BIOSTEAM: THE OPEN-SOURCE BIOPROCESS SIMULATION AND TECHNO-ECONOMIC ANALYSIS MODULES IN PYTHON

BY

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THESIS

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ABSTRACT

Preliminary techno-economic analysis (TEA) of a chemical process provides critical information on the economic feasibility, technological bottlenecks, and venture risks due to process uncertainties. Current TEA methods generally rely on proprietary software to evaluate two to three design configurations with single point sensitivity analysis. Such classical methods neglect the effect of process uncertainties and fail to evaluate the complete landscape of design decisions. The limited scope of current literature obscures comparisons between process evaluations and makes it difficult to predict how possible technological developments can impact the sustainability of a process. The main difficulties in adding rigorous uncertainty analysis is high computational time and low rate of successful convergence. Additionally, relying on proprietary software presents both an economic and intellectual barrier for evaluating emerging and conceptual processes. The Bioprocess Simulation and Techno-Economic Analysis Modules, BioSTEAM, is an open-source steady state process simulation package in python for preliminary TEA that will enable rigorous uncertainty analysis through its fast and flexible platform. BioSTEAM presents an intuitive toolset of objects that handle thermodynamic properties, material flows, unit operations, recycle systems, and process specifications. The applicability of BioSTEAM is demonstrated here in the context of a design for the co-production of biodiesel and ethanol from lipid cane. The evaluation of the lipid cane biorefinery in BioSTEAM closely matches a previous evaluation of the design using SuperPro Designer (a proprietary process simulation software). BioSTEAM is well documented and readily available at the Python Package Index, a repository for published Python packages. Although BioSTEAM has not yet incorporated many of the unit operation models presented in proprietary process simulators, its extendable and transparent architecture offers users the power to build new unit operation models and share their designs without any barriers. BioSTEAM may help foster a new open-source community that can accelerate advancements in the field of process design and simulation.

ACKNOWLEDGEMENTS

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CHAPTER 1

INTRODUCTION

1.1 The Need for a Community-Led Simulation Platform

Technological advancements for biorefineries are imperative for the commercialization of biofuels. Techno-economic analysis can reveal process bottlenecks and play a critical role in defining which areas of research should be prioritized. Current approaches to TEAs, however, present only single point evaluations that can lead to misinterpreted comparisons between process evaluations due to different assumptions on technological performance and cost correlations. Additionally, TEA reports are generally based on proprietary process simulation software (e.g., Aspen Plus, SuperPro Designer, Pro/II, CHEMCAD) that range from $1,000-2,000/yr lease. This economic barrier prevents independent groups from reassessing designs to quantity the impact of possible technological improvements. An intellectual barrier also becomes apparent when sharing user defined unit operations and process designs. Most steady state process simulators comply with the CAPE-OPEN standard, an interface blueprint that allows for interoperability between simulation software as well as building user defined unit operations while protecting intellectual property. However, there exist no community platform for sharing unit operations and process designs. Additionally, interfacing adds both computational overhead and development time for the user. These intellectual and economic barriers allow only a restricted set of groups to focus on process evaluation with no clear consensus on key assumptions. The field of process simulation and TEA would benefit from a community-led, open-source software with capabilities that can rival well-established simulation software. Such a software would need to be accessible, well documented, and easily extendable to motivate community involvement to share designs, build unit operation models, and make further improvements.

1.2 Available Open-Source Simulation Software

Several attempts have been made to build an open-source simulation software, most notably SIM42, OPSIM, and DWSIM. The SIM42 project is written in Python 2.2 and includes a thermodynamic server, OLLINTS, essential unit operations, and a flowsheet graphical user interface (GUI). The project was released in 2007 but unfortunately abandoned in 2011. It is difficult to continue the SIM42 project as it does not include a development roadmap and version 2.2 of Python is no longer supported by several applications. OPSIM is an open-source simulation software in development written in pascal. The project began in 2006, and after a decade long hiatus, occasional progress been made with the latest update in August 2018. The capabilities of OPSIM as a process simulator have not been tested as the software is still in its early development stages. DWSIM is a well-established, CAPE-OPEN compliant, open-source process simulation software written in in Visual Basic .NET and C sharp. DWSIM has emerged as a powerful alternative to proprietary simulation software. Since its release in 2008, 13 scientific and technical publications have cited DWSIM. The software includes a rigorous thermodynamic library, essential unit operations, and a capital cost estimation plugin for an additional, yet affordable, fee. Through its CAPE-OPEN interface, it is possible to externally call objects from DWSIM and implement them in another simulation platform. However, the inner architecture of DWSIM is not appropriately built and documented to foster community led development of the software by scientists and engineers moderately skilled in computer science.

1.3 BioSTEAM as a Community-Led Platform for Techno-Economic Analysis

This study showcases BioSTEAM as a fast and flexible platform for preliminary Techno-Economic Analysis. BioSTEAM is a published python package with a transparent and well documented API that facilitates both the creation of new unit operation types and the development of new production processes (Cortes-Pena and Guest 2019) A graphical user interface is not yet available for BioSTEAM, and its usage is mainly through a scriptive IDE. However, flowsheets of all streams, unit operations, and recycle systems can be instantaneously generated during the development of a production process. As a starting point to demonstrate the capabilities of BioSTEAM, a design for the co-production of ethanol and biodiesel from lipid cane is evaluated through BioSTEAM. The results of this evaluation (e.g., material and energy balances, utility requirements, capital cost, etc.) closely match a previous evaluation of the lipid

cane biorefinery in SuperPro Designer (Huang et al. 2016). Differences between both evaluations possibly arise from differences in both the thermodynamic basis and the cost estimation algorithms. BioSTEAM estimates mixture properties through classical mixing rules for computational efficiency. More rigorous thermodynamic packages may use equation of state (EOS) mixing rules that better reflect non-ideal mixing. The data and correlations used to perform cost estimations in BioSTEAM were obtained from a variety of sources which may not necessarily agree with the original design evaluation.

CHAPTER 2

SOFTWARE FRAMEWORK

2.1 Software Overview

BioSTEAM is an installable package written in Python 3.6 that allows the user to design and simulate a production process. An object-oriented approach is taken to organize and abstract implementation details. Data is contained as object attributes, while functional algorithms are stored as object methods. A unified modeling language (UML) class diagram in Figure 1. describes the objects that users interact with in BioSTEAM.

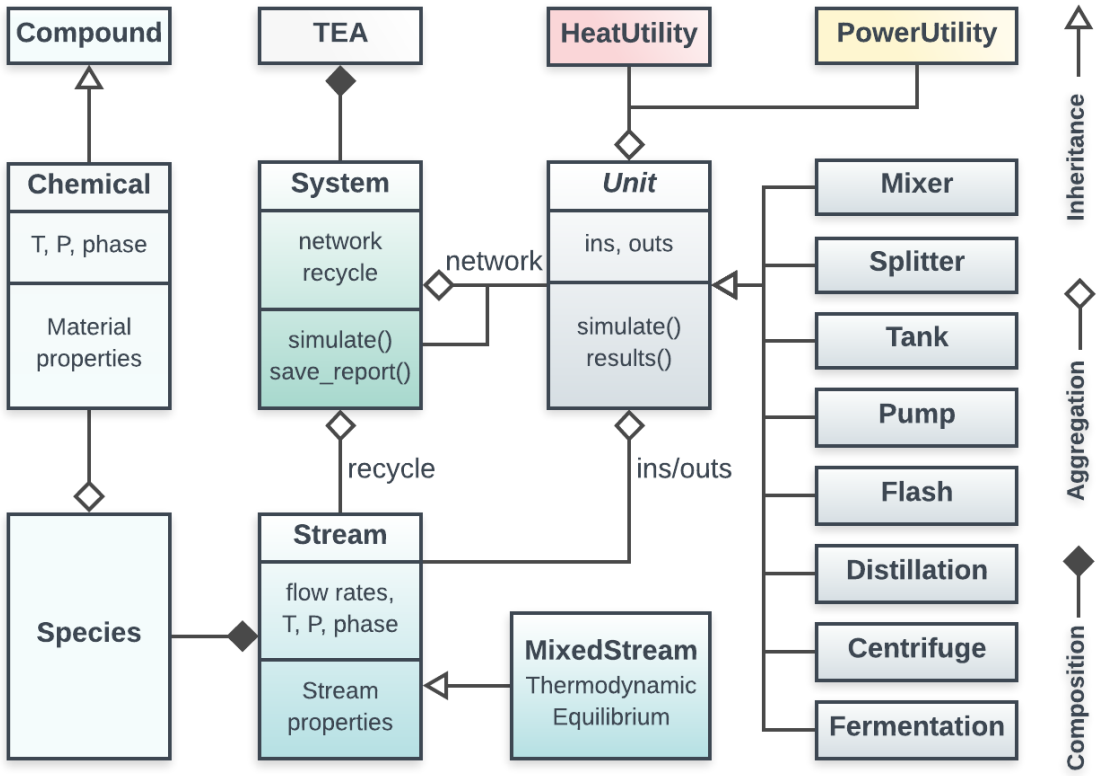

Figure 1. A simplified UML class diagram depicts the core classes of BioSTEAM. Only main attributes and methods are included. Some classes may include only a general description of attributes and methods. In aggregation relationships, the labels represent the attributes where the objects are stored.

