignocellulosic biorefineries, which have the following advantages [1, 3]:

1. Significant amount of lignocellulosic wastes, including wood and forest waste, agricultural waste (corn stover and cereal straw etc.), dedicated energy crops such as hybrid poplar and switchgrass, and municipal solid waste are available as feedstock.
2. Non-arable land can be used for planting dedicated fast-growing energy crops such as hybrid poplar and switchgrass.
3. Lignocellulosic biorefineries may contribute to 70% reduction in CO_2 emission and even up to 100% if electricity is co-generated so as to avoid using natural gas or coal.
4. With future advances, the production cost of cellulosic ethanol can be greatly decreased to 500 \$/CMGE from the current 1,000 \$/CMGE at the pilot scale, thus approaching the corn–ethanol cost in the next decade.

In general, biorefineries of starch to ethanol, sugarcane to ethanol, and biodiesel are referred to as *current* or *conventional* biorefineries due to their relatively mature technologies and being already commercially available. Another often-overlooked conventional biorefinery is the long-standing forest products and pulp and paper industry where thermochemical conversion processes have long been used for the production of cellulose fiber and energy and power. Expanding beyond cellulose fiber and current levels of energy production to include liquid fuels, chemicals, polymers, and additional energy from lignocelluloses offers a tremendous opportunity for a cost-competitive, environmentally sustainable future bioeconomy.

Lignocellulosic biorefineries can be classified as two major categories: basic lignocellulosic biorefinery (BLCBR) and integrated/advanced lignocellulosic biorefinery (ILCBR). BLCBR represents the simplest lignocellulosic biorefinery involving conversion of lignocellulosic feedstock into bioethanol with production of process steam and electricity or combined heat and power (CHP) by burner/boilers and steam turbines. BLCBR can comprise of the following process steps: feedstock handling, pre-treatment and conditioning/detoxification, saccharification and co-fermentation, product separation and purification, wastewater treatment, product storage, lignin combustion for production of electricity and steam, and all other utilities (Fig. 1) [4]. ILCBR is a more complex, integrated, or advanced process involving a biomass-based integrated gasification combined cycle (BIGCC) to produce biosyngas and combined heat (steam) and power (CHP) with both gas turbine and steam turbine [5–7], in addition to biochemical conversion of hemicelluloses to ethanol. The syngas can then be converted to methanol and DME as well as Fischer–Tropsch liquid transportation fuels (green diesel), etc. The above route can also be accomplished using pyrolysis of biomass to bio-oil instead of gasification to syngas [3, 8].

One of the most important ILCBR is integrated forest biorefinery (IFBR) based on current infrastructure of pulp and paper mills. This process (Fig. 2) involves pre-extraction of hemicelluloses prior to pulping (so-called value prior to pulping), isolation of short and long fiber after pulping, conversion of hemicelluloses, and the short fiber (cellulose) to ethanol in one or more bioreactors. The long fiber (cellulose) can be used for production of paper or other fiber-based materials such as biocomposites, but this is not included in the simulation. In addition, the black liquor after pulping and washing containing dissolved lignin can be gasified to produce biosyngas substituting for the Tomlinson recovery boiler system. The resulting biosyngas can be further synthesized to produce chemicals such as methanol, liquid transportation fuels such as DME, and green diesel, etc. Electricity and process steam can also be produced from biosyngas with high-efficiency gas turbine [9, 10].

