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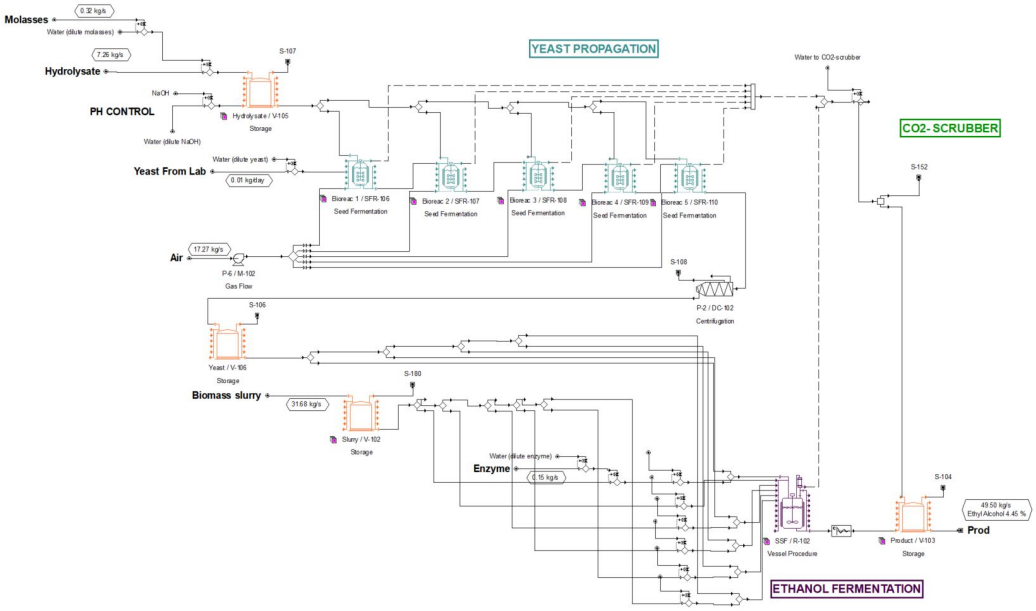

Design and Scheduling of a Bioreactor System Model for Production of 2G Ethanol

Master's Thesis in Innovative and Sustainable Chemical Engineering

Elin Wallin

Department of Biology and Biological Engineering
Chalmers University of Technology
Gothenburg, Sweden 2019

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Cover: A visual illustration of a bioreactor system producing ethanol. The image is of the SuperPro Designer model that was created in the project.

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Abstract

During the past 50 years, CO_2 emissions have increased by 90 %. Combustion of fossil fuel for energy and transportation and emissions from industrial processes are the two major contributors to these increased CO_2 emissions [14]. Because of increasing energy demand and the desire to reduce the CO_2 emissions, research to decrease our dependence on fossil-based products has grown during recent years. A way to decrease CO_2 emissions is to substitute fossil-based products with biomass-based products [18].

One of the products that can be produced from biomass is bioethanol. The process of converting biomass to bioethanol require multiple procedures due to the complex structure of the raw material [18]. These procedures can be classified into the following sections; pre-treatment section, bioreactor section and downstream section. In this thesis economic evaluation of a fed-batch bioreactor system, comprising of a yeast propagation procedures and a procedure for saccharification and fermentation (SSF), has been the focus.

To make an economical comparison between different scheduling cases a batch operating model in SuperPro Designer (SPD) was developed. A batch model has the advantage compared to a continuous model to give a more detailed analysis of the bioreactor section that accounts for the fed-batch behaviour and to account for time-dependency and sequencing of events.

The results from the model created indicates that there are economic advantages, decreased annual operating cost and equipment cost, to be gained from optimized scheduling of the process. Results from variation in reaction time for SSF and reactor volume shows that both these impacts the scheduling. Optimizing the scheduling of a industrial-scaled process based on data from lab-scale tests may be problematic since the time required for a certain process, such as SSF, may be different depending on the size of the process. If the time required to get high enough conversion in a SSF process increases for a a larger process the scheduling may be unfeasible, which gives that more reactors has to be purchased and included in the layout of the plant. The conclusion is therefore that scheduling using data from small-scale should allow for some flexibility.

Keywords: Bioethanol, Scheduling, SuperPro Designer, Fed-batch

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Elin Wallin, Gothenburg, January 2019

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Nomenclature

Abbreviations

1G	First Generation Bioethanol Production
2G	Second Generation Bioethanol Production
Case A	All SSF reactors operate in parallel, no equipment operate with staggered start times
Case B	Three SSF reactors operate with staggered start times
Case C	All parallel SSF reactors operate with staggered start times
Case D	All parallel SSF reactors and reactors for yeast propagation operate with staggered start times
CBM	Carbohydrate-Binding Modules
CIP	Clean-In-Place
EGC	Equipment Gantt Chart
OGC	Operational Gantt Chart
SPD	SuperPro Designer
SSCF	Simultaneous Saccharification and Co-fermentation
SSF	Simultaneous Saccharification and Fermentation
TEA	Techno-Economic Assessment
VBA	Visual Basics for Applications
VVM	Volume (of gas) per volume (of liquid) per Minute
WIS	Water-Insoluble Solids

1. Introduction

In the process of making our society more environmentally sustainable one interesting option is to move towards a society free from fossil-based products and energy. However, this requires developing methods that enable efficient biomass use. In biorefineries biomass can be converted into bioenergy and bio-based products, such as chemicals, materials and human food [2]. The biorefinery concept uses different technologies to separate the raw materials into their building blocks and then use these to obtain value added products [16]. The concept also gives the possibility to upgrade low-quality lignocellulosic biomass into valuable products [23].

Converting biomass to a range of products usually requires a lot more effort than using fossil-based material. This is e.g. due to the complexity and variation in composition of the material [16]. By taking advantage of the complex structure of lignocellulosic biomass some bio-based products are today available on the market, e.g. bioethanol and vanillin [3].

Bioethanol can be produced through fermentation of sugars in biomass, such as lignocellulose and algae, with the use of microorganisms [1]. Prior to fermentation pre-treatment and hydrolysis of the biomass is needed to obtain a solution containing fermentable sugars. After fermentation of sugars to bioethanol impurities are removed.

To develop new products using the complex structure of biomass in an efficient manner requires the development of processes both on a molecular scale and on an industrial scale. Once a concept has been proven promising in a small-scale environment, some tools are required in order to prioritize between different process options in a large-scale environment and help predict the outcome, so the most suitable alternative can be selected.

Tools helping with the process design, e.g. determining the workflow, equipment needs, and implementation requirements for a particular process, involve flowcharting and usage of process simulation softwares [4]. These types of tools may be used prior to building, expanding or retrofitting a process plant.

There are different programs that can help with this. One commonly used program is SuperPro designer (SPD), which is a software tool used to simulate industrial scale processes. The software is specialized in performing

techno-economic calculations [12]. SPD is the most widely used simulator in different industries such as pharmaceutical, biotech, specialty chemical, food and mineral [8].

1.1 Background

This master thesis is a part of an ongoing collaboration between the department of Resource Efficient Systems and Services at RISE and the divisions of Industrial Biotechnology and Environmental Systems Analysis at Chalmers University of Technology. The aim of this collaborative project is to evaluate the performance of a bioethanol production concept from economic and environmental perspectives.

As a part of this collaboration a continuous operating model of a biorefinery process for production of ethanol from second generations (2G) biomass has been constructed and used in order to analyse the effects of variations in process design has on economic performance and environmental impact.

In Figure 1.1 a block diagram of the multi-feed biorefinery process is shown. The block diagram contains the pre-treatment and the bioreactor section of the biorefinery. The bioreactor section consists of a process that produces yeast and a process that converts pre-treated biomass to ethanol through Simultaneous Saccharification and Fermentation (SSF).

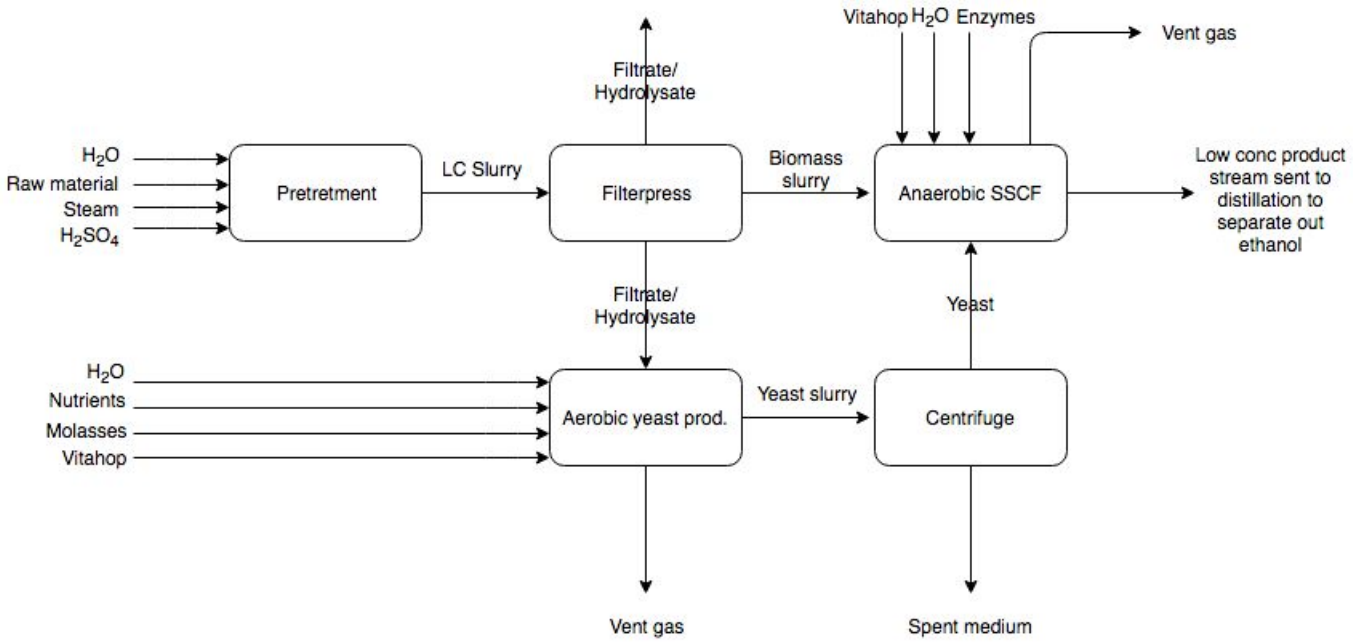

Figure 1.1: Flowchart of a biorefinery.