To complete TEA of a process, the user must create Species, Stream, Unit, and System objects. A Species object defines all the working compounds of the process. When a Species object is created, it identifies compounds by name (i.e., IUPAC or synonym registered in PubChem, InChI name, InChI key, PubChem CID, SMILES, and CAS) and retrieves all constant and temperature and pressure dependent coefficients from a database. The actual data for pure compound properties are stored as Compound objects within the Species object. The BioSTEAM Chemical class is an extension of the thermo package in Python (Bell 2016), which contains pure component data and material property equations. A Stream object is created by passing material flow rates by compound, a temperature, a pressure, and the phase. Using data from the Species object, Stream objects can estimate mixture thermodynamic and transport properties and perform both vapor-liquid equilibrium (VLE) and liquid-liquid equilibrium (LLE). Before performing any equilibrium calculation, a Stream object is cast to a MixedStream object to enable multiple phase flow rates. A Unit object stores input and output Stream objects as lists in the "ins" and "outs" attributes respectively. Unit subclasses (e.g., heat exchangers, distillation columns, flash vessels, etc.) have additional key arguments and attributes for detailed design and costing. The user should create Unit operations and connect streams as inputs and outputs appropriately. Additionally, the user must make any necessary adjustments to the available heating and cooling agents of the HeatUtility class (e.g., steam pressure, cooling water temperature, price) as well as the electricity price of the PowerUtility class. A System object serves to define a network of unit operations, functions, and subsystems, as well as a recycle stream if any. When a System object is simulated, each element in the network is run sequentially within an iterative solver until the recycle stream converges in terms of both material flow rates and temperature. The use of functions in the network allows for flexible behavior in the process to satisfy process specifications. Subsystems are simply System objects in the network that serve to define recycle loops and help separate key areas of the process. A TEA object can be created from a System object to perform cashflow analysis given a set of options.

2.2 Thermodynamic framework

Thermodynamic properties of pure compounds are estimated through the thermo package of the Chemical Engineering Design Library in Python (Bell 2016). The thermo package includes a database of (70,000+) chemicals taken from the PubChem database. Unfortunately,

only ~20,000 of those have even one chemical property apart from metadata (molecular weight, etc.). Peng Robinson is the default EOS of all pure components initialized by a Species object. To facilitate the calculation of mixture properties, BioSTEAM estimates mixture properties mainly by assuming a molar weighted average of the chemical property as well as other classical ideal mixing rules. For computational efficiency, reduced temperature coefficients of the EOS model are not recalculated at each temperature. Instead, BioSTEAM assumes the reduced temperature is constant unless specified otherwise. Excess thermodynamic energies due to high pressures are also neglected by default. Because a typical fuel ethanol biorefinery operates at moderate temperatures and pressures, these simplifications may not have a significant effect on process estimations. Phase equilibrium calculations are based on modified Raoult's law with activity coefficients estimated through Dortmund UNIFAC interaction parameters. Modified Raoult's law is suitable to estimate VLE of non-ideal mixtures under low to moderate pressures. At high pressure, gaseous non-idealities become more significant at higher pressures. UNIFAC interaction parameters are appropriate for compounds with low to moderate molecular weights. Structural effects become more significant at higher molecular weights. Modified Raoult's law is an appropriate VLE model for the lipid cane biorefinery because the biorefinery mainly concerns mixtures of highly polar compounds with low to moderate molecular weights (i.e., water, methanol, ethanol, and glycerol) at atmospheric pressures.

2.3 Unit Operations

BioSTEAM includes classes of all unit operation required to perform TEA of the lipid cane biorefinery. The modeling rigor and design detail varies greatly between unit operations. Essential unit operations including pumps, heat exchangers, flash vessels, and distillation columns are some of the most rigorously modeled and designed. Other unit operation models are based on component splits (i.e., a specified fraction of each component entering a unit is separated) and the purchase price is estimated using size factor correlations that are ultimately a function of material flow rates. Most unit operation cost correlations and models were adapted from design textbooks and literature (Seider et al. 2017, Apostolakou et al. 2009, Haas et al. 2006, Svrcek 1993).

A variety of pumps are available in BioSTEAM, including centrifugal, metering plunger, and screw pumps. By default, a pump type is selected based on the outlet pressure requirement,

the inlet pressure, and the flow rate. Precedence is given to centrifugal pumps. A standard motor size from the National Electrical Manufactures Association (NEMA) is selected such that it meets the power requirement after accounting for pump break and motor efficiency. A variety of vacuum systems based on air leakage and vapor suction are also available.

Heat exchangers are modeled using counter current configuration, a default pinch temperature of 5 ºC, and a default minimum temperature difference of 10 ºC between utility and process fluids before entry. These assumptions are enough to calculate the duty (heat transfer requirement) of a heat exchanger through an energy balance coupled with phase equilibrium, if necessary. The area requirement is then solved using the heat transfer equation with an overall heat transfer coefficient from tabulated heuristics and a log mean temperature difference (LMTD) correction factor estimated through the Fakheri equaition (Seider 2017).

Flash vessels are designed to minimize entrainment of liquid droplets in the vapor. Vapor liquid separation is accomplished in three stages. The first stage is at the inlet diverter, where the largest droplets impinge on the diverter and drop by gravity. The second stage is gravity separation of smaller droplets as vapor flows through the disengagement area. The final stage is mist elimination where the smallest droplets coalesce and fall by gravity. Design of the necessary disengagement area, minimum and maximum liquid levels, and the allowable vapor velocity is based on a heuristic procedure outlined in Chemical Engineering Progress (Svrcek et al. 1993). The purchase cost of a flash vessel is based on its weight, as calculated from its design requirements and the ASME pressure vessels code.

Distillation columns are modeled as binary separation columns, assuming all light and heavy non-keys are completely separated to the top and bottoms product respectively. McCabe-Thiele analysis is used to find both the number of stages and the reflux ratio given a ratio of actual reflux to minimum reflux and percent recoveries (Perry 2018). This method assumes that saturated liquid and vapor enthalpy curves are parallel throughout the column, and that the column operates at both adiabatic and isobaric conditions. The lipid cane biorefinery uses distillation columns for the separation of Ethanol/Water, Water/Glycerol, and Methanol/Water/Glycerol with Glycerol as a heavy non-key. Preliminary analysis showed that the theoretical number of stages using this method is off by less than +/-1 stage for all distillation systems at the given reflux ratio. More rigorous validation for the use of this method on these

systems would be necessary to perform optimization and sensitivity analysis around distillation column design and operation. The Murphree efficiency (i.e., tray efficiency) is based on the modified O'Connell correlation (Duss et al. 2018). The diameter is based on the tray separation and flooding velocity (Perry 2018).

CHAPTER 3

TECHNO-ECONOMIC ANALYSIS OF THE LIPID CANE BIOREFINERY

3.1 Lipid Cane Biorefinery Overview

In summary, the lipid cane biorefinery can be divided into 5 main areas: feedstock handling, oil/sugar separation, ethanol production, biodiesel production, and electricity co-generation system (Figure 2). The complete flowsheet with stream tables is presented in Appendix A. In feedstock handling, the lipid cane in belt conveyed to the biorefinery and shredded. During oil and sugar separation, the lipid cane is treated with hot water and proteases, then crushed to extract the juice. The bagasse is screened out, and the juice is further treated to remove impurities. The bagasse is burned to produce steam and electricity. The oil and sugar solution is separated by a settler. The sugar solution is fermented and distilled. The oil is trans-esterified with methanol and sodium methoxide catalyst to produce biodiesel and glycerol. The biodiesel centrifuged out, washed and vacuum dried. The glycerol is distilled to 80% by mass and sold as crude glycerol.