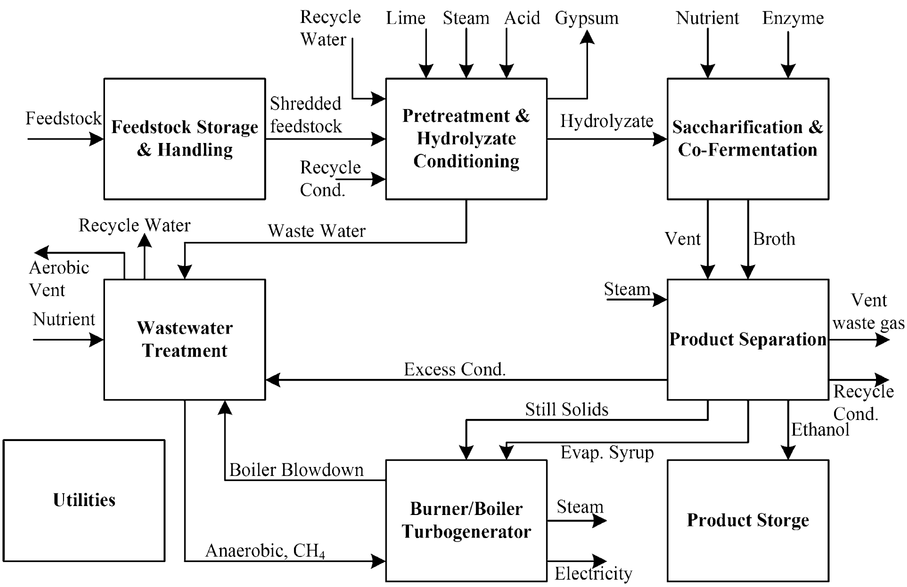


Fig. 1 Process block diagram for a basic lignocellulosic biorefinery [4]

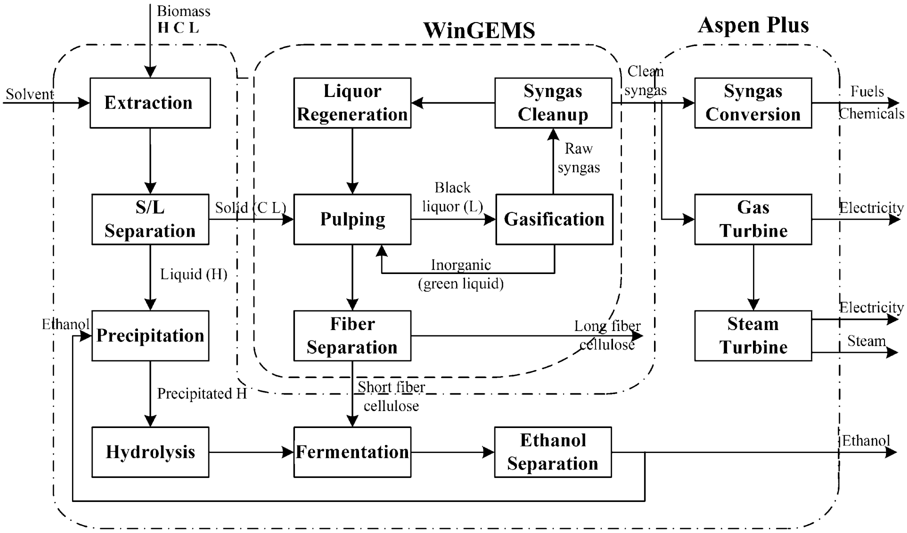


Fig. 2 Overall block diagram of a whole integrated forest biorefinery (*H* hemicellulose, *C* cellulose, *L* lignin; the block "pulping" includes the whole process in Fig. 3 except the recovery boiler which is replaced by a gasifier in Fig. 2)

IFBR is one of the top priorities as it offers the most promise for commercialization in the near future. In the United States, significant quantities of wood (approximately 200 million tons) are already used for pulp and paper manufacture; thus, the raw material handling and the know-how currently exist for modification to an IFBR. The existing facilities of the pulp mill can potentially lead to reduction in the overall capital investment of IFBR, compared to the completely new, stand-alone lignocellulosic biorefinery. In addition, the IFBR can take advantage of all the components of the feedstock to produce value-added multiple co-products, including power and process steam, a variety of chemicals, as well as the major products such as paper and bioethanol. The IFBR's replacement of Tomlinson boilers with black liquor gasifiers (BLG) can improve the energy efficiency, reduce CO_2 emissions, modify pulping strategies, and improve safety [11]. Therefore, IFBR can significantly increase profits and revenue.

Process modeling and analysis of the pulp mill-based IFBR involves process simulation of the pulping process [12, 13] and the non-pulping processes, including biochemical conversion of lignocelluloses into ethanol [4, 14, 15], etc.