The currently used model is a continuous model of the biorefinery process and it has been developed in the flow sheeting software SuperPro Designer (SPD), see appendix D for a visual illustration. At this stage the simulation assumes that the entire biorefinery process operates continuously. In reality, however, the bioreactor section of the biorefinery typically operates fed-batch. It is therefore of interest to develop a model accounting for the fed-batch behaviour, since it allows more detailed analyses and makes it possible to realistically investigate the scheduling of the process.

1.2 Specification of issue under investigation

This thesis focuses on creating a model of the bioreactor system in a process producing bioethanol from wheat straw. The bioreactor system operates in fed-batch mode while the rest of the process operates in continuous mode. To meet the requirement of operating partly in fed-batch and partly in continuous mode the fed-batch part of the model must be modelled such that enough material can be processed so that the rest of the process can operate continuously. The flow of biomass slurry, denoted solids in Figure 1.1 from the pre-treatment section, is constant at 9.0×10^5 tonnes/yr. and the bioreactor system should be designed such that there is no accumulation of biomass slurry.

The concept that is the foundation of the biorefinery process is that both the operation mode for yeast propagation and the operation mode for the SSF process are fed-batch. The pre-treatment process contrasts with the two other processes since it is in continuous mode. The main difference in operation between yeast propagation and the SSF procedure is in turn related to supply of material. To the SSF procedure biomass slurry mixture is fed at discrete time points while feeding of the hydrolysate mixture in the yeast propagation reactors occurs continuously.

1.3 Aim

The purpose of this work is to start developing a model in SuperPro Designer (SPD) that can be used to validate different scheduling alternatives for the bioreactor section. The long-term objectives are to be able to consider variation in equipment size and variation in time allocated for simultaneous saccharification and fermentation (SSF) in validation of different scheduling alternatives and also to come up with a strategy that enable economic evaluation of the biorefinery, that accounts for the fed-batch behaviour of the bioreactor section, using techno-economical assessment (TEA).

The short-term project aims are to develop a batch model in SPD for yeast produced in hydrolysate liquor and a batch model for the SSF reactor, and to schedule the operation of the bioreactor system such that the two models can be merged.

The questions that will be answered in this thesis are:

- How should scheduling be performed for the process to be as economically sustainable as possible?
- What happens to the scheduling if the time for the SSF reaction is varied?
- How does the size of the equipment affect the scheduling of the process?
- What the advantages and disadvantages of using a fed-batch model rather than a continuous model?

1.4 Limitations

The focus of this thesis was to create a model for the bioreactor section of a biorefinery. The bioreactor section in the biorefinery includes propagation of yeast and SSF of sugars to bioethanol using *Saccharomyces cerevisiae*. The composition of the inlet streams to the bioreactor section in the batch model was based on the streams exiting pre-treatment in the continuous model. These values were valid for using wheat straw of a certain composition as raw material in the continuous model. It would have been interesting to change the composition of the raw material and evaluate the impact it would have on the economy of the process. Unfortunately, this was not included due to time restrictions.

The reaction model that used in this thesis was the same as the one that was used in the continuous model, namely a stoichiometric model. The reason not to use a more advanced model was that the kinetic model developed to capture the behaviour of the SSF reaction [27] was not compatible with SuperPro Designer (SPD). Using the visual basic for applications (VBA) tool in Excel could create a possible way for transferring data from the kinetic model to SPD. This would be of interest once looking into the impact of variation in raw material composition.

In this thesis four different scheduling options was evaluated based on time utilization, size utilization, number of equipment required, size of equipment, operation cost and equipment cost. If more time was given it would be of great advantage to merge the biorector model with the pre-treatment and downstream sections of the biorefinary, since it would then be possible to compare different scheduling options based on net present value.

The optimal time for SSF of sugars to ethanol using *Saccharomyces cerevisiae* from an economical perspective was assumed to be 96 hours. However, since this assumption may not be true the effects of operating with different procedure time for SSF was investigated. The different process times tested in this thesis was limited to 90, 96 and 100 hours. If more time were available it would be of interest to investigate the impact variation in time will have for the entire biorefinary.

In this thesis volume and the number of parallel equipment was for a given maximum volume calculated by SPD. The maximum volume was assumed to be 1200 m^3, as in the continuous model. To gain a sense of the impact

of different maximum volumes a maximum volume of 3795 m^3 [7] was also used. If more time were available it would be of interest to get in contact with companies manufacturing SSF reactors to get inputs regarding costs and available sizes. The reason for selecting these two equipment sizes was that 1200 m^3 was selected for the continuous model and 3975 m^3 was used by The National Renewable Energy Laboratory (NREL) in their report Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol [7].

The vapor-liquid state of the components in the procedures was estimated using the default shortcut method [9]. If more time was available it would be of interest to change these settings to a rigorous method and to evaluate the different methods.

2. Theory

This chapter presents the relevant theory for this thesis. The first section aims to give a greater theoretical understanding for the concept that the model should be based on, hence in this section fermentation of biomass to ethanol and the propagation of yeast will be introduced. The later sections in this chapter aim to give the reader an introduction to process simulations and the SuperPro Designer (SPD) software.

2.1 Description of the bioethanol production process

During the last decades, concerns regarding global warming, fossil fuel depletion, and energy security resulted in a wide interest in renewable fuels. Bioethanol is an example of a product that can be used as a substitute for fossil fuel. Production of bioethanol today is mainly of the first generation (1G), with an average production of each plant in the US of 260,000 m^3/ year [29]. Currently, all industrial scale production of bioethanol are 1G biofuels. The drawback with 1G is that the feedstock is produsd using land area that could be used for food production, As an alternative, technology to produce second generation (2G) bioethanol is available and there are currently several demo plants available [29].

2G bioethanol is produced using lignocellulosic materials such as forestry residue, agricultural by-products and industrial waste [25] as feedstock. The technical and economic challenges that limit the production of 2G bioethanol are caused by the creation of inhibitory compounds during the harsh pretreatment of the feedstock [29]. This is required since ligocellulosic materials are stable which brings that biodegradation in nature is a slow process [37]. The challenge is to speed up this process without breaking down the sugars [29].

The term lignocellulosic biomass refers to plant materials which mostly contains cellulose, hemicellulose and lignin. The composition of lignocellulosic biomass, on a dry-weight basis, typically contains 40-55 % of cellulose, 25-50 % of hemicellulose, 10-40 % lignin and about 5 % of extractives and ash [17]. An example of lignocellulosic biomass that seems to be a promising raw material for 2G biofuel production is wheat straw. The wide availability and

low cost make wheat straw one of the agricultural residues with greatest potential [25].

Direct conversion of wheat straw to biofuels is difficult to accomplish as the main components, cellulose, hemicellulose and lignin, makes the material too intractable [17]. For instance, the structure of cellulose makes it insoluble in water. Its high resistance to hydrolysis is due to the crystalline structure and the embedding of hemicellulose and lignin with the cellulose fibres. The structure of hemicellulose is in contrary to cellulose a more branched polymer, which makes it less resistant to hydrolysis. Lignin is a hydrophobic aromatic macromolecule and it gives strength to the cell wall of the plant as it is covalently linked to hemicellulose [17].

Conversion of wheat straw to bioethanol requires multiple process steps due to its complex structure. After pre-treatment of the feedstocks four more steps are required and then product recovery to obtain bioethanol. Apart from pre-treatment and product recovery, cellulase production or enzyme production, yeast propagation, enzymatic hydrolysis and microbial fermentation are required [17], see Figure 2.1.

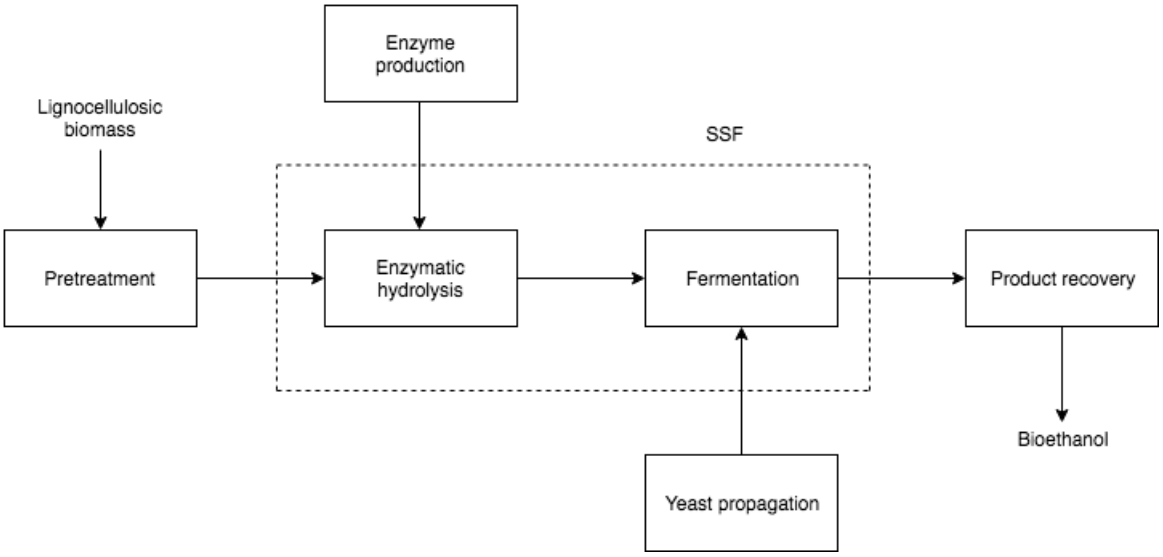

Figure 2.1: Flowchart of process steps for conversion of wheat straw to bioethanol.

To make enzymatic hydrolysis of lignocellulosic biomass possible, pre-treatment is required. The idea is to break the lignin seal, solubilize the hemicellulose and make the cellulose structure less crystalline [17]. To achieve complete

hydrolysis of cellulose into monomer sugars requires interaction of several enzymes collectively called cellulases [17], and mild reaction conditions, a pH slightly below 5 and a temperature between 45–50 ^{o}C [1]. The purpose of using a mixture of enzymes is that a combination of their properties is required. Some of the most common enzymes in the cellulase mixture are described in short in Table 2.1.

Table 2.1: Some of the most common enzymes in the cellulase mixture.

Enzyme	Short description
Cellobiohydrolase	Depolymerize and hydrolyze the crystalline regions in the cellulose from the ends of the chain [17].
Endoglucanase	Attack the amorphous parts of the cellulose chains, creating more free ends [17].
β-glucosidase	Hydrolyze cellooligosaccharides into monomer glucose [17].
Lytic polysaccharide monoxygenase (LPMO)	Can strongly promote the depolymerization of cellulose, by oxidative cleavage of glycosidic bonds [28].