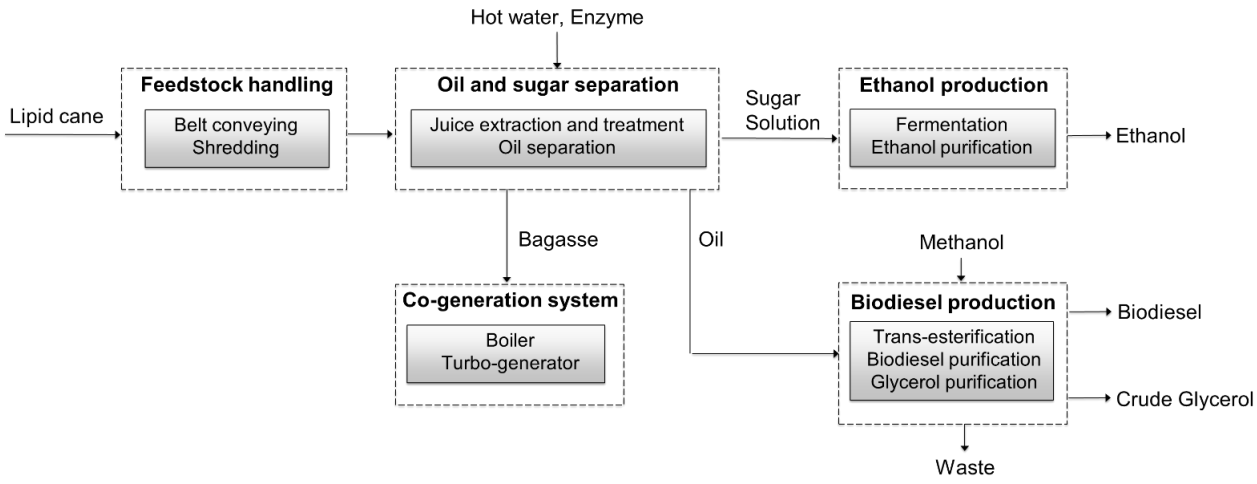

Figure 2. A simplified flowsheet depicts the 5 main areas of the lipid cane biorefinery.

In addition to these areas, the lipid cane biorefinery includes on-site recirculation of cooling water. The capital cost of the cooling tower and the electricity cost of water recirculation is also accounted for in Techno-economic analysis.

3.2 Techno-Economic Analysis Assumptions

All techno-economic assumptions outlined in the original evaluation of the lipid cane biorefinery were used in BioSTEAM's evaluation. The evaluation scripts are available as the lipidcane package in the Python Package Index (Cortes-Pena and Guest 2019). These assumptions include, but are not limited to, process specifications, utility conditions, chemical prices, labor, tax, and depreciation schedule. A key assumption by Huang et al. is the effect of lipid content on the overall composition of lipid cane. In summary, an energy balance is used to equivalate an increase in lipid content to a decrease in sucrose content. Because lipid is more energy dense than sucrose, there is a loss of biomass with an increase in lipid content. This loss is compensated by fiber to maintain the same biomass yield. The construction material for all centrifuges and vessels (i.e., mixing and storage tanks, flash vessels, and distillation columns) in the biorefinery is stainless steel SS304. This selection is based on previous TEA reports concerning ethanol and biodiesel production (Humbird et al. 2011, Apostolakou et al. 2009, Haas et al. 2006). While most unit operation cost correlations were adapted from design textbooks and literature, certain unit operations were cost based on six tenths rule exponential scaling including, shredders, crushing mills, fermentation reactors, and molecular sieves (Humbird 2011, Huang 2016). The scenarios evaluated in this report along with their respective assumptions are used to test BioSTEAM's predictions with the original evaluation and do not reflect the authors' judgement of the process.

3.3 Results and Discussion

The cost assessments presented in this study represent a preliminary (order-of-magnitude) evaluation. Preliminary evaluations are typically within +/- 30% of the actual venture cost and are used to make coarse choices between design alternatives. No detailed quotations are necessary for a preliminary evaluation. In general, the evaluation using BioSTEAM and the previous evaluation by Huang et al. in SuperPro Designer shows comparable results and trends. The main scenarios compared are at a feedstock lipid composition of 2%, 5%, and 10% dry

weight. BioSTEAM's economic assessment shows a more pronounced trend of increasing internal return on investment (IRR) with lipid content (Figure 3). The IRR of both evaluations are most similar at 5% lipid.

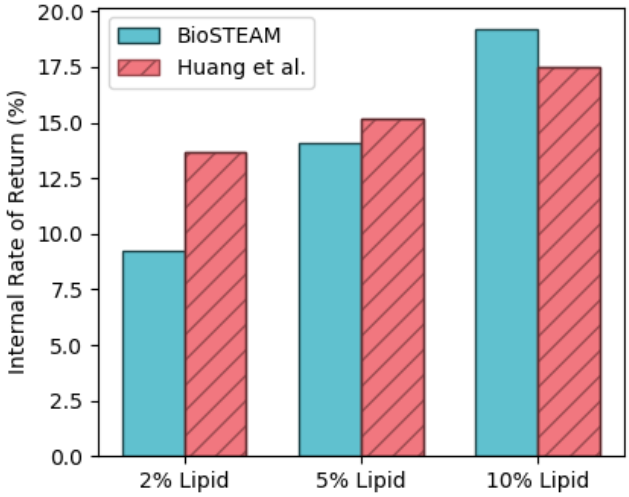

Figure 3. Bar chart of the IRR at 2%, 5%, and 10% feedstock lipid content as evaluated by BioSTEAM in this study and Huang et al. in SuperPro Designer. Both studies show an upward trend of increasing IRR with lipid cane content. This trend is more pronounced in BioSTEAM.

The material flows in BioSTEAM closely match the previous evaluation in SuperPro Designer with no significant difference in product yields as depicted in stream tables in Appendix A. Therefore, the economic differences must stem from capital cost and utility cost estimates. In general, the additional revenue of producing more biodiesel is offset by a higher capital investment. The detailed capital cost estimates show that BioSTEAM has a weaker trend of increasing capital cost with lipid content. Therefore, the lower sensitivity of capital cost to lipid content results in a stronger IRR sensitivity to lipid content in BioSTEAM.

Table 1. The itemized equipment cost of key areas are listed for 2%, 5%, and 10% feedstock lipid content. The capital cost increases with lipid content more pronouncedly in BioSTEAM.

	2% Lipid		5% Lipid		10% Lipid	
	BioSTEAM	Huang et al.	BioSTEAM	Huang et al.	BioSTEAM	Huang et al.
Feedstock handling	2.5	2.5	2.5	2.5	2.5	2.5
Oil/sugar separation	8	8.2	7.8	8.4	7.6	8.6
Ethanol production	8.6	10	8	8.5	7.1	7.5
Biodiesel production	2.2	1.4	2.4	2.3	2.7	3.4
Co-generation system	32.8	29.7	33.8	31.5	35.8	36
Storage	1.6	1.3	1.9	1.7	2.2	2
Utilities	1.7	1.7	1.8	1.7	1.8	1.9
Total equipment cost	57.7	54.9	58.5	56.6	59.8	61.9
Fixed capital investment (3x total equipment cost)	173.2	164.7	175.5	169.8	179.6	185.7
Working capital	8.6	8.2	8.7	8.5	8.9	9.3
Total capital investment	181.9	172.9	184.3	178.3	188.6	195

The steam utility requirement in BioSTEAM is almost 90,000 metric tons less than the previous evaluation in SuperPro Designer at 10% feedstock lipid content (Table 2). This result can be attributed to the differences in distillation column models. Distillation columns in the process consume more than half the total steam requirement. Huang et al. makes use of shortcut columns in SuperPro Designer. Shortcut methods, such as the Fenske-Underwood-Gilliland, assume a constant volatility across stages. However, the volatility of the highly polar mixtures present in the biorefinery vary greatly at different compositions. It is possible that the steam requirements in the original study are overly conservative due to the use of semi-rigorous methods for solving distillation columns.

Table 2. The steam and electricity requirements are listed at a 10% feedstock lipid composition. Demand is lower for steam and higher for electricity in BioSTEAM.