The objective of the present paper is to develop a comprehensive approach for modeling IFBR in order to achieve efficient design, simulation, and optimization of the whole integrated forest biorefinery and to be able to perform the overall techno-economic analysis.

In the following sections, an integrated method using two commercial process simulators Aspen Plus and WinGEMS and Microsoft Excel® as the communications interface between the simulators and a case study using the method are described. "Modeling of the Integrated Forest Biorefinery" introduces the comprehensive approach for modeling an integrated forest biorefinery and the mechanism of communications between Aspen Plus and WinGEMS with Excel as the communications interface. The case study is presented in "Case Study: Simplified IFBR", and the obtained results are given in "Results". Finally, the paper closes with conclusions in "Conclusions".

Modeling of the Integrated Forest Biorefinery

Comprehensive Approach for Modeling an Integrated Forest Biorefinery

As shown in Fig. 2 and described above, IFBR includes pulping process and black liquor gasification, in addition to hemicelluloses pre-extraction and hydrolysis, fermentation of hemicellulose sugars and the short fiber (cellulose), ethanol separation, biosyngas conversion, and power and steam production. Figure 3 shows the conventional Kraft pulping process. In this process, pre-heated wood chips enter a continuous digester where the lignocellulose components of wood chips undergo thermochemical pulping reactions with active pulping chemicals comprising mainly NaOH and Na_2S in pulping liquor called the white liquor. The solid portion of the cooked wood chips from the digester goes to pulp Washers to produce unbleached pulp. The liquid part from the digester, called weak black liquor, enters the multiple effect evaporators for concentrating the liquor, increasing its solids content. The resulting strong black liquor is then fed into the chemical recovery boiler for recovery of heat and inorganic chemicals (Na_2S and Na_2CO_3). This is followed by slaking and causticization with lime (CaO) from Lime Kiln to produce NaOH for recycling back to the pulping process. $CaCO_3$ produced in the Causticizer, after clarification, is washed by Mud Washer and then fed into the Lime Kiln to regenerate lime for reuse.

Process modeling of pulping itself is quite different from modeling of the conventional petrochemical processes in that the former involves modeling of continuous digester, Lime Kiln, and slaker, which contain slurry and inorganic chemicals. WinGEMS is a commercial process simulator widely used in modeling of pulp and paper processes for 30 years. All the blocks or modules (unit operations), including compound blocks, stream structure, stream components, physical properties, and chemical reactions, etc., in WinGEMS are well designed for simulating pulp and paper process operations. Since WinGEMS is focused on pulp and paper industry, modeling of pulping process was conducted using WinGEMS rather than the common chemical process simulators such as Aspen Plus, Hysys, and PRO/II, etc., as it offers significant advantages of more simplicity, higher model-developing efficiency, and more reliability. Besides, gasification, biosyngas cleanup, including sulfur removal, liquor regeneration, and pulping form a closed loop with inorganic chemicals recycled for reuse in

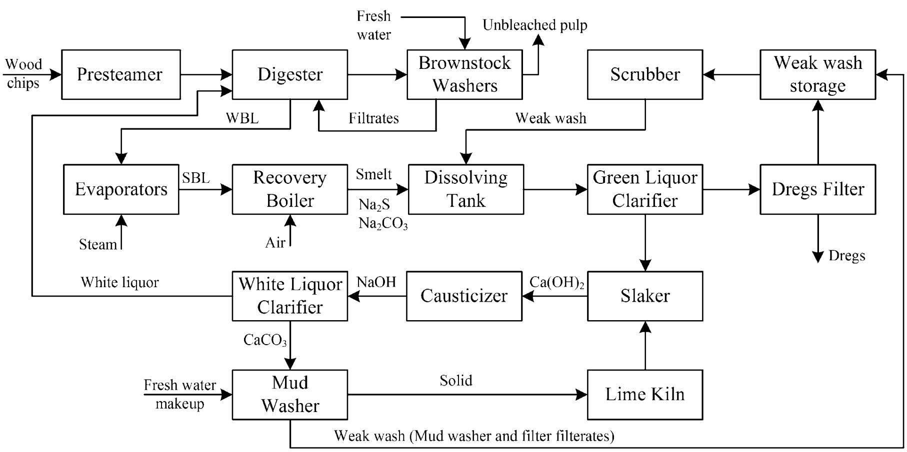


Fig. 3 Simplified block diagram of conventional Kraft pulping process

pulping. Modeling of some portions of this cycle excluding pulping using other process simulators will lead to complexity and difficulty in data transfer between these simulators and WinGEMS. Therefore, in this study, WinGEMS is used to simulate pulping, gasification, biosyngas cleanup, liquor regeneration, and fiber separation, as shown in Fig. 2.