Cellulase enzymes are supplied after pre-treatment to hydrolyse the material into fermentable sugars. This process is known as enzymatic hydrolysis. The time required to obtain fermented sugars depends on several things, but the features of cellulose that mostly affects the rate is its crystallinity and the accessible surface area [17].

Microbial fermentation is the process of converting sugars to ethanol. This process requires the use of a fermenting organism that convert all the sugars, to achieve favourable economics from the bioethanol process. The challenge with this is that during the pre-treatment process inhibitors are created, e.g. furfural, 5-hydroxymethylfurfural (5-HMF) and acetate [13]. It is therefore important to use a microorganism that has a high tolerance against these inhibitors [17].

One commonly used microorganism for converting sugars to ethanol is the yeast *Saccharomyces cerevisiae*. The native strain of *S. cerevisiae* is an excellent ethanol producer. However, to ensure that all sugars in the cellulosic biomass hydrolysate are converted to ethanol with high yield and at high concentration the yeast is metabolically engineered to broaden the substrate range. Native *S. cerevisiae* can only ferment hexose monomers in the cellulosic biomass hydrolysate and not pentose sugars, cellobiose, or xylobiose [11].

To enable producing ethanol at high concentration high water-insoluble solids (WIS) concentration during simultaneous saccharification and co-fermentation (SSCF) processing of biomass [30] is required. However, to operate at a high WIS concentration entails operating at a high viscosity. This makes mass transfer less efficient. Operating at a high WIS concentration also gives that the content of inhibitors increases, which makes inhibition of yeast more obvious compared to a lower WIS concentration [30].

Simultaneous saccharification and fermentation (SSF) is, as the name implies, a process in which saccharification of the pre-treated biomass and fermentation of sugar occur together. SSF offers several advantages compared to separate hydrolysis and fermentation. One advantage is that SSF reduces end-product inhibition of hydrolytic enzymes. The economic advantages of SSF have been estimated to reduce the capital investment by more than 20 % with SSF compared to separate hydrolysis and fermentation processes. SSF also favours co-fermentation (SSCF) of hexose, e.g. glucose, and pentose, e.g. xylose, by recombinant *Saccharomyces cerevisiae*. It is favourable since the concentration of glucose can be kept low. Giving a balanced rate of released and consumed glucose via hydrolysis and fermentation [30].

Because of decreased mass transfer and increased inhibition of yeast the ethanol yield and productivity of the process decreases as fermentation proceeds. Research has therefore been dedicated to decreasing these negative effects and to enhance the productivity of bioethanol production. One concept that has been developed to increase yeasts tolerance towards inhibitors uses parts of the hydrolysate stream in the propagation of yeast. The hydrolysate stream is a by-product that is produced when biomass after pre-treatment gets separated to one thick slurry that is used for SSF and hydrolysate. The point of doing this is that when yeast is propagated on hydrolysate it learns to survive such environment [30].

Most biological products are produced in batch or fed-batch mode [24]. Fed-batch is a strategy midway between batch and continuous mode. In fed-batch a batch culture with an initial low working to total volume ratio is supplied with a nutrient feed. Unlike continuous culture no material is removed from the reactor during operation. One well documented use of operating in fed-batch compared to batch and continuous is to produce a high cell mass. This can be achieved since processes operating in fed-batch mode operate under pseudo steady state conditions [22].

The fed-batch culture is useful if it is appropriate to prolong a phase of batch

culture for optimal product formation. This type of fed strategy might also be beneficial when a substrate concentration threshold exists above which product formation is inhibited or repressed [22]. In yeast propagation fed-batch culture avoids the waste of carbon source, molasses or glucose, and maximize yeast accumulation by applying a feed composition and rate which maintain the glucose concentration below the threshold value [22].

2.2 Scheduling

Scheduling involves breaking down a project into component activities and then estimating their duration. The complexity of a scheduling task can be as simple as a few events in a calendar or involve scheduling an elaborate network containing of thousands activities [20]. Scheduling includes more than determining the duration of a project. The three questions that scheduling helps to answer are; what is the expected duration of the project? what resources are required? and what can be accomplished? Optimized scheduling becomes a trade-off between time, goals and resources. [20]

In some chemical plants, such as plants producing bio-fuel, the process may consist of both continuous and batch procedures. For chemical processes operating partly or entirely in batch mode scheduling is the core of the production. Scheduling is of importance for improving the productivity of batch processes. The decision-making process for improving productivity includes determining the locations, times and sequencing of processing activities with finite units and resources to achieve a certain objective [31].

There are different methods available for optimizing the scheduling of batch processes. Some of the different models available can be classified as global event-based, unit-specific-event based, slot-based and precedence-based models [31]. These different approaches for optimizing scheduling can be used in high-level modeling systems for mathematical optimization like general algebraic modeling system (GAMS). One problem with optimization is that most of the objectives requires inputs that may vary. For example, if the objective is to maximize the profit the price of raw material is likely to have great impact on the solution for optimal scheduling and the price for raw material is likely to vary throughout the lifetime of the process.

SuperPro Designer (SPD) is an example of a simulation program in which the user has the ability to improve the scheduling based on process limitations.

For example time, equipment and raw material are resources that may limits the scheduling.

2.3 SuperPro Designer

Simulation can be used to evaluate a process by creating a model that capture the behaviour characteristics of an actual process. Through these simulations, estimations of a real process can be computed. However, all details of the real process can never be included. Focus when creating a model is to include all aspects crucial for the evaluation and leave out all details that are of low importance [9].

SuperPro designer (SPD) is a flowsheet driven software in which design, economic evaluation and environmental impact can be estimated for a variety of different processes for steady-state conditions. Some of the advantages with SPD compared to programs like Excel and Matlad are that SPD have pre-defined databases for chemical components, mixtures, equipment and resource and gives the user a better overview of the process through a visual representation of the process [19].

Two commonly used designations in SPD modelling are unit procedure and unit operations. Each piece of equipment in a batch process can perform different unit procedures, e.g. a reactor can be used both to execute a procedure that converts A and B to C and D and a second procedure that converts C and E to F. Each procedure requires a recipe of actions that is called unit operations. For example, to perform a procedure in which A and B are converted to C and D requires the following operations; first charging of component A and B to the reactor vessel, followed by reaction, then a transfer out operation to empty the vessel and finally cleaning.

Apart from SPD there are also other simulation tools available for modelling of batch operating plants. For example, BATCH and Aspen Batch Process Developer are two batch process simulation tools that can be used to model multiple batches of multiple products. One drawback with these tools is that they require long time to generate solutions because they do detailed material and energy balances for all the simulated batches. Another tool for simulation of batch processes is the Discrete-event simulation (DES) [9].

In the flowsheet of SPD each unit procedure can be seen as equipment-like icons. Within each of these unit procedures all operations associated with

that procedure can be set by the user. For every operation within a procedure, the simulator includes a mathematical model that performs material and energy balance calculations. Based on the results of these balances, the software performs equipment sizing calculations [19]. Most of these calculations only involves solving sets of algebraic equation. Some however include solving differential equations e.g. if kinetic reactions or rigorous vapor-liquid calculations are required [9].

In SPD the simulation order of each operation is based on the flowsheet representation of the process and not their relative scheduling sequence which is set by the user. The scheduling calculations are always done after the completion of the mass and energy balances. The order is decided in such way that when solving a procedure all input streams to the procedure are already known either because they are direct process inputs or because they are outputs of previously solved procedures [9].

The simulation engine in SPD prepares for the iterative calculations by adjusting all properties of the intermediate streams to zeroes, except those selected as tear streams [9]. Tear streams are those streams which are given initial guessed values which can be used to calculate values for the remaining streams [32]. For the streams selected as tear streams the simulation engine generates an initial guess for the state variables x_1, x_2, x_3... x_n, i.e. the composition and temperature. The initial guess of the tear streams in SPD can be specified by the user based on current properties of all tear streams, all properties of the tear streams are reset to zero or customize the strategy such that different initialization strategies are used for each of the tear steams [9].

The program then solves all the elements in each partition in the predetermined order until a new set of values is generated for all the tear stream variables, $g(x_1)$, $g(x_2)$, $g(x_3)$... $g(x_n)$. Based on the originally guessed values and the generated values a new set of values can be generated. To determine if a new iteration should be executed the generated set of stream properties are compared to the guessed set of states. If the values are sufficiently close convergence has been achieved and no more iterations are required. Else, a new iteration is started unless the maximum number of iterations is exceeded. To generate the next guessed value the most commonly used method is successive substitution, the generated values for the tear stream variables are used as the next guess, this method sometimes leads to diversion. In such case Wegstein's next guess estimation could be considered for obtaining the next guess [9].

To determine that convergence has been reached the relative division between a guessed value for a variable and a calculated value, see equation 2.1, is calculated. If the relative division is lower than a set tolerance, the variable is considered as converged. Setting the tolerance value to lower values, will enforce a tighter matching between the guessed and calculated values and therefore will allow for smaller errors but it may take longer to converge [9].

$$Relative\ Deviation(RD) = \left| \frac{(Guessed\ Value - Calculated\ Value)}{Guessed\ Value} \right| \quad (2.1)$$

Modelling of processes operating in batch or fed-batch mode are best accomplished with batch process simulators that can account for time-dependency and sequencing of events. Batch process simulation is a computer modelling technique used for design, analysis, and optimization of batch manufacturing processes. Batch processes are common in industries that produce low-volume, high-value products such as pharmaceuticals, fine chemicals, biochemicals, food, consumer products, etc. [8].

At the start-up process of a new project in SPD the user selects operation mode, batch or continuous. Biochemical processes usually operate in batch or fed-batch mode, in contrast to typical petrochemical processes which operate continuously [35]. Continuous processes are also common in other industries that handle large throughputs. Compared to operating continuously, where a piece of equipment performs the same task all the time, in batch mode equipment operates cycle-wise [35]. In SPD it is required that all procedures at least have one operation in their recipe for the material and energy balances to be executed. If there is only one operation in the recipe the procedure are simulated to operate continuously and if more then one operation in the procedure then it is modeled to operate batch wise [9].