Utilities at 10% Lipid	Steam MT yr^{-1}	Consumed electricity MWhr	Surplus electricity MWhr
BioSTEAM	568,923	114,569	260,985
Huang et al.	656,000	52,644	208,000

Because the steam requirement is lower in BioSTEAM, more electricity can be produced by the turbo-generator. The electricity requirement in BioSTEAM, however is two times higher than the evaluation in SuperPro Designer. This result is possibly due to conservative estimates in power requirements for the cooling tower, mixing tanks, and centrifuges. Even with these differences in utility requirements, the operating cost of BioSTEAM closely matches the evaluation by Huang et al. (Table 3). The annual costs of feedstocks and chemicals may be different between studies because original study reported prices with only two significant digits.

Table 3. The annual costs of the biorefinery are listed at a 10% feedstock lipid composition.

Annual costs at 10% lipid	BioSTEAM 10^6 USD yr^{-1}	Huang et al. 10^6 USD yr^{-1}
Feedstock	56.0	55.3
Chemicals	7.1	6.2
Utilities	0.6	0.2
Labor	3.5	3.5
Supplies	2.3	2.4
General works	2.0	2.0
Capital charges (Depreciation)	9.0	9.3
Co-product credit	-18.2	-14.6
Total operating cost	62.3	64.3

The production costs of ethanol and biodiesel in BioSTEAM closely match with the previous evaluation in SuperPro Designer. Production costs in BioSTEAM also display a stronger

sensitivity to differences in lipid composition (Figure 4), which agrees with the effect of lipid composition on IRR.

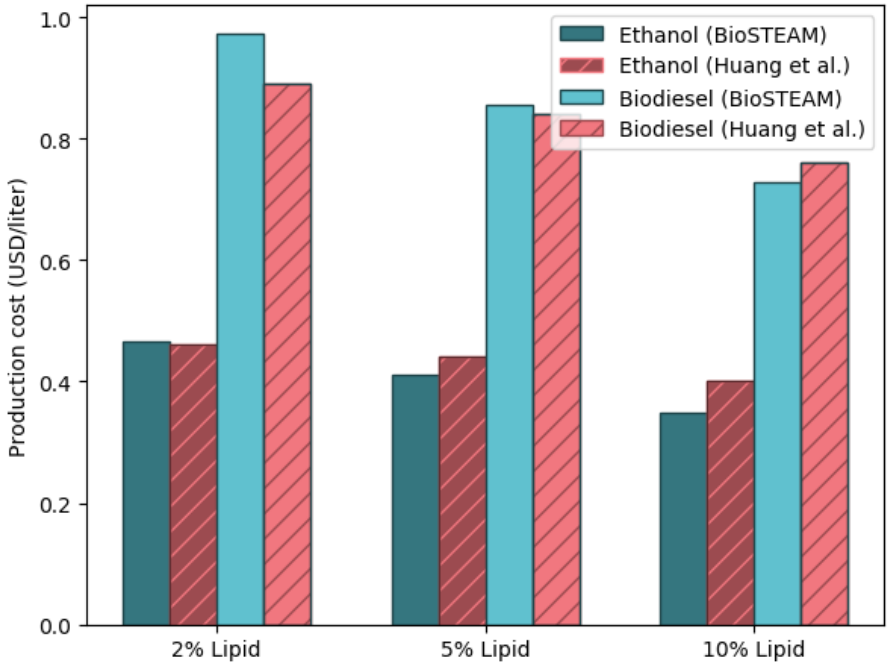

Figure 4. Bar chart of ethanol and biodiesel production costs at 2%, 5%, and 10% feedstock lipid composition, as evaluated in BioSTEAM and by Huang et al. in SuperPro Designer.

Single point sensitivity analysis around uncertain parameters illustrates the effect of different assumptions between BioSTEAM and the previous evaluation in SuperPro Designer (Figure 5). Sensitivity around all parameters appear to have similar magnitudes, except for both lipid extraction rate and annual crushing capacity.

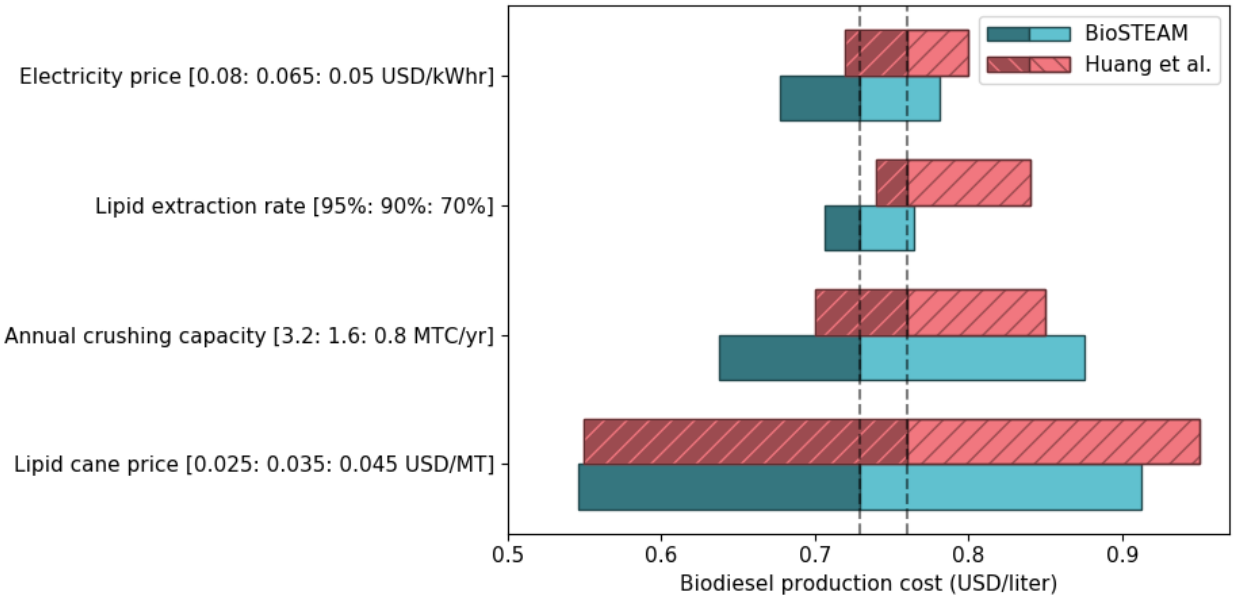

Figure 5. The bar chart shows single point sensitivity analysis of biodiesel production cost to key parameters at 10% feedstock lipid content. BioSTEAM displays higher sensitivity to annual crush capacity and lower sensitivity to lipid extraction rate compared to the previous study in SuperPro Designer.

Differences in sensitivity may arise from the different design and cost models implemented in BioSTEAM as well as from the difference in production cost at the baseline (i.e., the sensitivity center point). In general, however, a more rigorous uncertainty analysis around all parameters used in lipid cane biorefinery would provide a more transparent overview of the process. Current work in BioSTEAM is aimed at incorporating global uncertainty analysis as one of its main features.

3.4 Computational Efficiency

The lipid cane biorefinery includes 4 recycle systems, 93 unit operations, and 88 streams. BioSTEAM can complete the simulation of the whole biorefinery and solve for the internal rate of return (IRR) within ~750 millisecond without any initial recycle estimates, and within ~130 millisecond to reevaluate the solved biorefinery system. These measurements were made using an Intel Core i7-8750H CPU at 2.20GHz processor and a 16.0 GB RAM. Although it may seem contradictory for a process simulation platform built on a dynamic programing language like Python to have fast performance in comparison to software built on compiled languages with

static-typing, BioSTEAM takes a wide range of approaches to skip unnecessary calculations, cache and reuse information, and speed up simulation. Given a set of simulation arguments, Unit objects calculate and store the simulation parameters that will be used across runs during convergence. Additionally, unit operations only perform the necessary calculations required for mass and energy balances during recycle convergence. Only after a System object has finished converging, design requirements and capital cost of unit operations are found. In thermodynamic equilibrium calculations of a Stream object, the last equilibrium solution is used as an initial estimate for the next. Lastly, for unit operations that do not make changes to Stream objects, input and output Stream objects share the same data space instead of copying data. This last efficiency approach not only speeds up simulation, but also decreases the memory needs.

CHAPTER 4

BIOSTEAM ROADMAP

The core components of BioSTEAM, as presented in the UML diagram, are considered a stable framework for future versions. Except for Unit subclasses, all public attributes and method which constitute the application program interface (API) will be maintained in future versions as well. Future developments to unit operations are geared towards separations. More rigorous models for multi-component distillation are critical for predicting separations of a wider set of compounds. Additionally, accurate thermodynamic models for solid-liquid, liquid-liquid, and vapor-liquid-liquid equilibrium will be incorporated to enable the evaluation of wider set of bioproducts. Currently, BioSTEAM's liquid-liquid equilibrium model cannot guarantee a correct prediction due to difficulties in finding a stable minimum of the objective function.