In general, many non-pulping process unit operations such as ethanol separation and biosyngas conversion, etc. are difficult to be efficiently modeled by WinGEMS since WinGEMS is not as powerful and flexible as common simulators such as Aspen Plus. Therefore, Aspen Plus is used for modeling the other non-pulping processes (Fig. 2) in this study. For the same reasons, gasification can be more efficiently modeled by Aspen plus rather than WinGEMS. However, as described earlier, the inorganic chemicals recovered by gasification need to be recycled to the digester for pulping. Hence, WinGEMS was chosen for modeling gasification, thus avoiding exchange of any recycle stream, i.e., recycling of inorganics back to pulping between WinGEMS and Aspen Plus model. This minimizes the number of values to be transferred between WinGEMS and Aspen Plus during the multiple iterative calculations of the cycle for effective convergence of the results, avoiding possible transferring errors in simulation results. To some extent, this method solves the problem of synchronization between two softwares, which is rather difficult to deal with.

Since Excel can easily exchange data with both WinGEMS and Aspen Plus, Excel was chosen as the common platform for interfacing and exchanging data between the two simulators. The following section will discuss the mechanism of communications between Aspen Plus and WinGEMS based on Excel.

Mechanism of Communications Between Aspen Plus and WinGEMS

Communication Between WinGEMS and Excel

The communication between WinGEMS and Excel is based on dynamic data exchange (DDE) technology, including the use of the execution scripts in WinGEMS and the use of WinGEMS Excel add-in macros and/or WinGEMS toolkit functions in Excel [16].

WinGEMS contains a scripting language, simply called script, allowing the user to customize execution, define scenarios, or perform a specific action at a particular time. The scripts can be used to send/write specified unit parameters and stream data in WinGEMS to specified cells of an Excel worksheet and read/retrieve data from specified cells in an Excel worksheet to specified unit parameters and stream data in WinGEMS.

In addition, both WinGEMS Excel add-in and WinGEMS toolkit allows for transfer of data (to and from) and control of any WinGEMS simulation from an Excel spreadsheet, including browsing for WinGEMS process values from Excel, running different simulation scenarios using spreadsheet values, and using the Excel Solver to find an optimum value of a function of one or more simulation parameters. Briefly, the user can set/edit the parameters of WinGEMS modules (unit blocks) and streams in one or more spreadsheets of Excel and then run the user's WinGEMS program from Excel. Once the calculation is complete, WinGEMS can send back the results to Excel. This enables easier integration of Excel's features such as statistics, finances, plotting, and optimization, etc. with WinGEMS.

Specifically, with the WinGEMS Excel add-in, the user can send values from Excel to WinGEMS, e.g., write a cell value from the Excel worksheet to a WinGEMS block or stream parameter using the "WinGEMSPut" Excel macro from the Formula Bar. The user can also send values from WinGEMS to Excel, e.g., read a block or stream parameter value into a worksheet cell, using the "WinGEMS" Excel macro from the Formula Bar. WinGEMS toolkit consists of a number of programming functions for sending commands

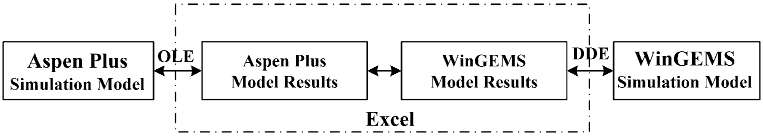


Fig. 4 Simplified diagram of communication between Aspen Plus and WinGEMS

to WinGEMS, providing the user another way to communicate with WinGEMS from Excel based on VBA programming [16].