There are several differences between modelling a continuous process and a batch process in SPD. An equipment with a continuous procedure does not have the ability to host more than one procedure since a continuous procedure, by definition, operates without interruptions. Another difference is that a continuous unit procedure consists of only a single unit operation, whereas a batch procedure may consist of multiple operations. As a result, accounting for cleaning of equipment is less straight forward for procedures operating continuously than for procedures operating batch wise. In Batch

mode both steam-in-place (SIP), which is usually done prior to operation when it is crucial for the environment in the equipment to be sterile, and clean-in-place (CIP), which is commonly used as the final operation in the recipe of an equipment, can easily be accounted for.

CIP is an operation used to account for cleaning of complete items of a plant or pipeline circuit without dismantling or opening of the equipment [5]. There are multiple recipes available for optimal CIP of a process. The optimal CIP for a certain process is often dependent on the product and the requirements associated with it. In Table 2.2, an example of a cleaning recipe is presented.

Table 2.2: Example of a recipe for a Cleaning-In-Place operation [10] [34] [15].

Cleaning step	Cleaning Agent	Duration [min]	Temp [$^{\circ}C$]	Vol. flow rate [$m^3/(h \times m)$]
Pre-rinse	Water	10	45	35
Caustic Cleaning	4 wt.% NaOH	30	75	35
Rinse	Water	5	45	35
Desinfect	Water	5	95	35
Cooling	Water	10	25	35

In modelling it is likely that there are uncertainties in some of the variables used in the model. A common way of analysing variability of a set of critical independent parameters effects on various outputs can be accomplished through sensitivity analysis [33]. To help validate the sensitivity of different parameters in processes modelled in SPD a tool that allows SPD to interoperate with other windows applications, e.g. MS Excel, can be used. This feature allows the user to manipulate variables in an existing model of a process without interacting with SPD directly, which makes it possible to analyse a model without knowledge about SPD. Some of the parameters in SPD that can be modified are flow rates, utility cost, degree of conversion, and number of staggered equipment sets [9]. The tool can be designed such that it records variation in different economic parameters such as equipment cost, annual equipment cost, payback time and net present value.

2.3.1 Scheduling in SPD

In SPD there are three different levels of scheduling. The first one is operational scheduling, which gives the possibility to implement various relations

between operations in the same procedure or between different procedures. For instance, CIP of a vessel is suitable to schedule after emptying the vessel.

Figure 2.2 illustrates an example of an operations Gantt chart (OGC) in SPD. An OGC can be used to ensure that operations are scheduled as intended. All procedures and operations are stated on the left side of the chart. The blue bars are known as activity summary bars and represent a composite activity, e.g. a procedure. Green bars are known as elementary activity bars and represent single activities, e.g. an operation in a cycle.

The circled operations in the top left corner in Figure 2.2 are scheduled such that they start at the beginning of each new batch. The second circle, counting from left to right, indicates an operation that is scheduled to start at the completion of an operation in a different procedure. The operations in the third circle are scheduled to start simultaneously with the start of a previous operation in the same procedure. Finally, the last circled operation marks that an operation starts at the completion of the previous operation in the same procedure.

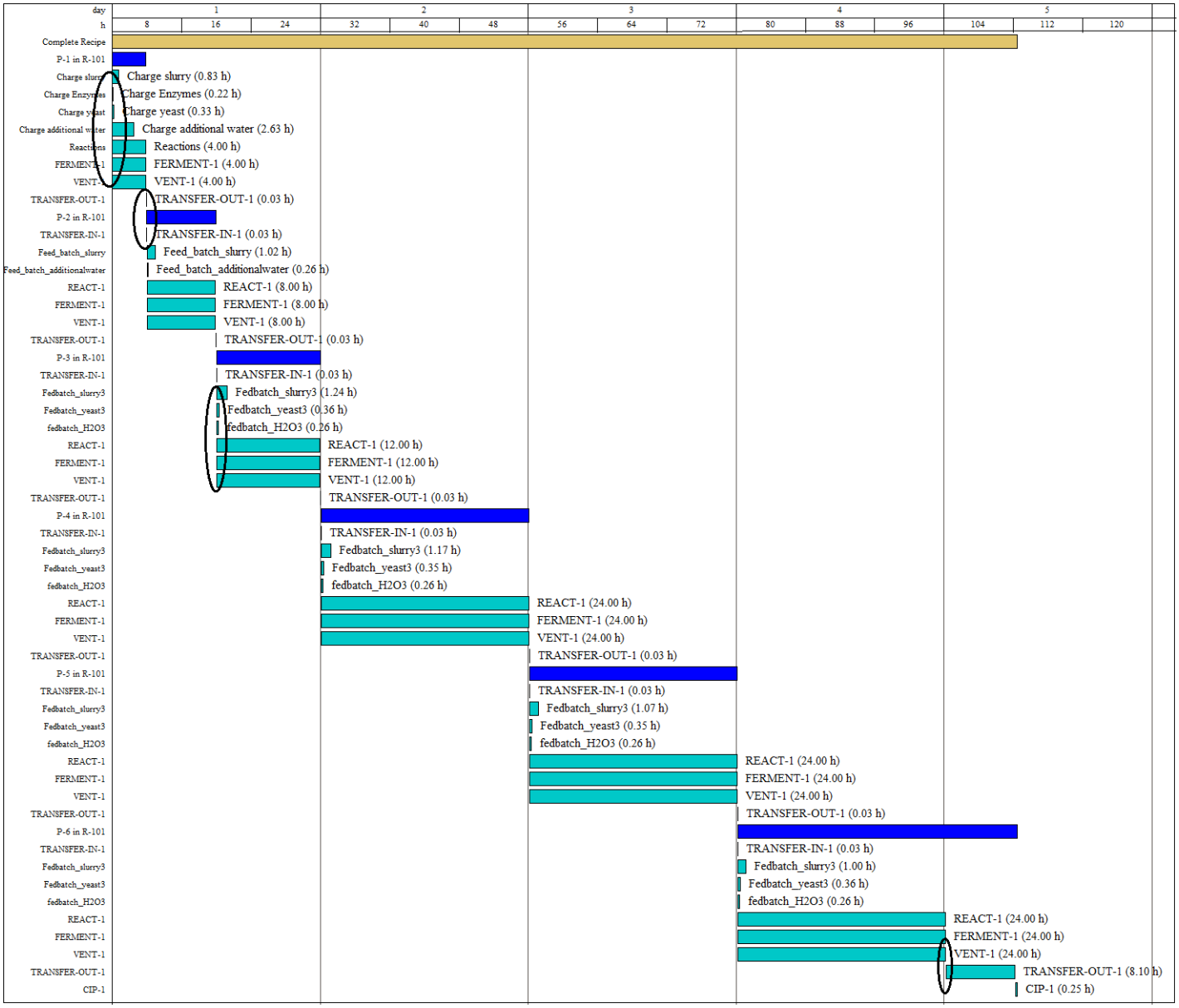

Figure 2.2: Example of an operations Gantt chart in SPD.

The second type of scheduling, procedure scheduling, involves determining the number of cycles to be executed per process batch to complete the unit procedure. In case the operation mode is continuous then the number of cycles is automatically assumed to be one.

There are a few tools in SPD that can be used to optimize scheduling of a process. The above mentioned OGC can, apart from being used to indicate

that each operation and procedure are scheduled to be executed in a logical way in relation to each, other also be used to indicate the bottleneck procedure of the process. Bottleneck equipment is the equipment with the longest cycle time. The piece of equipment that is scheduled as the bottleneck equipment determines the minimum recipe cycle time and the maximum possible number of batches per year. Knowledge about the bottleneck equipment of the process helps the SPD operator to improve the scheduling of the process.

Another chart that can be used to help improve the scheduling is the equipment occupancy chart (EOC). This tool can help with identification of bottleneck procedures. Similar to the OGC, EOC is way of visualizing the execution of a batch process as a function of time. As mentioned, the bottleneck procedure is the process with the longest occupancy time, hence has the shortest gap between consecutive batches. In an EOC in SPD all continuously-operating equipment are displayed as aligned blocks with no gaps between them since such procedures by definition has no downtime.

2.3.2 Economic evaluation and cost analysis in SPD

To evaluate the economic feasibility of a project or to compare different technology applications providing the same use from an economic perspective techno-economic assessment (TEA) can be used. In principle TEA is a variety of methods that enables comparison between costs and benefits of e.g. a project. Example of methods used for TEA are net present value and internal rate of return [26].

The cost assessment of a project can be classified into capital-related cost and operation-related cost. Capital-related costs comprise annual miscellaneous costs (insurance, local taxes and factory expenses), annual cost for infrastructure and costs related to initial investments. The costs related to the raw material, labour and maintenance are included in the operation-related costs [26]. The beneficial assessment of a plant may be more than the earnings from selling of the main product, e.g. in a biorefinery the benefits is the combined benefit of all product and in some cases include the benefits also of selling carbon credits [26].

Prior to economic validation of a process it is important to supply the model with quality data, since a program working on inaccurate data will only yield misleading results. For example, in SPD some of the predefined economic parameters are based on estimations from the pharmaceutical industry. Eco-

nomical evaluations of other industries may therefore not be possible with the default data. It is possible to avoid using these predefined values in SPD and make better estimations using your own defined correlations based on the power-law, see equation 2.2.

$$C = C_0(\frac{Q}{Q_0})^a \tag{2.2}$$

where C is the cost of a piece of equipment with a capacity equal to Q and C_0 is the base cost of a piece of equipment with a base capacity of Q_0. Costs and capacities for flat bottom tanks, seed fermenters and stirred reactors are available in table 2.3 [7].

Table 2.3: Parameters to estimate equipment costs for flat bottom tanks, seed fermenters and stirred reactors using the power-law equation, see equation 2.2, with 2009 as the reference year [7].

Equipment	Low end capacity [m^3]	High end capacity [m^3]	Base capacity (Q_0) [m^3]	Base cost (C_0) [€]	Exponent (a)
Flat Bottom Tanks	0	50000000	2000 m^3	565000 €	0.7
Seed Fermenters	0	0.1	0.08	37700	0.7
Seed Fermenters	0.1	1	0.77	58300	0.7
Seed Fermenters	1	10	7.74	78800	0.7
Seed Fermenters	10	100	77.40	176000	0.7
Seed Fermenters	100	1000	774.00	590000	0.7
Stirred Reactor	0	4000	3870	793360	0.6

3. Methods

This chapter is divided into four sections to give a better overview of the working procedure of this project. The chapter begins by describing the development of the bioreactor model in SPD. Later sections in this chapter describe the method for economic evaluation and cost analysis of the bioreactor system.