The thermodynamic implementation details that are hidden to the user are subject to considerable change in future versions. Mainly, BioSTEAM needs to make available more thermodynamic models for estimating mixture properties and thermodynamic equilibrium. For example, implementing EOS mixture models would provide more accurate prediction of mixture properties that would enhance accurate design of unit operations. Incorporating EOS mixture models would also address gaseous non-idealities in equilibrium models. The future thermodynamic framework of BioSTEAM will implement the Species object as a flexible thermodynamic package for Stream objects to depend on. Stream objects will interface with the Species object for modular implementation of thermodynamic models.

The implementation details of the Unit class is considered a stable and transparent framework for creating new Unit subclasses. The creation of new unit operation classes will continue to function in future versions of BioSTEAM. Complete documentation with examples is available for the development on new unit operations (Cortes-Pena and Guest 2019).

At the flowsheet level, System objects are also stable. Currently, System objects require that the user specify a recycle stream, and the order that units in the network run. Future efforts will focus on automatically ordering the sequence and identifying recycle streams for iterative

convergence. This development would enhance user experience in developing a production process. Currently, System objects have the option to use either fixed point or Wegstein iterative solvers. Other iterative solvers such as Broyden's method can be incorporated for faster convergence of non-linear systems.

Capital cost estimation in BioSTEAM is limited to the Lang factor method, whereby the total fixed capital investment is estimated by multiplying the total purchase cost of all units by a Lang factor particular to the process. For dynamic assessment of different technologies and configurations, the use factored-cost methods is more appropriate. For each piece of equipment, the factored-cost method estimates the direct costs of materials and labor, as well as indirect costs of installation as a factor of the free on board (f.o.b.) purchase cost of the equipment. Future versions of BioSTEAM will make this method available for all unit operations.

A crucial limitation in classical TEA reports is that their preliminary nature is not subject to rigorous uncertainty and sensitivity analysis. Incorporating these analyses would enhance comparison between different product and process designs. Although most process simulation software are equipped with tools to analyze techno-economic uncertainties, these tools are difficult to implement for the complete landscape of scenarios. The main limitations are low convergence success rate, and high computation time. Future versions of BioSTEAM will offer a straight forward way of adding parameter distributions, while maintaining convergence success, and minimizing computational burden.

CHAPTER 5

CONCLUSION

BioSTEAM presents a viable alternative process simulation software for fast and flexible preliminary TEA. The simulation of the lipid cane biorefinery includes mass and energy balances for large a set of chemical species, solving rigorous vapor-liquid equilibrium, solving rigorous unit operations models, and converging multiple recycle systems. BioSTEAM is capable of simulating this complex biorefinery in less than a second. The unit operation models and thermodynamic framework was shown to provide comparable results to the previous evaluation of the lipid cane biorefinery in SuperPro Designer. However, further developments must be made to this open-source software for it can rival well-established simulation software and benefit the general scientific community. The downloadable version of BioSTEAM in the Python Package Index (PyPI) is a stable prerelease that can be improved and extended to allow the evaluation of other production processes. With its accessible, well documented, and easily extendable framework, BioSTEAM has the potential to become a community led platform for process simulation and TEA. BioSTEAM may foster community involvement to share designs, build unit operation models, and standardize the field of process design.

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APPENDIX A

FLOWSHEETS AND STREAM TABLES

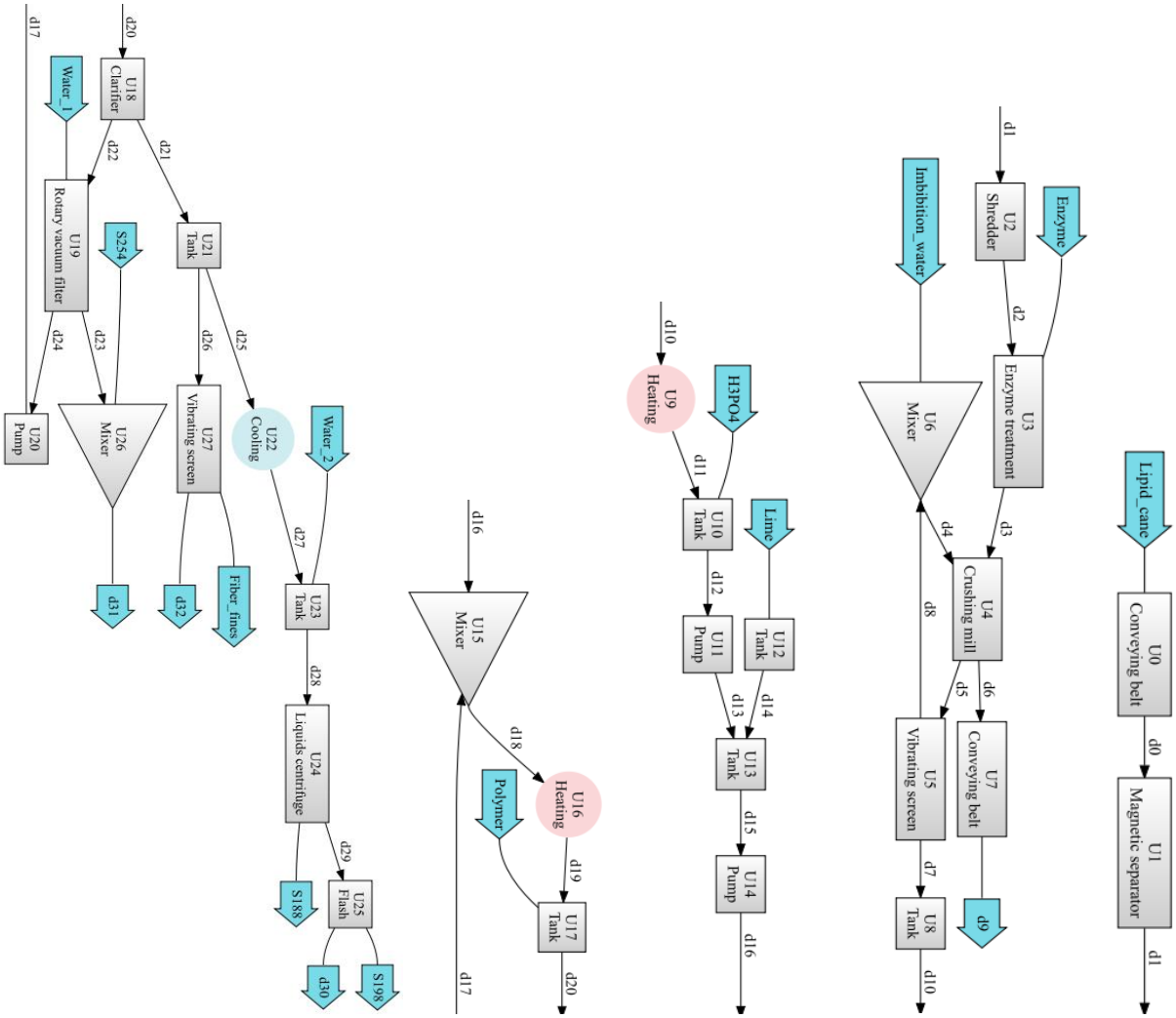

Figure 6. Flowsheet for feedstock handling and oil and sugar separation. The flowsheet is split to fit in the page.

Table 4. Stream table for feedstock handling and oil/sugar separation.

	H3PO4	Lime	Polymer	Water_1	Water_2	Fiber_fines	Combustibles
Source	-	-	-	-	-	U27	-
Sink	U10	U12	U17	U19	U23	-	BT*
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	25.00	25.00	25.00	90.00	85.00	99.00	58.54
flow (kg/min)	1.46	42.22	0.01	256.63	22.50	9.68	2375.02
Composition:							
- Glucose	0.000	0.000	0.000	0.000	0.000	0.007	0.001
- H3PO4	0.850	0.000	0.000	0.000	0.000	0.000	0.000
- Flocculant	0.000	0.000	1.000	0.000	0.000	0.001	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Lignin	0.000	0.000	0.000	0.000	0.000	0.000	0.099
- Solids	0.000	0.000	0.000	0.000	0.000	0.000	0.035
- Sucrose	0.000	0.000	0.000	0.000	0.000	0.080	0.009
- CaO	0.000	0.131	0.000	0.000	0.000	0.000	0.002
- Ash	0.000	0.000	0.000	0.000	0.000	0.000	0.022
- Cellulose	0.000	0.000	0.000	0.000	0.000	0.000	0.186
- Hemicellulose	0.000	0.000	0.000	0.000	0.000	0.000	0.109
- Lipid	0.000	0.000	0.000	0.000	0.000	0.000	0.007
- Water	0.150	0.869	0.000	1.000	1.000	0.912	0.529

*BT refers to the boiler and turbo-generator in the electricity co-generation area.

