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Evaluation of the Open Source Process Simulator DWSIM for Bioprocess Simulation

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Abstract

In the recent times, the application of process simulation software has found its way to the simulation of bioprocesses. Presently, bioprocesses are simulated and technoeconomic analysis is performed in commercially available software for such as SuperPro Designer®, Aspen Plus® etc. These softwares are not freely available and therefore, there exists a need for an open source software for the simulation of bioprocesses. Furthermore, the chemical process softwares show compatibility issues, when used for bioprocesses. More recently, an open source process simulator called DWSIM was introduced for the simulation of chemical processes. However, the applicability and compatibility of DWSIM for complex bioprocess simulation involving microbial biomass has not been reported yet. Therefore, the present study evaluates and reports the simulation results of the bioethanol production process developed by NREL (National Renewable Energy Laboratory, USA), performed in DWSIM. The simulator results were compared to those of existing commercial software, and the results showed good agreement with the literature. This suggests that DWSIM could be a promising alternative for bioprocess flowsheeting and simulation, and further technoeconomic analysis.

Keywords

flowsheeting, bioprocess simulation, DWSIM, bioethanol, open source software, technoeconomic analysis

1 Introduction

Biotechnologists have always tried to identify computational methods available for efficient practical applications. With the evolution of both hardware and software for computing, bioprocess engineers are attracted to the recent advances in the same for use in bioprocessing. Bioprocesses are developed through a combination of media optimization, process optimization, process design, and control. This can be a tedious task if performed manually, but becomes easier when software is used [1]. The significance of computational tools lies in their ability to solve complex problems in bioprocessing that would otherwise be difficult to address [2]. There are three interrelated areas of particular importance in bioprocessing, namely process simulation, process monitoring, and process analysis. The major contribution of bioprocess software is in simulating bioprocesses to maximize profits by predicting and operating the most efficient processes [3], i.e. technoeconomic analysis. This involves demonstrating how laboratory and pilot plant data can be captured and used to build a flowsheet model, estimate process economics, and identify priorities for process improvement [4, 5].

Software-based simulation plays a key role in the design of bioprocess plants. There are numerous commercially accepted software options available, such as Aspen Plus®, Aspen HYSYS®, ProSim Plus®, SuperPro Designer® and UniSim®. These software are used to simulate chemical and bioprocesses [6–9], but their high cost makes them difficult to acquire. Most of the chemical process softwares also present compatibility issues with biological processes. To address this, the present study focuses on using open-source software like DWSIM, which is freely accessible. Open-source software provides distinct advantages in modeling dynamic processes with its user-friendly interface. This accessibility makes it a preferred choice for researchers and professionals. The collaborative and transparent nature of open-source software fosters innovation, serving as a valuable resource for diverse applications [10]. In contrast to commercial simulators, open-source alternatives offer benefits for simulating multidisciplinary plants, allowing access and modification of source code. They are particularly accessible to rural

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communities. While commonly used for dynamic simulations, they have untapped potential for steady-state simulations [11]. Use of open-source software, hence, can aid in promoting the transfer of technology and dissemination of information in both educational and trade sectors, enabling a better understanding of various processes [12].

Medeiros, a software developer, created the open-source chemical process simulator, DWSIM. As it is freely available, it allows users to understand the workings of chemical process systems. The advantage of using DWSIM is its compatibility with various platforms such as Windows, Linux, macOS, Android, and iOS, enabling the user to perform steady-state and dynamic simulations with thermodynamic models and unit operations. The user interface is user-friendly and features advanced property packages. The latest version of DWSIM includes a new feature called the dynamic property, which enables users to integrate Python scripts into the flow sheet to calculate relevant parameters [13]. DWSIM introduced Version 7, featuring DWSIM Pro with extensions like additional unit operations and property packages. It allows modification of individual units and entire calculation routines in the flowsheet. DWSIM supports customization of communication between unit operations and the flowsheet, as well as between operations. Notably, it excels in creating entire unit operations as custom plugins [14]. This enhances the applicability of the software for a wide range of processes, including bioprocesses. Several studies have reported the application and comparison of DWSIM with other process modeling softwares for chemical processes [15, 16]. More recently, Elavazhagan et al. [17] have reported the application of DWSIM for the simulation of biodiesel production by transesterification. However, the same has not been reported yet for complex biological processes involving microbial systems such as fermentations, which require creation of biological compounds, adoption of relevant property packages and creation of unit operations compatible for such biological processes. Therefore, the present study was conducted with the following objectives:

- Create components and custom unit operations in DWSIM for a well-known ethanol production bioprocess involving microbial fermentation.
- Simulate the bioethanol production process in DWSIM and validate with the literature.