3.1 Developing the model of the bioreactor system

The creation of the model was done iteratively, meaning that input and the model were improved as new knowledge was gained. During the initial stage of the development of the model two separate models were created, one of the SSF reactor and the other of the yeast propagation reactor system. The focus was to capture the behaviour of the SSF reactor and in each of the yeast propagation reactors separately.

During the creation of these two models all pure components and stock mixtures required were first specified. Once all components were specified, all procedures were connected in a logical manner and all operations associated with the respective procedure were added.

After creating two successfully operating models they were merged. A stream controller was added at the outlet of the SSF reactor, between the SSF reactor and the storage vessel named Product Storage in Figure 3.1. The stream controller was made to adjust the amount of hydrolysate entering the yeast propagation section, such that the mass fraction of yeast in the stream leaving the SSF reactor remained at 0.3321 %, to obtain a similar concentration as the one in the continuous model [27].

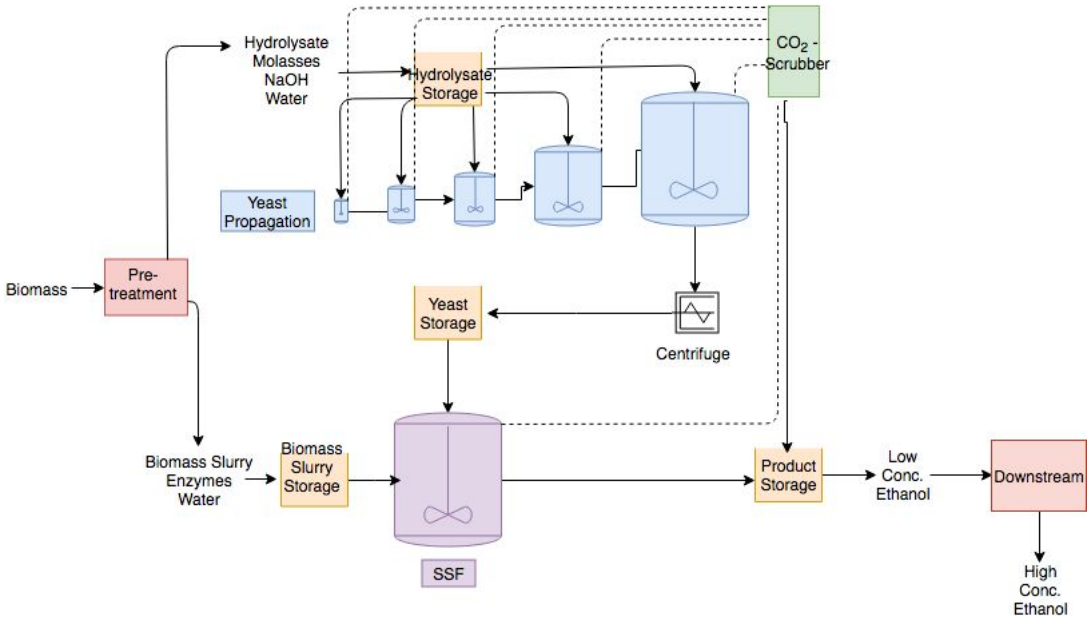

Figure 3.1: Flowchart of a biorefinery.

3.2 Detailed design of the yeast propagation seed train

The yeast propagation seed train was modeled such that a mixture containing hydrolysate, molasses,sodiumhydroxide and water was created. Firstly, hydrolysate was mixed with diluted molasses (250 g molasses/l) to obtain a ratio between molasses mixed in to the amount of xylose in the hydrolysate stream of 1.14. The hydrolysate stream is an intermediate steam in the continuous model [27] with a composition as in Table 3.1.

Table 3.1: The composition of hydrolysate entering the bioreactor section, with reference temperature of $25°C$.

Component	Percentage [wt.%]	Concentration [kg/m^3]
Acetic-acid	1.43	14.38
Extractives	0.6342	6.39
Furfural	0.11	1.09
Molasses	0.25	2.55
HMF	0.03	0.27
Sodium hydroxide	0.00	0.02
Soluble lignin	0.28	2.81
Succinic acid	0.27	2.73
Water	93.14	938.36
Xylose	3.86	38.92

The process stream, containing hydrolysate and molasses, was modelled such that it was continuously fed to a flat bottom tank, denoted hydrolysate storage. A sodium hydroxide solution was symbolically added to the hydrolysate storage, it was assumed that the pH would remain constant if the concentration of NaOH in the tank remained at approximate 0.2 wt.%.

The hydrolysate storage tank was connected to each of the five seed fermenters, used to scale up the yeast production. The scale up factor for the reactors where approximately 10, hence the model was made such that the stream exiting the hydrolysate storage was divided to achieve this scale up. The seed fermenters were modelled to work in sequence with a residence time of 24 hours, a transfer time of 30 minutes between each of these reactors and a CIP time of 60 minutes between new batches, see table 2.2 for the recipe of the CIP. The model was made such that apart from hydrolysate supplied air was also continuously supplied at a rate of 1 VVM. One additional stream containing yeast from lab was added to the first fermentation procedure.

The last seed fermenter was connected to a continuous operating decanter centrifuge. The centrifuge was modelled such that the cells were separated from most of the water to increase the concentration of yeasts in the solution. The centrifuge was connected to a continuous flat bottom tank procedure, denoted yeast storage.

3.3 Detailed design of the SSF fed-batch reactor

The model of the SSF fed-batch reactor was created such that the stream containing the thicker biomass slurry, with a composition as in table 3.2, from the last pre-treatment step was sent to a continuous flat bottom tank for storage, denoted biomass slurry storage, at a rate of 9.0×10^5 tonnes/yr.

Table 3.2: The composition of biomass slurry entering the bioreactor section, with reference temperature of $25°C$.

Component	Percentage [wt.%]	Concentration [kg/m^3]
Acetic-acid	0.88	10.05
Ash	4.24	48.36
Cellulose	16.91	192.68
Extractives	0.39	4.47
Furfural	0.07	0.76
Molasses	0.16	1.78
Hemicellulose	2.53	28.84
HMF	0.02	0.19
Lignin	9.93	113.17
Insoluble protein	4.58	52.23
Sodium hydroxide	0.00	0.01
Soluble lignin	0.17	1.96
Water	57.56	655.84
Xylose	2.39	27.20

The stream exiting the biomass slurry storage was split into six fractions and water, yeast and enzymes were added at different amount as in table 3.3. The enzymes were modelled to consist of 85 wt.% of insoluble protein and 15 wt.% of biomass and were diluted to a water content of 94.7 wt.%. These six streams were connected to a stirred reactor procedure.

Table 3.3: Amount of biomass slurry, yeast mixture, water (with the unit of m^3 water added/ m^3 in the process stream) and enzymes (excluding water and with the unit of kg enzyme solution/ kg cellulose in process stream) added to the SSF procedure at each of the six feeding operations.

Time	Biomass Slurry [wt.%]	Yeast mixture [wt.%]	Water [m^3/ m^3]	Enzymes [kg/kg]
0 hr	14.28	34.59	4.20	0.20
4 hr	19.50	0	0.03	0
12 hr	18.83	16.42	0.02	0
24 hr	17.52	16.42	0.00	0
48 hr	15.59	16.42	0.03	0
72 hr	14.28	16.42	0.03	0

The SSF procedure was designed such that material was added at six times. Each transfer in operation of material was followed by one reactor operation and one fermentation operation. The sixth fermentation operation was followed by 30 minutes transfer out operation and 60 minutes CIP operation. The SSF procedure was connected to a continuous flat bottom tank procedure, denoted product storage unit.

In the SSF procedure the reaction were defined as in reaction 1, reaction 2 and reaction 3 and the heat of reaction for all reactions were assumed to be zero. The stoichiometric coefficient in the reaction expressions are on mass basis.

$$162.16\,\text{Cellulose} + 18.02\,H_2O \longrightarrow 180.16\,C_6H_{12}O_6 \quad \{1\}$$

$$132.00\,\text{Hemicellulose} + 18.02\,H_2O \longrightarrow 150.13\,\text{Xylose} \quad \{2\}$$

$$180.16\,C_6H_{12}O_6 \longrightarrow 92.14\,C_2H_5OH + 88.02\,CO_2 \quad \{3\}$$

The efficiency of the reactions in the SSF procedure was obtained using a kinetic model earlier created in the project [27]. The values in the kinetic model were converted from yield to conversion and included in the SPD model.

The vent gases from the seed fermenters and the SSF procedure were connected to a CO_2-scrubber. The CO_2-scrubber was made of a custom mixing unit that supplies water to the venting gases, such that the ratio between

the amount of water supplied to the amount of carbon dioxide in the CO_2-scrubber was 1.3. The scrubber also contained a two-way component splitting operation that was set to remove 100 % of all CO_2, nitrogen and oxygen. The steam with a lower CO_2 concentration was connected to the product storage unit.

Apart from above named storage tanks virtual tanks, in the sense that they were not displayed in the flowsheet, were supplied. Five supply tanks were added to store raw material and receiving tanks were added to store aqueous waste products from all CIP operations in the process.

To ensure that the flows generated were comparable with the amount of material used in the demo tests, which were executed earlier at the biorefinery demo plant in Örnsköldsvik, the flow of the biomass slurry in the model was adjusted to enable comparison with the amount of material supplied per batch in demonstration plant [27].

3.4 Scheduling

To validate that all operations and procedures were operating as intended OGC and EOC were generated. These charts were also used to identify the bottleneck equipment. Based on bottleneck equipment and number of SSF procedures three cases with different scheduling were constructed. For the first case (Case B) equipment operating with staggered starting times were added the original case (Case A). The number of equipment operating with staggered starting times were such that a new SSF procedure was started each 25.5 hours. To ensure that the throughput remained constant the flow of the biomass slurry was fixed at 9.0×10^5 tonnes/yr., as in the continuous model. The second scheduling (Case C) was such that all parallel equipment in Case A were operating with staggered starting times. The residence time in the storage units was adjusted in these cases such that the residence time was equal to the time between the start of consecutive batches.

The EOC for both Case B and Case C showed a change in bottleneck equipment, hence the third scheduling was made like Case C with the difference that the parallel units required for all seed fermenters were scheduled to operate with staggered starting times.

3.5 Economic evaluation and cost analysis of the bioreactor system

In the early phase of modelling the default values were used to estimate capital and investment costs for the bioreactor system. With time some of the economic parameters were adjusted according to table 2.3, appendix E and the material of construction for all equipment was changed to 304SS, which is a commonly used grade of austenitic stainless steel [36].