Communication Between Aspen Plus and Excel

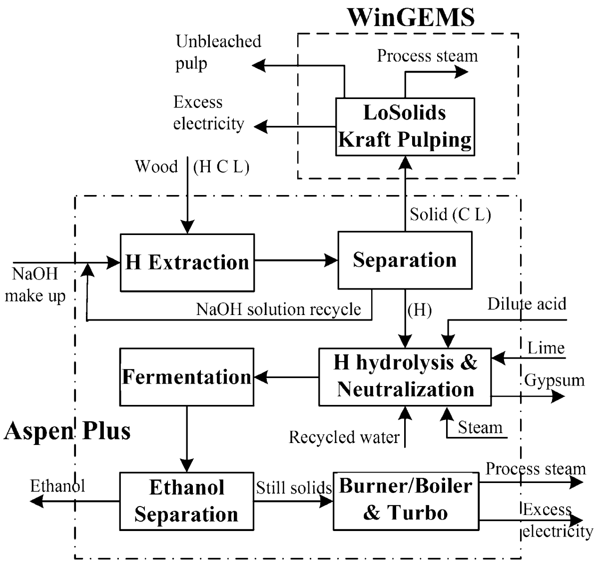
The Aspen Plus User Interface supports Microsoft's object linking and embedding (OLE) Automation (ActiveX™) technology, which enables the user to transfer data easily to and from other Windows applications such as Excel [17].

There are two ways to use the OLE Automation technology to exchange data between Aspen Plus and Excel. One is to create active links between Aspen Plus and Excel. With OLE, active links from input or results fields in Aspen Plus process models (the link source) to Excel spreadsheets (the link container) can be created. The links will update the Excel spreadsheets when the Aspen Plus model is modified. In addition, active links from Excel spreadsheets (source) to input fields in Aspen Plus models (container) can also be created. Another way is to enable Excel (client) to interact with Aspen Plus, which is taken as an OLE Automation Server, by programming with VBA in Excel. In this way, the inputs and the results of Aspen Plus simulations are communicated to Excel [17].

Communication Between Aspen Plus and WinGEMS

Since data can be transferred between Aspen Plus simulation model and Excel by OLE technology and between WinGEMS simulation model and Excel by the DDE technology as

Fig. 5 Block diagram of a simplified IFBR (*H* hemicellulose, *C* cellulose, *L* lignin)



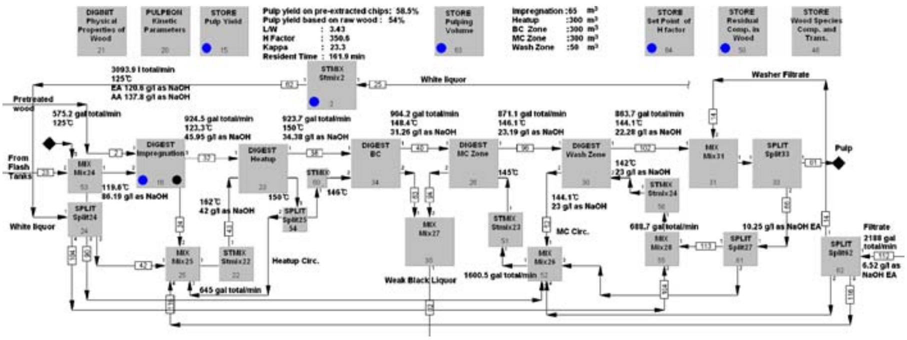


Fig. 6 Flowsheet of LoSolids digester system

described above, Aspen Plus can communicate with WinGEMS through Excel as a common interface/platform (Fig. 4). In other words, the simulation data from Aspen Plus model in an Excel spreadsheet and the simulation data from WinGEMS model in the same or different Excel spreadsheet can easily be shared with each other within Excel. For example, Aspen Plus is able to send a stream flow rate in the Aspen process model into a specified cell in an Excel worksheet from which WinGEMS retrieve the data to a specified stream in the WinGEMS model and vice versa. Thus, a seamless, efficient, real-time data exchange between the two process simulators has been successfully achieved.