2 Methodology

2.1 Ethanol production process

The process of ethanol production from lignocellulosic biomass as described in the NREL (National Renewable Energy Laboratory, USA) report [18] was used for simulation (Fig. 1). The process involves dilute acid pretreatment of corn stover biomass, enzymatic saccharification of the cellulose and fermentation of the six and five carbon sugar compounds to ethanol. The major auxiliary processes involve handling and storage of feedstock, purification of product, wastewater treatment and lignin combustion.

2.2 Software input

The Aspen flowsheet of NREL process (Fig. 1) consists of 9 areas viz. A100 (feed handling), A200 (pretreatment and conditioning), A300 (enzymatic hydrolysis and fermentation), A400 (enzyme production), A500 (distillation dehydration solid separation), A600 (wastewater treatment, WWT), A700 (storage), A800 (burner/boiler turbogenerator) and A900 (utilities). For simulation in DWSIM, the major steps that involve the biological processes in areas A200 (pretreatment and conditioning), A300 (enzymatic hydrolysis and fermentation) and A500 (distillation dehydration solid separation) were only considered. The omission of other areas was made up by introducing appropriate recycle streams or input streams.

2.3 Reactants

All the reactants involved were given as input in DWSIM (version 7.5) [19], either from the existing list (Chemsep) or after creating them using the Compound Creator Wizard available in the software. This creation involved the entry of molecule ID, constant properties, temperature dependent properties and molecular structure in the Compound Creator Wizard window manually or by importing data from JSON files available in online repositories such as Pubchem [20]. Data for the manual entry of the molecular properties were obtained from the online repository Chemeo [21]. Table 1 gives the details of the existing compounds and the added compounds in the software. Furthermore, the details of the major properties of the compounds added new to the software are summarized in Part D of the Supporting Information.

2.4 Property package and unit operations

Following the recommendation of the thermodynamic decision tree discussed by Carlson [22], Peng Robinson thermodynamic property package was chosen for the simulation. The software calculates the thermodynamic properties of the compounds as explained in Section 2.1.1 of the DWSIM user guide [23]. Subsequently the flow sheet was generated by adding unit operations and material streams. The units for mixer, cooler, heater, heat