Table 4. Continued

	Emission	Lipid_cane	Enzyme	Imbibition_water	d0	d1
Source	BT	-	-	-	U0	U1
Sink	-	U0	U3	U6	U1	U2
Phase	gas	liquid	liquid	liquid	liquid	liquid
T (degC)	25.00	25.00	25.00	65.00	25.00	25.00
flow (kg/min)	2375.02	5555.56	16.67	1450.39	5555.56	5555.56
Composition:						
- Glucose	0.001	0.006	0.000	0.000	0.006	0.006
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000
- Flocculant	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000
- Lignin	0.099	0.042	0.000	0.000	0.042	0.042
- Solids	0.035	0.015	0.000	0.000	0.015	0.015
- Sucrose	0.009	0.073	0.000	0.000	0.073	0.073
- CaO	0.002	0.000	0.000	0.000	0.000	0.000
- Ash	0.022	0.010	0.000	0.000	0.010	0.010
- Cellulose	0.186	0.079	0.100	0.000	0.079	0.079
- Hemicellulose	0.109	0.047	0.000	0.000	0.047	0.047
- Lipid	0.007	0.028	0.000	0.000	0.028	0.028
- Water	0.529	0.700	0.900	1.000	0.700	0.700

Table 4. Continued

	d2	d3	d4	d5	d6	d7	d8	d10
Source	U2	U3	U6	U4	U4	U5	U5	U8
Sink	U3	U4	U4	U5	U7	U8	U6	U9
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	25.00	50.00	61.47	53.79	53.79	53.79	53.79	53.79
flow (kg/min)	5555.56	5572.22	2219.60	5632.24	2159.58	4863.03	769.21	4863.03
Composition:								
- Glucose	0.006	0.006	0.002	0.007	0.001	0.007	0.006	0.007
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Flocculant	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Lignin	0.042	0.042	0.006	0.004	0.106	0.001	0.017	0.001
- Solids	0.015	0.015	0.000	0.000	0.039	0.000	0.000	0.000
- Sucrose	0.073	0.073	0.024	0.079	0.009	0.080	0.069	0.080
- CaO	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ash	0.010	0.009	0.001	0.001	0.024	0.000	0.004	0.000
- Cellulose	0.079	0.079	0.011	0.007	0.198	0.003	0.031	0.003
- Hemicellulose	0.047	0.047	0.006	0.004	0.116	0.002	0.018	0.002
- Lipid	0.028	0.027	0.008	0.027	0.008	0.028	0.024	0.028
- Water	0.700	0.701	0.941	0.872	0.500	0.879	0.830	0.879

Table 4. Continued

	d11	d12	d13	d14	d15	d16	d17	d18
Source	U9	U10	U11	U12	U13	U14	U20	U15
Sink	U10	U11	U13	U13	U14	U15	U15	U16
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	70.00	70.00	70.00	25.00	69.61	69.61	98.43	83.66
flow (kg/min)	4863.03	4864.48	4864.48	42.22	4906.70	4906.70	4530.13	9436.83
Composition:								
- Glucose	0.007	0.007	0.007	0.000	0.007	0.007	0.007	0.007
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Flocculant	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Lignin	0.001	0.001	0.001	0.000	0.001	0.001	0.000	0.001
- Solids	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Sucrose	0.080	0.080	0.080	0.000	0.079	0.079	0.077	0.078
- CaO	0.000	0.000	0.000	0.131	0.001	0.001	0.000	0.001
- Ash	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Cellulose	0.003	0.003	0.003	0.000	0.003	0.003	0.001	0.002
- Hemicellulose	0.002	0.002	0.002	0.000	0.002	0.002	0.000	0.001
- Lipid	0.028	0.028	0.028	0.000	0.028	0.028	0.001	0.015
- Water	0.879	0.879	0.879	0.869	0.879	0.879	0.914	0.896

Table 4. Continued

	d19	d20	d21	d22	d23	d24	d25	d26
Source	U16	U17	U18	U18	U19	U19	U21	U21
Sink	U17	U18	U21	U19	U26	U20	U22	U27
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	99.00	99.00	99.00	99.00	98.43	98.43	99.00	99.00
flow (kg/min)	9436.83	9436.84	4970.79	4466.06	215.43	4530.13	136.34	4834.45
Composition:								
- Glucose	0.007	0.007	0.007	0.007	0.001	0.007	0.000	0.007
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Flocculant	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Lignin	0.001	0.001	0.000	0.002	0.032	0.000	0.000	0.000
- Solids	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Sucrose	0.078	0.078	0.078	0.079	0.016	0.077	0.000	0.080
- CaO	0.001	0.001	0.000	0.001	0.026	0.000	0.000	0.000
- Ash	0.000	0.000	0.000	0.000	0.007	0.000	0.000	0.000
- Cellulose	0.002	0.002	0.000	0.003	0.060	0.001	0.000	0.000
- Hemicellulose	0.001	0.001	0.000	0.002	0.036	0.000	0.000	0.000
- Lipid	0.015	0.015	0.027	0.001	0.000	0.001	0.997	0.000
- Water	0.896	0.896	0.888	0.904	0.821	0.914	0.003	0.913

Table 4. Continued

	d27	d28	d29	S188	S198	S254
Source	U22	U23	U24	U24	U25	-
Sink	U23	U24	U25	-	-	U26
Phase	liquid	liquid	liquid	liquid	gas	liquid
T (degC)	70.00	74.99	74.99	74.99	74.00	25.00
flow (kg/min)	136.34	158.84	134.77	24.07	0.24	0.02
Composition:						
- Glucose	0.000	0.000	0.000	0.000	0.000	0.000
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000
- Flocculant	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000
- Lignin	0.000	0.000	0.000	0.000	0.000	0.000
- Solids	0.000	0.000	0.000	0.000	0.000	0.000
- Sucrose	0.000	0.000	0.000	0.000	0.000	0.000
- CaO	0.000	0.000	0.000	0.000	0.000	0.000
- Ash	0.000	0.000	0.000	0.000	0.000	1.000
- Cellulose	0.000	0.000	0.000	0.000	0.000	0.000
- Hemicellulose	0.000	0.000	0.000	0.000	0.000	0.000
- Lipid	0.997	0.856	0.998	0.056	0.056	0.000
- Water	0.003	0.144	0.002	0.944	0.944	0.000