Case Study: Simplified IFBR

Based on the above-described comprehensive approach to integrated biorefinery process modeling using an effective data exchange protocol using Excel, a case study is presented in this section. A simplified process of the whole IFBR is chosen for the case study (Fig. 5 and Fig. 2). The case study considers the conventional Kraft pulping (LoSolids) with Tomlinson boiler for steam (heat) and inorganic recovery rather than BLG. This is essentially the first phase in the comprehensive modeling of the whole IFBR.

Table 1 Model inputs for Kraft pulping simulation.

Name		Value	Unit
EA charge		28	%
Sulfidity		25	%
L/W		3.43	m^3/Mg
White liquor split	IV	70	%
	BC	10	%
	MC	10	%
	Wash	10	%
Digester impregnation outlet temp.		123.3	°C
Digester heatup outlet temp.		150.0	°C
Digester BC outlet temp.		148.4	°C
Digester MC outlet temp.		146.1	°C
Digester wash outlet temp.		144.1	°C

Table 2 Data of pre-extracted wood stream transferred from Aspen Plus to WinGEMS through Excel.

Name		Value	Unit
Flow rate of pre-extracted wood stream		147.7	Mg/h
Suspended solids		50.9	wt.%
Temperature		90.0	°C
Composition	Lignin	24.4	wt.%
	Carbohydrates	67.5	wt.%

In the case study, aspen wood is used as feedstock at a flow rate of 145.833 dry Mg/h (1 Mg=10^6 g). The composition of aspen wood and the operating conditions of all the sub-processes modeled by Aspen Plus (refer to Fig. 5) are kept the same as what was reported in earlier study [14]. The conventional pulping process, detailed in Fig. 3, is modeled by WinGEMS as shown in Fig. 5. Figure 6 shows the WinGEMS flowsheet of the corresponding LoSolids digester system, the core system of the pulping process for this case study. This continuous digester was based on the work by Walkush and Gustafson [12]. A five-effect evaporator (figure not shown) was used in the pulping.

The major model inputs for conventional Kraft pulping simulation are shown in Table 1. Chip size distribution considered here is the same as what was used by Walkush and Gustafson [12].

Table 3 A worksheet CommWithWinGEMS of excel as a communication interface.

	A	B	C	D	E	F	G	H	I
1	To WinGEMS					From WinGEMS			
2	Chip Feed					Major Results			
3	Pre-extracted chips flow rate		147749	kg total/hr		Pulping Yield		54.0	%
4	Suspended solids		50.9	cons%		Liquor-to-chip ratio		3.43	
5	Temperature		363.2	K		H factor		350.6	
6	Composition	Lignin	24.4	%wt		Kappa number		23.3	
7		Carbohydrates	67.5	%wt		Pulp	Flow rate	352	Mg total/hr
8	Chip Size	Chip 1 thickness	3	mm				1056.6	od Mg/day
9		Chip 2 thickness	4.5	mm			Suspended solid	12.5	cons%
10		Chip 3 thickness	9	mm			Cellulose	77.6	%
11		Chip 1 length	15	mm		Black Liquor	Flow rate	318.8	Mg total/hr
12		Chip 2 length	20	mm			Temperature	261.2	K
13		Chip 3 length	25	mm			Total tit. Alkali	118.9	g/l as NaOH
14	Chip Percent	Chip 1	15	%			Effective alkali	181.8	g/l as NaOH
15		Chip 2	79.2	%			Sulfidity	38.8	%
16		Chip 3	5.8	%			Total Diss. Solid	65.0	%mass
17	White Liquor					Steam Consumed or Generated			
18	EA charge		0.28	frac as NaOH				MJ/hr	MMBtu/hr
19	Sulfidity		25	%		Chip presteaming		14474	13.7
20	Digester Configuration					STMIX1		16484	15.6
21	WL Split	IV	70	%		STMIX2		40185	38.1
22		BC	10	%		STMIX3		-2648	-2.5
23		MC	10	%		STMIX4		49305	46.7
24		Wash	10	%		STMIX5		34137	32.4
25	Volume	Impregnation	65	m^3		Evaporators		219278	207.9
26		Heatup	300	m^3		Flash Tank (B6)		7851	7.4
27		BC	300	m^3		Flash Tank (B7)		3588	3.4
28		MC	300	m^3		Smelt Dissolving		24109	22.9
29		Wash	50	m^3		LPS Turb		429619	407.3
30		Total volume	1015	m^3		LPS Scrubber		3588	3.4

CommWithAspenPlus / **CommWithWinGEMS** / Summary / DataProcessing / Pret

Table 4 Major results from aspen PLUS to excel.