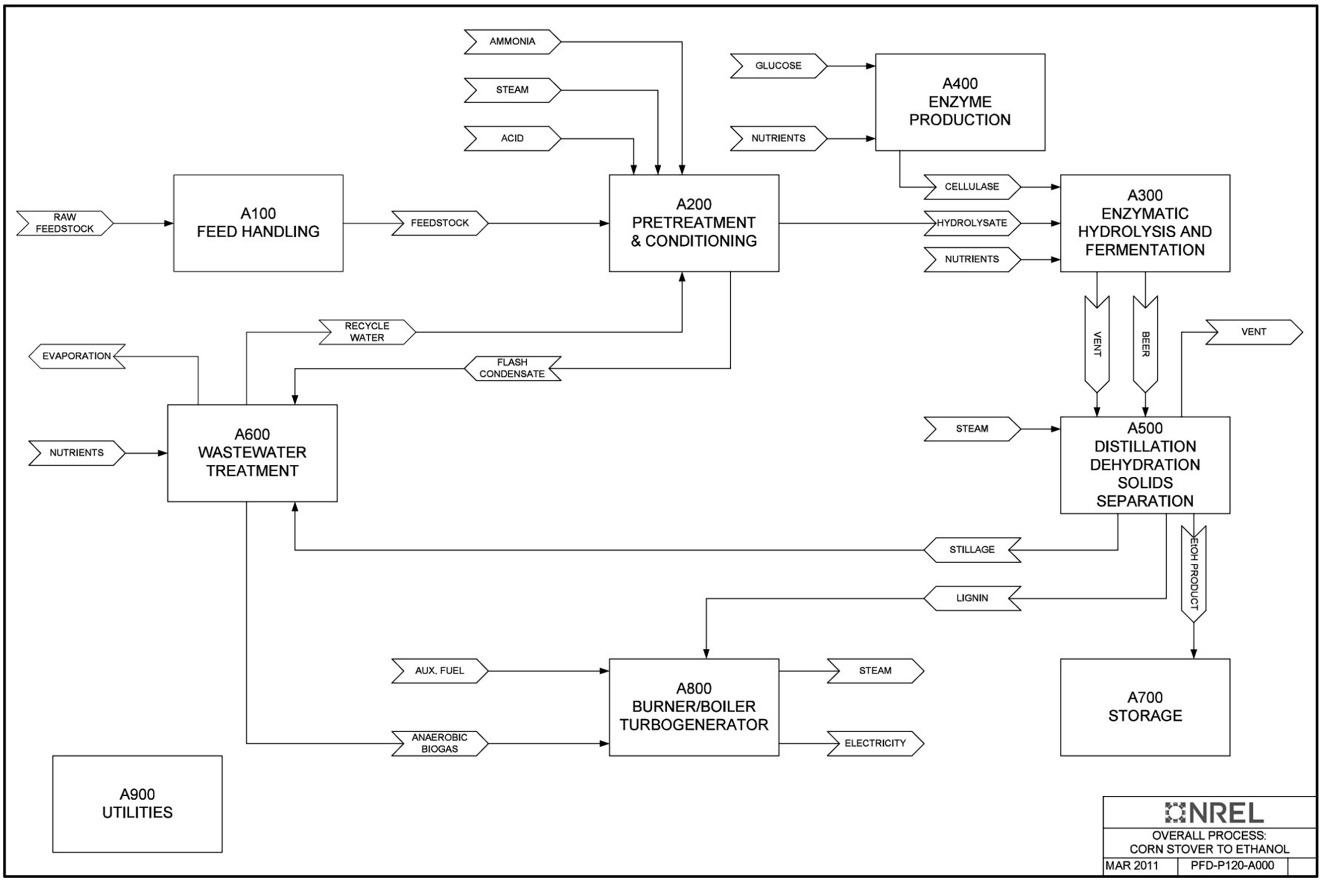

Fig. 1 Ethanol production process reprinted with permission from the National Renewable Energy Laboratory [18]

Table 1 Reaction components used for simulation

Compound	Additional details*
Existing compounds in the software	
Ethanol	MW: 46
Water	MW: 18
Cellulose	MW: 163
CO_2	
Ammonia	
Sulphuric acid	
O_2	
Furfural	
Added compounds in the software	
Glucose	MW: 180
Xylose	MW: 150
Xylan	MW: 132; Formula $C_5H_8O_4$ (monomer)
Lignin	Modelled as vanillin $C_8H_8O_3$
Other sugars (arabinose, mannose, galactose, cellobiose, sucrose)	Arabinose, mannose and galactose modelled as glucose; cellobiose modelled as sucrose
Sugar polymers (glucose oligomers & xylose oligomers)	MW of glucose oligomers: 162; MW of xylose oligomer: 132; Modelled as glucose and xylose
Protein	MW: 22; Formula: $CH_{1.57}O_{0.31}N_{0.29}S_{0.007}$; Modelled for corn protein, cellulose
Biomass	MW: 23; Formula: $CH_{1.64}O_{0.39}N_{0.23}S_{0.0035}$; Modelled for WWT sludge, *Zymomonas mobilis* from fermentation, *Trichoderma reesei* from cellulase production

* MW – molecular weight

exchangers, rectifiers etc. already existed in the DWSIM library. However, the units for the reactions of saccharification, fermentation, and distillation were user-defined (as described in Section 2.5) to simulate the process. The process flow sheet also included a few recycle water streams viz. rectifier bottom to pretreatment tank, saccharified slurry to inoculum, ethanol water vapour to rectifier bottom, scrubber bottom to distillatory vessel.