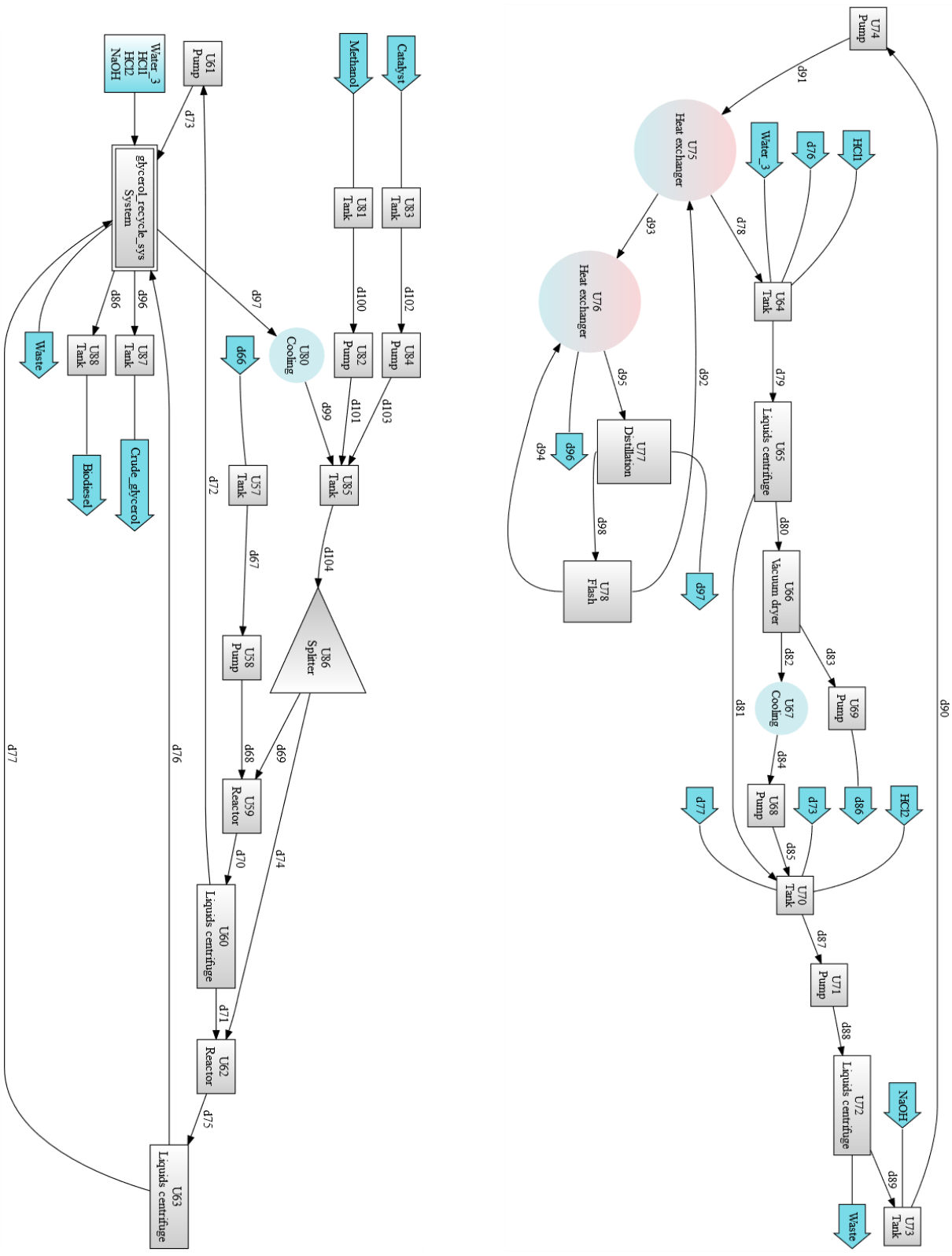

Figure 7. Flowsheet for biodiesel production. The flowsheet on the left is the complete biodiesel production system with a subsystem called “glycerol_recycle_sys”. This subsystem is represented in the flowsheet on the right.

Table 5. Stream table for the biodiesel production section

	Methanol	Catalyst	Water_3	HCl1	HCl2	NaOH	Crude_glycerol	Biodiesel
Source	-	-	-	-	-	-	U87	U88
Sink	U81	U83	U64	U64	U70	U73	-	-
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	25.00	25.00	60.00	25.00	25.00	25.00	6.26	58.35
flow (kg/min)	3.01	2.53	4.08	0.36	0.36	0.67	19.63	146.18
Composition:								
- Lipid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Methanol	1.000	0.750	0.000	0.000	0.000	0.000	0.000	0.000
- Glycerol	0.000	0.000	0.000	0.000	0.000	0.000	0.773	0.000
- Biodiesel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	1.000
- Water	0.000	0.000	1.000	0.650	0.650	0.000	0.193	0.000
- NaOH	0.000	0.000	0.000	0.000	0.000	1.000	0.034	0.000
- HCl	0.000	0.000	0.000	0.350	0.350	0.000	0.000	0.000
- NaOCH3	0.000	0.250	0.000	0.000	0.000	0.000	0.000	0.000

Table 5. Continued

	d66	d67	d68	d69	d70	d71	d72	d73	d74
Source	U25	U57	U58	U86	U59	U60	U60	U61	U86
Sink	U57	U58	U59	U59	U60	U62	U61	U70	U62
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	74.00	74.00	74.00	58.74	60.00	60.00	60.00	60.00	58.74
flow (kg/min)	134.52	134.52	134.52	32.27	188.31	163.74	24.57	24.57	3.19
Composition:									
- Lipid	1.000	1.000	1.000	0.000	0.071	0.081	0.005	0.005	0.000
- Methanol	0.000	0.000	0.000	0.982	0.145	0.100	0.443	0.443	0.982
- Glycerol	0.000	0.000	0.000	0.000	0.073	0.005	0.528	0.528	0.000
- Biodiesel	0.000	0.000	0.000	0.000	0.708	0.814	0.005	0.005	0.000
- Water	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- NaOH	0.000	0.000	0.000	0.000	0.002	0.000	0.017	0.017	0.000
- HCl	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- NaOCH3	0.000	0.000	0.000	0.018	0.000	0.000	0.000	0.000	0.018

Table 5. Continued

	d75	d76	d77	d78	d79	d80	d81	d82	d83
Source	U62	U63	U63	U75	U64	U65	U65	U66	U66
Sink	U63	U64	U70	U64	U65	U66	U70	U67	U69
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	gas	liquid
T (degC)	60.00	60.00	60.00	101.58	61.25	61.25	61.25	58.35	58.35
flow (kg/min)	169.07	149.53	19.54	6.16	159.37	146.54	12.83	0.36	146.18
Composition:									
- Lipid	0.008	0.008	0.007	0.000	0.008	0.000	0.093	0.000	0.000
- Methanol	0.113	0.013	0.877	0.003	0.012	0.002	0.122	0.973	0.000
- Glycerol	0.013	0.001	0.107	0.001	0.001	0.000	0.008	0.000	0.000
- Biodiesel	0.866	0.979	0.007	0.000	0.918	0.997	0.011	0.000	1.000
- Water	0.000	0.000	0.000	0.996	0.061	0.000	0.755	0.027	0.000
- NaOH	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000
- HCl	0.000	0.000	0.000	0.000	0.001	0.000	0.010	0.000	0.000
- NaOCH3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 5. Continued

	d84	d85	d86	d87	d88	d89	d90	d91	d92	d93
Source	U67	U68	U69	U70	U71	U72	U73	U74	U78	U75
Sink	U68	U70	U88	U71	U72	U73	U74	U75	U75	U76
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid	gas	liquid|gas
T (degC)	58.35	58.35	58.35	59.99	59.99	59.99	59.31	59.31	103.66	1.26
flow (kg/min)	0.36	0.36	146.18	57.66	57.66	55.04	55.71	55.71	6.16	55.71
Composition:										
- Lipid	0.000	0.000	0.000	0.025	0.025	0.000	0.000	0.000	0.000	0.000
- Methanol	0.973	0.973	0.000	0.519	0.519	0.544	0.537	0.537	0.003	0.537
- Glycerol	0.000	0.000	0.000	0.263	0.263	0.276	0.272	0.272	0.001	0.272
- Biodiesel	0.000	0.000	1.000	0.007	0.007	0.000	0.000	0.000	0.000	0.000
- Water	0.027	0.027	0.000	0.172	0.172	0.180	0.178	0.178	0.996	0.178
- NaOH	0.000	0.000	0.000	0.008	0.008	0.000	0.012	0.012	0.000	0.012
- HCl	0.000	0.000	0.000	0.004	0.004	0.000	0.000	0.000	0.000	0.000
- NaOCH3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 5. Continued

	d94	d95	d96	d97	d98	d99	d100	d101
Source	U78	U76	U76	U77	U77	U80	U81	U82
Sink	U76	U77	U87	U80	U78	U85	U82	U85
Phase	liquid	liquid|gas	liquid	gas	liquid	liquid	liquid	liquid
T (degC)	103.66	2.07	6.26	64.54	102.49	64.54	25.00	25.00
flow (kg/min)	19.63	55.71	19.63	29.93	25.78	29.93	3.01	3.01
Composition:								
- Lipid	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Methanol	0.000	0.537	0.000	1.000	0.001	1.000	1.000	1.000
- Glycerol	0.773	0.272	0.773	0.000	0.589	0.000	0.000	0.000
- Biodiesel	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Water	0.193	0.178	0.193	0.000	0.385	0.000	0.000	0.000
- NaOH	0.034	0.012	0.034	0.000	0.026	0.000	0.000	0.000
- HCl	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- NaOCH3	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 5. Continued

	d102	d103	d104
Source	U83	U84	U85
Sink	U84	U85	U86
Phase	liquid	liquid	liquid
T (degC)	25.00	25.00	58.74
flow (kg/min)	2.53	2.53	35.46
Composition:			
- Lipid	0.000	0.000	0.000
- Methanol	0.750	0.750	0.982
- Glycerol	0.000	0.000	0.000
- Biodiesel	0.000	0.000	0.000
- Water	0.000	0.000	0.000
- NaOH	0.000	0.000	0.000
- HCl	0.000	0.000	0.000
- NaOCH3	0.250	0.250	0.018