Name	Value	Unit
Ethanol (99.4%)	1.583	Mg/h
Steam requirement in non-pulping process	63,038	MJ/h
Net power requirement in non-pulping process	2,741	kWh/h

With the integrated method mentioned above using Excel as the communication interface, Aspen Plus simulation model was run first, and the obtained results were transferred to the worksheet named CommWithAspenPlus (data not shown) in a specified Excel file. Among these results, the data of pre-extracted wood stream (Table 2) containing mainly cellulose and lignin was shared by another Excel worksheet called CommWithWinGEMS (Table 3) in the same Excel file. This data and the major inputs and parameters for the pulping model (Table 1) listed under the title of "To WinGEMS" on the worksheet CommWithWinGEMS were then read by WinGEMS for its pulping simulation model. Next, WinGEMS pulping was run, and the results were sent back to the worksheet CommWithWinGEMS and listed under the title of "From WinGEMS".

Results

The major simulation results of Aspen model and WinGEMS model are listed in Tables 4 and 5, respectively. Data from these two tables are transferred from WinGEMS and Aspen Plus simulation models into Excel worksheets. The simulation results show that the integrated method works very well with high efficiency and reliability in modeling the simplified IFBR.

From Tables 4 and 5, it is found that net steam and power generated by the whole process (including both pulping and non-pulping processes) are 10,393 MJ/h and 16,273 kWh/h, respectively. In addition to fiber product, ethanol was also produced (13,308 Mg/year). Current model does not estimate electricity consumption during the pulping process, i.e., power required for pumps, chipping, etc. Even though this is expected to be low, it may be easily incorporated based on historic pulp and paper operations data. It can be seen from Table 5 that the traditional pulping process outputs/results, i.e., pulp yield, H factor, and Kappa number are at commercially realistic levels. The typical range of these parameters can refer to literature [18]. Note that the pre-extracted wood chips rather than

Table 5 Major results from WinGEMS to excel worksheet.

Name		Value	Unit
Pulp	Flow rate	44.0	OD Mg/h
	Cellulose	77.7	wt.%
Pulping yield		54.0	%
H factor		350.6	
Kappa number		23.3	
Black liquor	Flow rate	318.8	Mg total/h
	Total diss. solids	65.0	wt.%
Net steam generated in pulping		73,431	MJ/h
Hogfuel consumption in Lime Kiln		5.2	Mg/h
Power generated in pulping process		19,014	kWh/h

un-extracted normal wood chips were utilized for pulping in this case study. Efforts are underway updating the kinetic model and pulping process operating conditions based on laboratory experimental data on pulping of pre-extracted wood chips. It should be noted that, even though the case study presented here for the integrated approach was used in modeling of the simplified IFBR process, it is equally applicable for modeling of the complex IFBR. This effort is currently underway.

Conclusions

An integrated approach, i.e., using integrated/combined Aspen Plus and WinGEMS and Excel as a common communications interface platform, for comprehensive modeling of the whole IFBR has been successfully developed. Results from a case study using a simplified IFBR process were found reasonable. The simulation results show that the integrated method is efficient and reliable in modeling of the simplified IFBR. The method presented here is equally applicable for modeling the complex IFBR processes, including BIGCC or black liquor gasification combined cycle, biosyngas conversions into liquid fuels and chemicals, and fiber separation, etc. Efforts are currently underway in modeling the complex, whole integrated forest biorefinery with multiple products and co-products, including energy and fuels. This general integrated approach will play an increasingly important role in the design and development of the future fully integrated lignocellulosic biorefinery of the twenty-first century bioeconomy.

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