2.5 Reactions and reactors

The reactions and their rates of conversions were obtained from the NREL report for pretreatment hydrolysis, enzymatic hydrolysis, seed train reactions and co-fermentation reactions (summarised in Part A of the Supporting Information). The inlet flow rates of the components were obtained from the NREL report for simulation. Since the default conversion reactors and CSTRs available with DWSIM had restrictions with the number of input and output streams, to suit the requirement of pretreatment tank, saccharification and fermentation tank, seed fermenter and distillation column, custom unit operations with python script were used to simulate the same. To perform this, the Dummy Unit Operation was selected from the Object Palette in the flowsheet window of the software. After renaming the new unit operation in the Information tab, the Python Script Editor window was opened to input the necessary Python script. The scripts are detailed in Part B of the Supporting Information). The details related to the size of these units are also mentioned in the NREL report.

2.6 Simulation and comparative study

The overall flow sheet of the bioethanol production process that was simulated in DWSIM is given in Fig. 2. The step-by-step flowsheet is presented in Part C of the Supporting Information for better visibility. The streams considered for the analysis were the properties of the outputs from pretreatment (pretreated liquid, blow down slurry, flash tank, hydrolysate, saccharified slurry, fermented liquid, distilled ethanol vapor, rectifier ethanol vapor and dehydrated ethanol. Once the flowsheet was solved, the outlet mass flow rates of each component was obtained from each section and compared with the ASPEN simulated values available in the literature [18]. Further, the difference between the values was calculated using Eq. (1) and reported as error percentage and used for analysis.

$$\%\text{error} = \frac{|a-b|}{100} \tag{1}$$

Where a is the mass flow rate (kg/h) obtained from ASPEN simulation and b is the mass flow rate (kg/h) obtained from DWSIM simulation.

3 Results and discussion

3.1 Simulation results

The results of the mass flow rates of the process reaction components after DWSIM simulation, as well as the values available in the literature are compared in Fig. 3. The percentage of error in the overall mass flow rates ranged between 1 and 8.6, as summarized in Table 2. The highest error was observed for pretreated liquid, contributed by ethanol. Ethanol's contribution to the error percentages was reflected consistently in other streams as well. A deviation of the simulation results was expected to occur due to the omission of certain areas in the original process. Therefore, the recycle stream from the distillation that was directly routed to the pretreatment has led that error to show an effect on other areas.

Because of the omission of the cellulase enzyme production step in DWSIM simulation, the saccharified slurry produced at the end of the simultaneous saccharification and fermentation step is not recycled for cellulase seed production. This has resulted in an error of around 13% in the protein flow rate in saccharified slurry.

3.2 Comparison between Aspen and DWSIM

The report detailed the simulation of biochemical conversion of lignocellulosic biomass (corn stover) to ethanol through a sequential reaction process using DWSIM and a comparison with ASPEN Plus. The simulation process involved the pretreatment of lignocellulosic biomass to separate the cellulose from lignin. And then, the resulting product from the pretreatment reaction was subjected to hydrolysis and fermentation to convert into the desired product ethanol. Simulation of the same process resulted in a minor deviation in DWSIM in comparison with ASPEN Plus. This is primarily because of the omissions of certain reactions from the main process, a few differences in software and their facilities to simulate. Although DWSIM is a chemical process simulator, because of its latest feature of the dynamic property, it was able to simulate any process using Python script editor [13]. Unlike other chemical process software where users have trouble inserting bioreactors and biological compounds, in DWSIM, through Python codes, the user can insert the customized reactors and compounds to simulate the process of interest.