To simplify a comparison between the batch model and the continuous model water was assumed to be fully recirculated, hence the cost of water was set to zero. The cost of electricity was also assumed to be zero, as electricity is produced in a downstream part of the process.

After addition of estimated cost parameters to the model a VBA code for summering the results of the five different models was created. The VBA code was made such that the expense of all materials in the process easily could be adjusted in excel for all models. The operating time for the sixth fermentation and reactor operation in the SSF procedure were changed. Simultaneously with changed reaction time the conversions for all reactions in the SSF reactor automatically were updated.

During economical evaluation of the process a high-power demand was observed, which gave a high utility cost. By using the power chart for single batches in SPD the most power intense operation was localized. The most power demanding operation was located as the agitation demand during fermentation in the SSF procedure, a default value in SPD 3 kW/m^3. This value was compared to the default value for agitation in a continuous model and the power demand showed to be significantly lesser at 0.05 kW/m^3 for no obvious reason, hence the value was changed accordingly.

3.6 Sensitivity Analysis

The SSF reactor procedure was, as mentioned earlier, divided into different operations; six transfer in, six reactions, six fermentations, one transfer out and one CIP operation. Variation in time for the SSF reactor procedure was done by changing the operation time for the last reaction and fermentation operation in the procedure. The operating time for these two operations were adjusted such that the total time of the procedure was 90, 96 and 100 hours

(excluding transfer out and CIP), hence the operation time of the last reaction and fermentation operations was adjusted to 18, 24 and 28 hours.

Conversion of the reactions were simultaneously adjusted with changing reaction time using a kinetic model earlier created in the collaborative project [27]. The kinetic model was such that it gives the yield for different times, hence before implementing it into SPD model the yield was expressed as conversion.

Table 3.4 contains the conversions, for 90, 96 and 100 hours procedure time respectively. In the model the conversions presented in Table 3.4 were only included in the last fermentation and reaction operations. To obtain a final conversion as in the table the conversion for all other reaction and fermentation operations in the SSF reactor were set to zero.

Table 3.4: Variation in conversion as the residence time in the SSF reactor varies.

Reaction/Conversion	At 90 hr [%]	At 96 hr [%]	At 100 hr [%]
Hydrolysis of Cellulose	77	78	79
Hydrolysis of Hemicellulose	0.01	0.01	0.01
Glucose to Ethanol	91	91	91
Glucose to Glycerol	0.7	0.7	0.7
Xylose to Ethanol	0.01	0.01	0.01
Xylose to Xylite	14	14	14
Xylose to Glyce	20	20	20

To evaluate the size impact on the scheduling, the reactor size of the SSF reactor was changed from 1200 m^3 to 3795 m^3. Validation of Case A showed that fewer parallel reactors were required for 3795 m^3, the number of parallel equipment decreased from 16 to 6. The number of staggered equipment for Case C and Case D was therefore changed to 5.

4. Result and Discussions

This chapter combines the result and discussion of the thesis. In the first section below results and discussion regarding the development of the SPD model of the bioreactor system are given. This is followed by result and discussion regarding scheduling, comparison between the fed-batch and the continuous bioreactor model, variation in reaction time and lastly variation in equipment size.

4.1 Model

A visual illustration of the bioreactor system created in SPD is available in Figure 4.1. Different sections of the model have different colours to enhance the understanding. The procedures in orange are all part of the storage section, the teal coloured procedures belong to the yeast propagation section, the ethanol fermentation section includes only one procedure which has the colour of plum. The remaining procedures are shown in black and are all part of the main section of the bioreactor system.

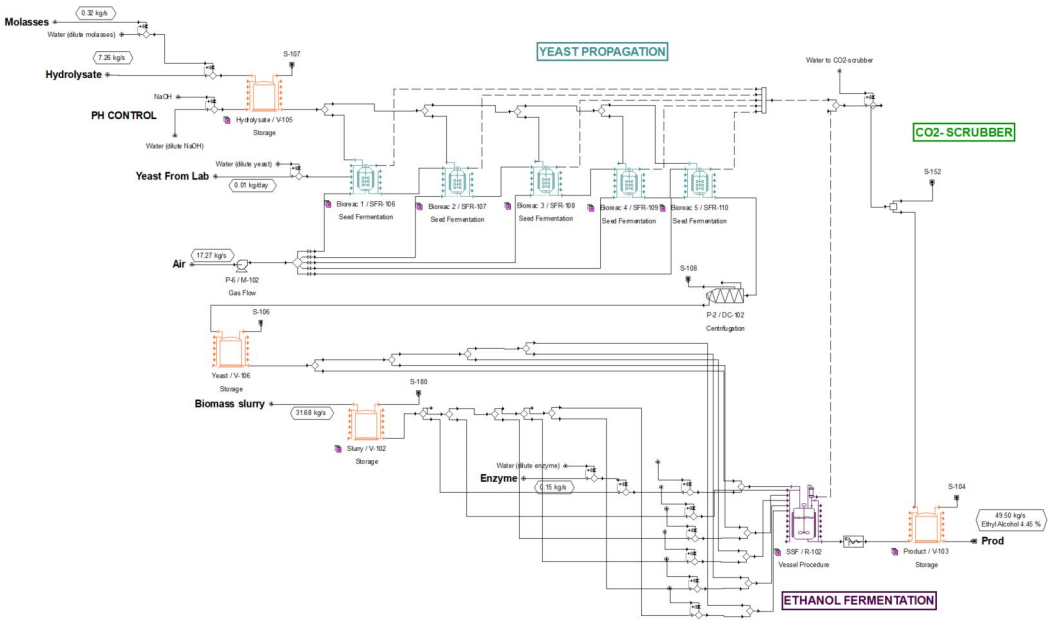

Figure 4.1: Flow chart of the bioreactor system.

According to the results from the demo testing [27] yeast should be added such that the amount of yeast in the SSF is 0.02 g cells / g WIS. To easier

implement this in the SPD model the WIS concentration was assumed to be 10 wt.% [21] of the content. The amount of yeast produced was therefore such that the concentration of yeast out of the SSF reactor was 0.2 wt.%. However, 0.2 was not the value used in the final model since the continuous model had a different value and a comparison was assumed to be easier if the same value was selected. The value selected was therefore 0.3321 wt.%. It was also found during validation with values from the demo that 0.3321 was a more suitable value than 0.2 wt.%.

CIP is an example of an operation that has been provided with uncertain inputs. The recipe used for cleaning includes pre-rinsing, cleaning with hot caustic solution, rinsing, steam for disinfection and finally cold water for cooling down the equipment. According to some literature, it is beneficial to use acid cleaning occasionally to remove mineral scale [5], this was however not included. The recipe for CIP used in the model was based on the cleaning procedure used for cleaning the demo equipment [34] with complementary data from SPD example files. The example used was of a brewery with a fermenter volume of 350 m^3 [15].

Looking at the scheduling of the process the main parameter of interest was the time required. In this case the time required was assumed to be one hour, which was based on that the time required for cleaning the demo plant was 30 minutes and the assumed cleaning time in the SPD example file was about 90 minutes. The reasons for using 60 minutes was that a shorter cleaning time in the demo plant would be required since the equipment in the model was larger, the time required to clean the equipment in the brewery example was assumed to be larger since the cleaning requirements for breweries are likely to be harsher.

It was also necessary to make certain assumptions regarding conversion in the yeast production section. For conversions of cellulose to glucose and hemicellulose to xylose 97 % and 95 % were selected, respectably. This assumption was slightly different from the continuous model, in which 100 % conversion was assumed. Since there has not been done any demo testing, for the yeast section of the process, there are no data available that can be used for validating the result of this section.

Table 4.1 provides a summary of the material demand, with raw material requirements listed per year, per batch and per main product (MP), i.e. ethanol. These values are based on the demands for Case A.

Table 4.1: Material consumed in the bioreactor system, for Case A and for 96 hours SSF procedure.

Material	Material/ year [kg/yr.]	Material/ batch [kg/batch]	Material / MP [kg/kg MP]
Biomass slurry	8.79×10^8	1.11×10^7	14.4
Hydrolysate	2.01×10^8	2.55×10^6	3.30
Air	4.79×10^8	6.06×10^6	7.84
Yeast from lab	1.97	2.49×10^{-2}	3.22×10^{-8}
Water	5.73×10^8	7.26×10^6	9.39
Sodium hydroxide	3.47×10^4	4.39×10^2	5.68×10^{-4}
CIP NaOH	5.38×10^7	6.80×10^5	0.88
Enzymes	4.25×10^6	5.38×10^4	6.96×10^{-2}
Molasses	8.86×10^6	1.12×10^5	0.15

In table 4.2 data used for validating the model and the corresponding from the demo plant experiments are shown. The values in this compilation show that the total amount of yeast in the model was lower than the amount supplied in the demo. The reason for not adjusting for this difference was that yeast supplied was defined based on the amount used in the continuous model and since a part of the aim of this thesis was to compare with the continuous model no adjustment was made. To estimate the impact that this has on the result temporarily adjustment was made, such that the concentration of yeast in the stream leaving the SSF reactor was changed from 0.3 % to 0.5 %. This gave a total yeast supply of 22.7 l/batch. At large scale, i.e. if the amount of biomass slurry to be processed was 9×10^5 tonnes/yr. or 7.9×10^5 m^3/ yr., using a concentration 0.3321 wt.% rather than 0.2 wt.% increased the number of equipment required in the bioreactor section.

Table 4.2: Validation results from model with values from demo.

Parameter	Unit	SPD Model	Demo *
Biomass slurry feed 1	kg/batch	449	449
Biomass slurry feed 2	kg/batch	613	614
Biomass slurry feed 3	kg/batch	592	592
Biomass slurry feed 4	kg/batch	551	551
Biomass slurry feed 5	kg/batch	490	490
Biomass slurry feed 6	kg/batch	449	449
Tot biomass slurry	kg/batch	3145	3145
Water feed 1	l/batch	1439	1536
Water feed 2	l/batch	9	8
Water feed 3	l/batch	8	8
Water feed 4	l/batch	8	8
Water feed 5	l/batch	9	8
Water feed 6	l/batch	9	8
Tot water	l/batch	1482	1576
Yeast feed 1	kg/batch	5.2	8.3
Yeast feed 2	kg/batch	0	0
Yeast feed 3	kg/batch	2.5	3.9
Yeast feed 4	kg/batch	2.5	3.9
Yeast feed 5	kg/batch	2.5	3.9
Yeast feed 6	kg/batch	2.5	3.9
Tot yeast	kg/batch	15.2	23.9
Enzyme feed 1	l/batch	93	80
Ethanol Conc. prod.	g/l	46	68

* The tests were performed in the biorefinery Demo Plant in Örnsköldsvik, Sweden.