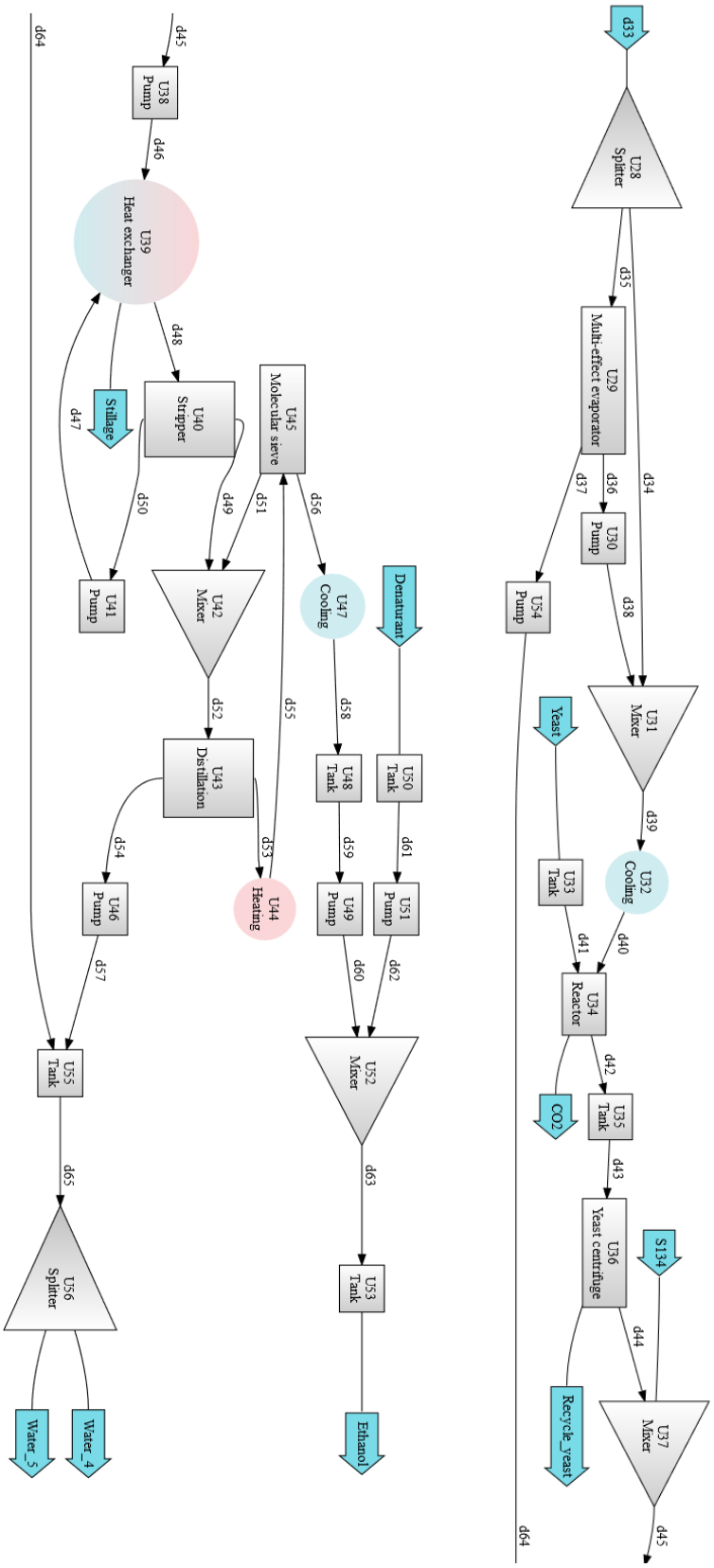

Figure 8. Flowsheet for ethanol production. The flowsheet is split to fit in the page.

Table 6. Stream table for the ethanol production section

	Stillage	Water_4	Water_5	CO2	Denaturant	Yeast	Ethanol	Recycle_yeast
Source	U39	U56	U56	U34	-	-	U53	U36
Sink	-	-	-	-	U50	U33	-	-
Phase	liquid	liquid	liquid	gas	liquid	liquid	liquid	liquid
T (degC)	36.68	100.00	100.00	32.00	25.00	25.00	81.18	32.00
flow (kg/min)	1625.07	66.06	80.74	193.18	3.84	599.25	205.96	255.91
Composition:								
- CO2	0.000	0.000	0.000	1.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.027	0.972	0.068
- Water	0.972	1.000	1.000	0.000	0.000	0.687	0.009	0.268
- Glucose	0.027	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Sucrose	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Octane	0.000	0.000	0.000	0.000	1.000	0.000	0.019	0.000
- DryYeast	0.001	0.000	0.000	0.000	0.000	0.286	0.000	0.664

Table 6. Continued.

	d33	d34	d35	d36	d37	d38	d39	d40	d41
Source	U27	U28	U28	U29	U29	U30	U31	U32	U33
Sink	U28	U31	U29	U30	U54	U31	U32	U34	U34
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	99.00	99.00	99.00	70.13	84.45	70.13	95.15	22.00	25.00
flow (kg/min)	4823.5	1278.2	3545.2	462.2	3083.0	462.2	1740.4	1740.4	599.2
Composition:									
- CO2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.027
- Water	0.913	0.913	0.913	0.334	1.000	0.334	0.759	0.759	0.687
- Glucose	0.007	0.007	0.007	0.054	0.000	0.054	0.020	0.020	0.000
- Sucrose	0.080	0.080	0.080	0.612	0.000	0.612	0.221	0.221	0.000
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Octane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- DryYeast	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.286

Table 6. Continued.

	d42	d43	d44	d45	d46	d47	d48	d49	d50
Source	U34	U35	U36	U37	U38	U41	U39	U40	U40
Sink	U35	U36	U37	U38	U39	U39	U40	U42	U41
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid	gas	liquid
T (degC)	32.00	32.00	32.00	31.68	31.68	100.00	85.95	89.78	100.00
flow (kg/min)	2146.5	2146.6	1890.6	1974.0	1974.0	1625.1	1974.0	348.9	1625.1
Composition:									
- CO2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.101	0.101	0.106	0.102	0.102	0.000	0.102	0.574	0.000
- Water	0.798	0.798	0.870	0.875	0.875	0.972	0.875	0.426	0.972
- Glucose	0.020	0.020	0.023	0.022	0.022	0.027	0.022	0.000	0.027
- Sucrose	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Octane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- DryYeast	0.080	0.080	0.001	0.001	0.001	0.001	0.001	0.000	0.001

Table 6. Continued.

	d51	d52	d53	d54	d55	d56	d57	d58	d59
Source	U45	U42	U43	U43	U44	U45	U46	U47	U48
Sink	U42	U43	U44	U46	U45	U47	U55	U48	U49
Phase	gas	gas	gas	liquid	gas	gas	liquid	liquid	liquid
T (degC)	115.00	93.60	78.38	100.00	115.00	115.00	100.00	76.85	76.85
flow (kg/min)	61.64	410.55	263.75	146.80	263.75	202.12	146.80	202.12	202.12
Composition:									
- CO2	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.629	0.582	0.906	0.000	0.906	0.991	0.000	0.991	0.991
- Water	0.371	0.418	0.094	1.000	0.094	0.009	1.000	0.009	0.009
- Glucose	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Sucrose	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Octane	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- DryYeast	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000

Table 6. Continued.

	d60	d61	d62	d63	d64	d65	S134
Source	U49	U50	U51	U52	U54	U55	-
Sink	U52	U51	U52	U53	U55	U56	U37
Phase	liquid	liquid	liquid	liquid	liquid	liquid	liquid
T (degC)	76.85	25.00	25.00	81.18	84.45	100.00	25.00
flow (kg/min)	202.12	3.84	3.84	205.96	3083.04	146.80	83.33
Composition:							
- CO2	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Ethanol	0.991	0.000	0.000	0.972	0.000	0.000	0.000
- Water	0.009	0.000	0.000	0.009	1.000	1.000	1.000
- Glucose	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Sucrose	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- H3PO4	0.000	0.000	0.000	0.000	0.000	0.000	0.000
- Octane	0.000	1.000	1.000	0.019	0.000	0.000	0.000
- DryYeast	0.000	0.000	0.000	0.000	0.000	0.000	0.000