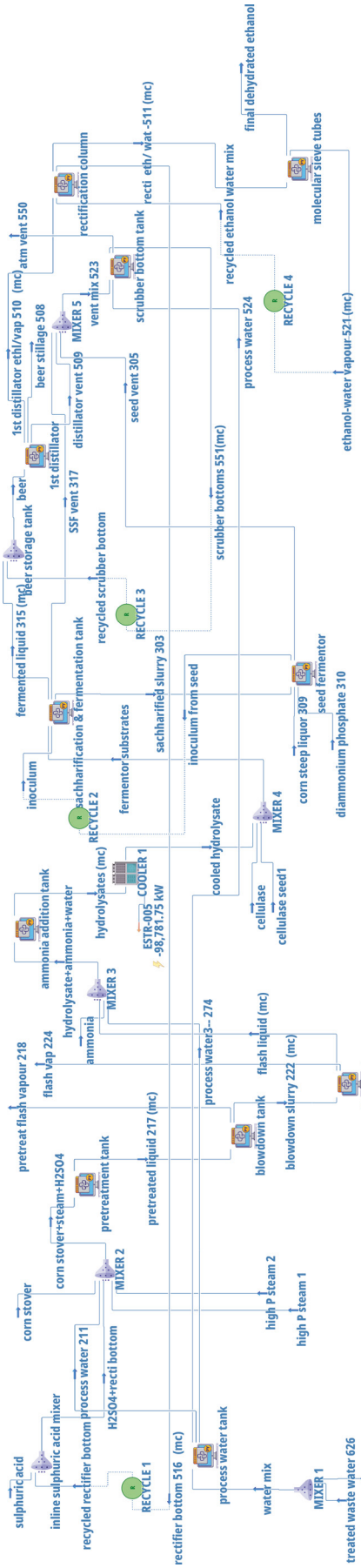

Fig. 2 Overall flowsheet of bioethanol production

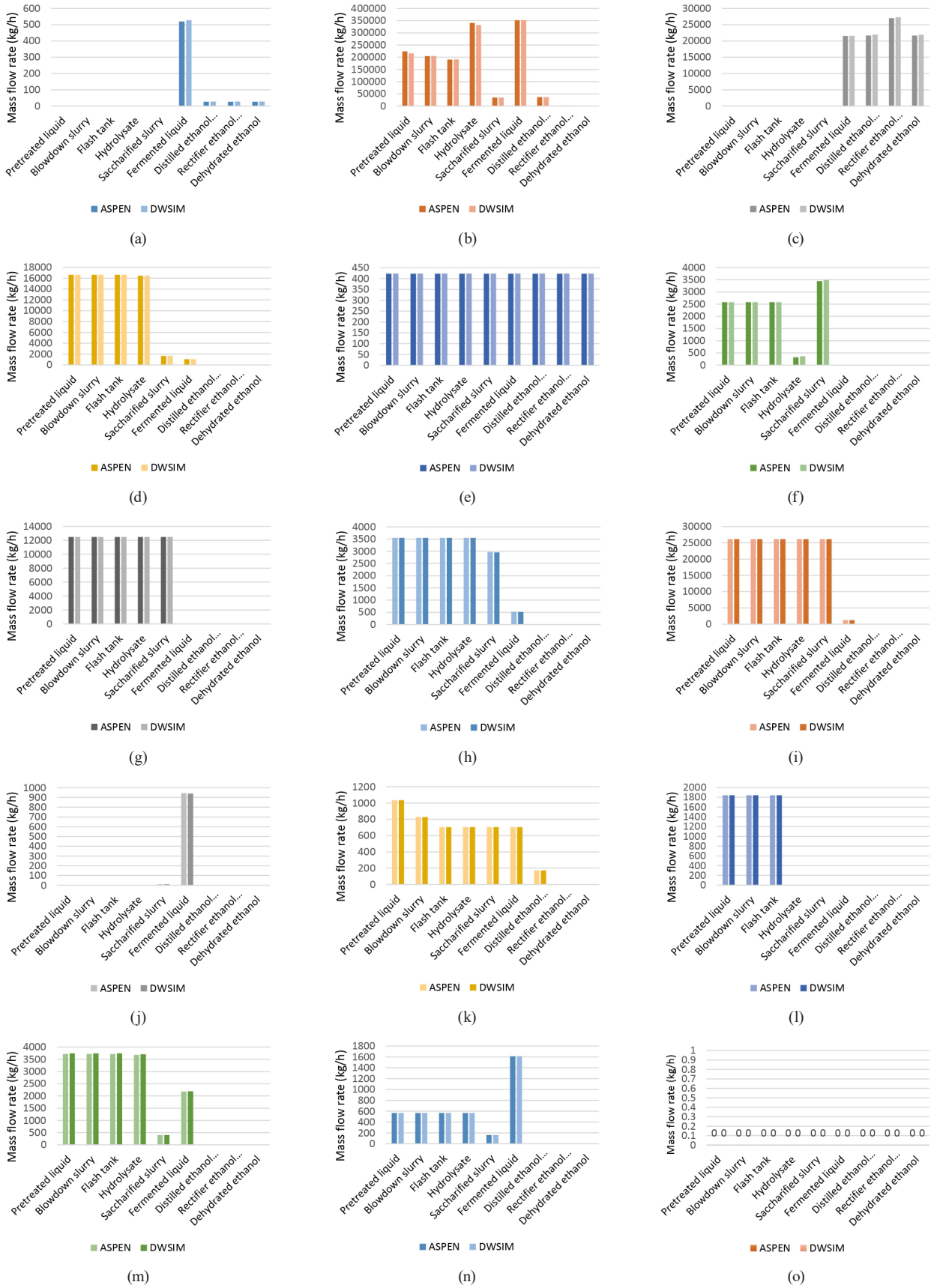

Fig. 3 Comparison of mass flow rates of bioethanol production process in DWSIM and ASPEN: (a) CO_2, (b) water, (c) ethanol, (d) xylose, (e) xylan, (f) protein, (g) lignin, (h) glucose, (i) cellulose, (j) biomass, (k) furfural, (l) sulphuric acid, (m) other sugars, (n) sugar polymers, (o) ammonia

Table 2 Error of mass flow rates of each stream

		Stream (values are in %)								
Sl. No.	Component name	Pretreated liquid	Blowdown slurry	Flash tank	Hydrolysate	Saccharified slurry	Fermented liquid	Distilled ethanol vapor	Rectifier ethanol vapor	Dehydrated ethanol
1	CO_2	0.0	0.0	0.0	0.0	0.0	1.5	4.2	4.2	4.2
2	Water	3.6	0.4	0.4	2.6	0.1	0.1	0.9	0.8	0.7
3	Ethanol	13.9	2.5	14.5	14.5	9.6	0.3	1.2	1.1	1.1
4	Xylose	0.0	0.0	0.0	0.0	0.5	0.3	0.0	0.0	0.0
5	Xylan	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6	Protein	0.0	0.0	0.0	0.0	13.5	1.3	0.0	0.0	0.0
7	Lignin	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
8	Glucose	0.0	0.0	0.0	0.0	0.5	0.7	0.0	0.0	0.0
9	Cellulose	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
10	Biomass	0.0	0.0	0.0	0.0	0.4	0.5	0.0	0.0	0.0
11	Furfural	0.0	0.0	0.0	0.0	0.0	0.3	0.4	0.0	0.0
12	Sulphuric acid	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
13	Other sugars	0.6	0.6	0.6	0.6	0.0	0.6	0.0	0.0	0.0
14	Sugar polymers	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
15	Ammonia	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Total mass flow rate	8.6	6.2	6.5	7.1	4.8	5.8	1.0	1.1	1.1