4.2 Scheduling

The results given in this section are all based on the case where the SSF reactor´s procedure time was 96 hours, excluding the time required for transferring material out of the reactor and the time allocated for CIP of the equipment.

The assumptions made for all equipment operating in batch mode were that transfer of material from one vessel to another always takes 30 minutes and the amount of time allocated for cleaning between each batch takes one hour. It is likely that the larger and the more material in the vessels the longer time will be required for cleaning and transportation.

For CIP the time was assumed to be equal for all equipment operating in batch mode. The recipe for cleaning was also assumed to be the same. Based on this assumption scheduling of CIP SKID, the set of equipment that supplies all cleaning circuits with the necessary flow, temperature, and conductivity for the correct amount of time through automated control [6], was excluded. Thereby, the scheduling of equipment required for CIP was not considered an issue. This assumption should be reconsidered if different cleaning recipes are required.

The operational Gantt chart of the process can be seen in Figure 4.2. In this Gantt chart only fed-batch procedures were included, since these procedures were the only procedures that had a start and finish time that could be scheduled. On the left side of the figure, description of the procedures are available. The right side of the figure shows how these procedures are scheduled relative to each other. The OGC of the process shows that first all the bioreactor procedures, starting with the smallest to the largest bioreactors, are propagating yeast and once enough yeast has been produced the SSF procedure starts. The time between bioreactor 5 and the SSF procedure was included to consider the residence time of the centrifuge.

In the lower left corner of Figure 4.2 the procedure with the longest duration, the bottleneck equipment, is indicated with a symbol of a blue triangle with an exclamation mark in it. In this case the symbol indicates that the current bottleneck, equipment before adjustments has been done to the scheduling, is the SSF reactor. the bottleneck equipment can also be identified by comparing the length of the different bars (i.e. by comparing the cycle times) in the figure, the bar for the SSF reactor is almost 98 hours while less the 26 hours for the remaining procedures.

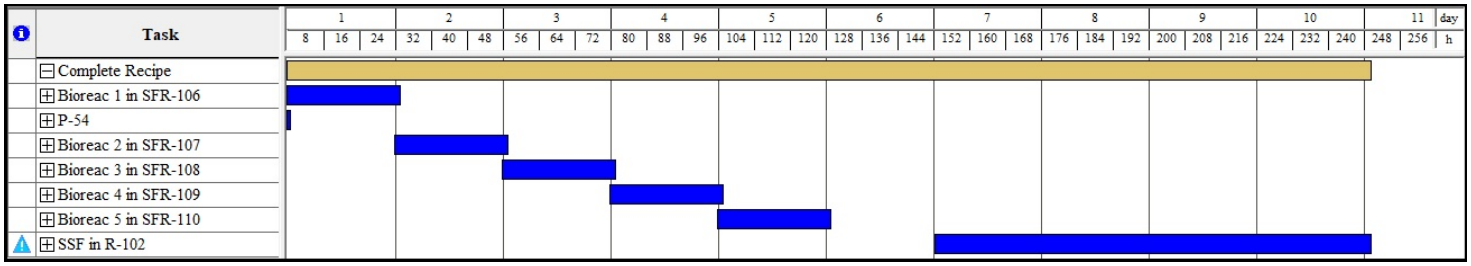

Figure 4.2: Operational Gantt chart on procedure level of the bioreactor system.

The Equipment Occupancy Chart (EOC) of 10 batches for Case A is available in Figure 4.3. The EOC shows that the equipment limiting the number of batches that can be completed per year was R-102, which contained the SSF procedure, since there were no gaps between the finish time of one batch and the start time of the next batch. The gap between the bars of SFR-106 to SFR-110 indicates that they have an idle time of almost 98 hours.

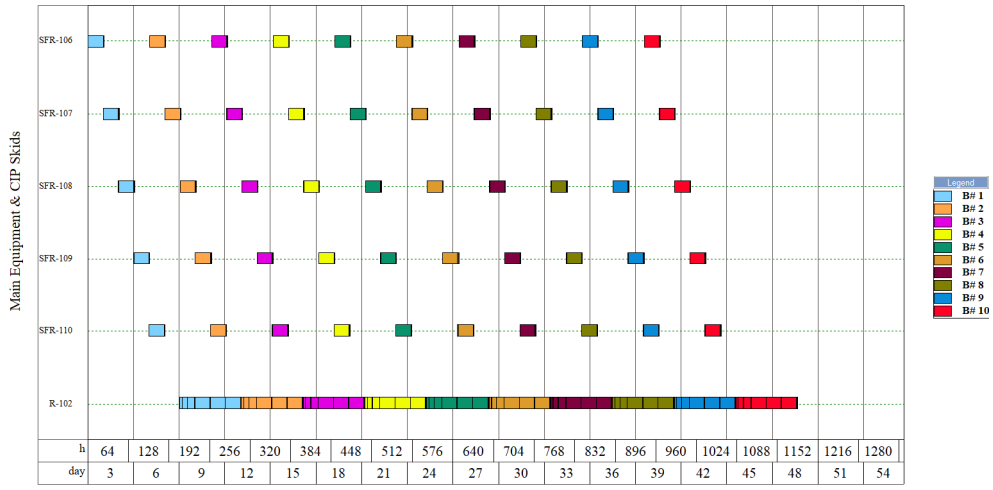

Figure 4.3: Equipment occupancy chart of the bioreactor system for Case A.

Through simulations in SPD the number of parallel reactors, i.e. number of SSF reactors starting simultaneously, was calculated to be 17 Case A. This means that in order to process a certain amount biomass, in this case 9.0×10^5 tonnes/yr, and with a maximum volume of 1200 m^3 for each the SSF reactors 17 reactors were required.

The EOC of the bioreactor system where the number of staggered units was such that the idle time of the reactors propagating yeast was zero, Case B, is available in Figure 4.4. Reduction of idle time makes it possible to use the annual operating time more efficiently. Through simulations in SPD the time between the staggered starting times of SSF reactors to remove the lag time between the completion of one batch of a yeast reactor and the start of the next was calculated to be almost 26 hours. This gave that five reactors started with 26 hours interval. The total amount of SSF reactors required for this scheduling was 20 pcs.

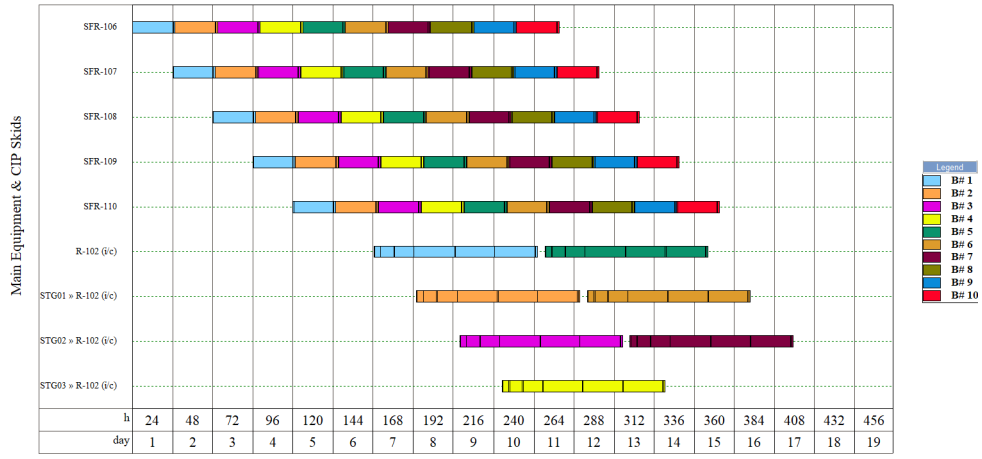

Figure 4.4: Equipment occupancy chart of the bioreactor system for Case B.

The EOC for the bioreactor system where all 17 SSF reactors operated in staggered mode, Case C, is available in Figure 4.5. The time between the start of two staggered procedures was 5.74 hours.To schedule the system this way the SSF reactor had to modeled to operate the SSF procedure independent on the procedures in the yeast train. This gives that the different colored bars in the yeast train in Figure 4.5 do not correspond to the similar colored bars in the SSF reactor part of the process. To validate that enough yeast was produced the different flows of hydrolysate in Case A and Case C were compared and the conclusion was that they were equal.

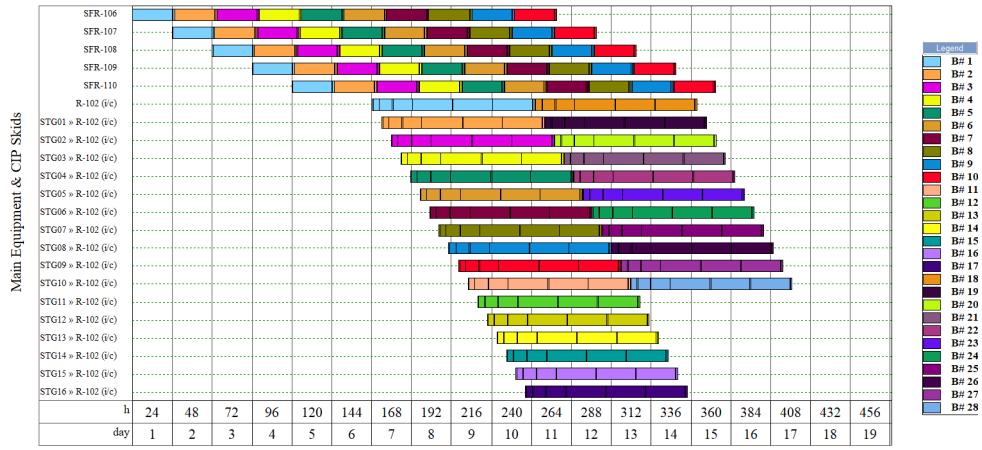

Figure 4.5: Equipment occupancy chart of the bioreactor system for Case C.

The EOC in Figure 4.6 is similar to the EOC in Figure 4.5 but with an important difference, the two parallel yeast trains required to process enough

yeast were also operating with staggered start times, hence a yeast train was started every 12.75 h compared to every 25.5 h.