In the present study, the flow rate deviations are less than 10% and therefore the DWSIM simulation results are acceptable. It has been proven from this study that free and open-source chemical process simulator DWSIM was able to complete tasks similar to the commercial software, Aspen Plus. This study also reports that DWSIM can simulate not only chemical processes but also bioprocess.

4 Conclusion

The study was performed out of the necessity of finding an open-source software for bioprocess simulation. Presently, there are no free open source software available, exclusively for bioprocess simulation. But, this could be compensated for, by utilizing the freely accessible DWSIM. Although DWSIM is used only for chemical process simulation, the same is compatible for bioprocess simulation, as is evident from the study. However, the use of DWSIM is restricted to flowsheeting and material and energy balance calculations. Presently, advanced simulations viz. equipment specification, technoeconomic analysis, sensitivity analysis etc. can only be performed in commercial process simulation software.

Statements and declarations

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Conflict of interest

The authors declare that they have no conflict of interest.

CrediT Author statement

Siddhi Sreemahadevan: Conceptualization, Methodology, Writing – Original Draft Preparation, Writing, Reviewing and Editing, Visualization, Supervision. Krishnapriya Velusamy Sivakumar: Software, Validation, Data Curation, Investigation. Menjith Palanisamy: Software, Validation, Data Curation, Investigation.

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