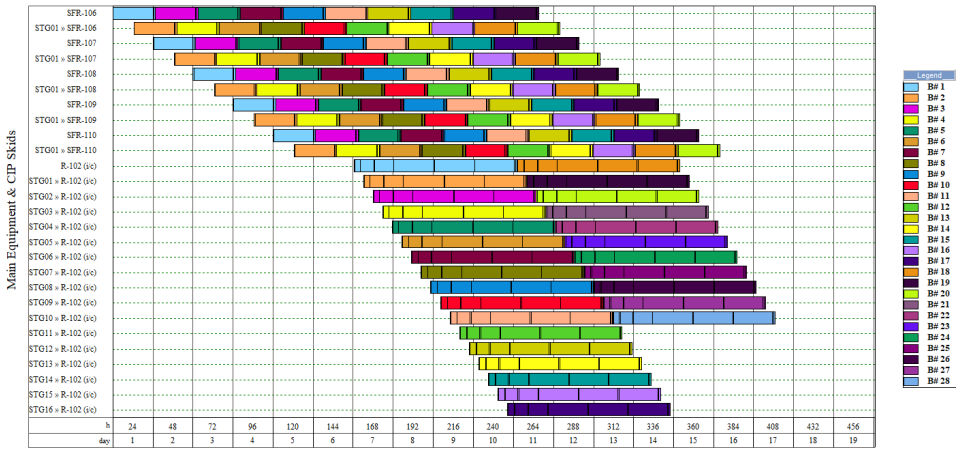

Figure 4.6: Equipment occupancy chart of the bioreactor system for Case D.

Table 4.3 aims to give an overview of the impact that the use of units operating with staggered start times had on equipment, annual operating cost, annual time utilized and annual amount of ethanol produced.

The values in table 4.3 indicate that from an economical perspective operating parallel equipment with staggered start times is beneficial. The reason for decreased equipment cost was most likely related to that less equipment is required to produce the same amount of ethanol in the models with more equipment operating out of phase. As the table shows the operating cost also lesser, this probably due to increased facility dependent costs, see appendix E.

Table 4.3: Impact of operating parallel equipment with staggered start times, for a 96 hours SSF procedure.

Parameter	Unit	Case A	Case B	Case C	Case D
Bottleneck equipment		R-102	SFR-110	SFR-110	SFR-110
Equipment cost	M€	7.3	4.7	4.2	4.1
Operating cost	M€/yr.	10.2	8.2	7.9	8.1
Time utilized	hr/yr.	7847	7897	7897	7909
Produced ethanol	tonnes/yr.	8.2×10^4	8.1×10^4	8.1×10^4	8.1×10^4
Number of Equipment	pcs	62	41	37	37

Decreasing the idle time for the reactors used to propagate yeast may be of less economical benefit compared to what the result of the simulation indi-

cates. The reason for this is that there are a few advantages with idle time, the first one is that the process has time to adapt to changes, for example it may take more than 30 min to empty a reactor in a real life plant. The second advantage with idle time is that the time the reactors are not used can be used for storage, hence minimizing the demand for storage vessels.

4.3 Comparison between continuous and fed-batch bioreactor systems

Table 4.4 contains the material demands for the bioreactor section in the continuous model and the material demand for Case A in the fed-batch model. The comparison was for the conversion associated with a procedure time of 96 hours in the SSF reactor, and water and sodium hydroxide demand for CIP operations in the fed-batch model are not included in the table.

There were a few differences between the two models regarding the demand of different components. This is since some of the parameters were defined differently. The difference is also due to that the demand in the two models were defined differently. For instance table 4.4 shows a distinct difference in the amount of sodium hydroxide fed to the two models. The intention was to define the demand in the batch model such that similar amount was supplied to both systems but during the development of the batch model the value changed. This was not seen as a severe error since the amount of sodium hydroxide supplied for pH regulation was only included symbolically and by changing the flow of sodium hydroxide for Case A to 27 kg/h the number of equipment remained constant since the sodium hydroxide demand was small relative to the demand of other components. The inequality will therefore have no major impact on the scheduling nor the economy of the bioreactor section.

Table 4.4: Data from the bioreactor section of the continuous model and the fed-batch model for Case A excluding the amount of material required for cleaning, for a SSF reaction time of 96 hr.

Parameter	Unit	Continuous	fed-batch
Tot Biomass slurry	kg/s	31.7	31.7
Hydrolysate	kg/s	8.0	7.3
Tot Water	kg/s	25.3	19.7
Yeast from Lab	kg/day	0.004	0.006
Tot enzymes	kg/s	0.15	0.15
Molasses	kg/s	0.35	0.32
Air	kg/s	19.0	17.3
Sodium hydroxide	kg/hr	27.0	4.5

Table 4.5 shows the result from the continuous model and the fed-batch model for Case A. Comparing the result of these two models indicates that using a continuous model to predict the outcome of a fed-batch process may underestimate equipment and operation costs. Underestimation of these costs can result in erroneously estimated profitability of the entire project.

Table 4.5: Comparison of results from the continuous and the fed-batch model for Case A, for a SSF reaction time of 96 hr.

Parameter	Unit	Continuous	fed-batch
Equipment Cost	M€	5.2	7.3
Annual Operating Cost	M€/yr.	6.2	10.4
Annual Time Utilized	hr/yr.	7920	7847
Ethanol production	tonnes/yr.	7.3×10^4	6.1×10^4

4.4 Sensitivity analysis

Changes in time of SSF and conversion of the reactions are likely to impact both the scheduling and the economy of the process. Investigating the impact of variation in these parameters is of importance, since it is a possibility that 96 hours SSF is not the optimal. In table 4.6 and in table F.1 the result of having a SSF time of 90, 96 and 100 hours for Case A to Case D are shown.

For continuous operations the size and time utilization were 100 %. All continuous operations are therefore excluded from table 4.6. The time utilization for the bottleneck equipment was also equal to 100 % but they are included

in the table.

Table 4.6: Variation in reaction time's impact on relative size and relative time utilization for Case A, Case B, Case C and Case D.

		90 hours		96 hours		100 hours	
Case	Procedure	Size [%]	time [%]	Size [%]	time [%]	Size [%]	time [%]
A	SSF Reactor	100	100	100	100	100	100
	Bioreactor 1	99.23	27.87	99.23	26.15	99.23	25.12
	Bioreactor 2	99.15	27.87	99.15	26.15	99.15	25.12
	Bioreactor 3	99.12	27.87	99.1	26.15	99.12	25.12
	Bioreactor 4	99.12	27.87	99.12	26.15	99.12	25.12
	Bioreactor 5	99.12	27.87	99.12	26.15	99.12	25.12
B	SSF Reactor	100	89.71	100	95.59	100	99.51
	Bioreactor 1	99.23	100	99.23	100	99.23	100
	Bioreactor 2	99.15	100	99.15	100	99.15	100
	Bioreactor 3	99.12	100	99.12	100	99.12	100
	Bioreactor 4	99.12	100	99.12	100	99.12	100
	Bioreactor 5	99.12	100	99.12	100	99.12	100
C	SSF Reactor	100	93.77	100	99.92	100	104.02
	Bioreactor 1	99.23	100	99.23	100	99.23	100
	Bioreactor 2	99.15	100	99.15	100	99.15	100
	Bioreactor 3	99.12	100	99.12	100	99.12	100
	Bioreactor 4	99.12	100	99.12	100	99.12	100
	Bioreactor 5	99.12	100	99.12	100	99.12	100
D	SSF Reactor	100	93.77	100	99.82	100	104.02
	Bioreactor 1	99.23	100	99.23	100	99.23	100
	Bioreactor 2	99.15	100	99.15	100	99.15	100
	Bioreactor 3	99.12	100	99.12	100	99.12	100
	Bioreactor 4	99.12	100	99.12	100	99.12	100
	Bioreactor 5	99.12	100	99.12	100	99.12	100

For both Case C and Case D the utilization time was greater than 100 %. The result of having a utilization time greater than 100 % is better visualized in the EOC, Figure 4.7. This figure shows the EOC for Case C at an operation time of 100 hours. In this figure an overlap of different bars can be seen. This indicates that the SSF procedure overlapped with itself across multiple batches. There are two alternative reasons for this conflict. Either there are not enough staggered units of host equipment R-102 to avoid this conflict or the recipe cycle time may be too short.

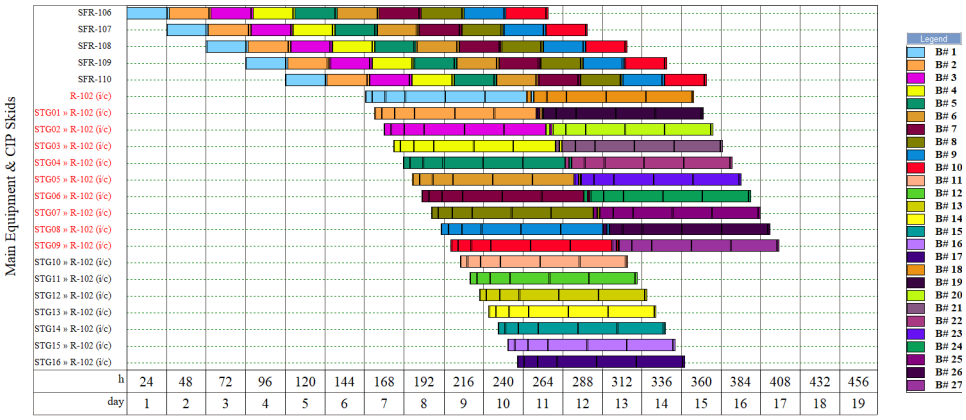

Figure 4.7: Equipment occupancy chart of Case C at a process time of 100 hours.

Table 4.6 shows that the time utilization for Case B is close to reaching 100 % for an operation time of 100 hours. This implies that if the time would be more than 100 hours it is likely that scheduling will be a problem in this case as well.

The amount of time material had to be stored was approximated such that it was made independent of the duration of the SSF procedure. This assumption probably affected the result for Case A the most since in the other cases material was taken out of the storage units at fixed time intervals. For Case A the design of the storage units was based on the cycle duration of the SSF procedure, hence it was fixed at 97.5 hours (96 hours SSF, one-hour cleaning, 30 min transfer out). This was not changed for 90 and 100 hours SSF.

Table F.1 indicates that the total number of equipment and the size of equipment decrease for increased number of equipment operating with staggered starting times. This is most obvious for equipment V-102, biomass storage, the number of equipment decreased from seven to one and the size required from 1600 m^3 to 670 m^3. There were, however, almost no differences in volume and number of equipment required for variation in SSF process time. Even so, this is no proof that reaction time has no impact on these parameters. In fact, it is likely, that the number of reactors will increase if the reaction time is long enough. The reason for this is that long residence time in the SSF reactor requires that more material gets processed simultaneously to ensure that the average amount of biomass slurry remains at 9×10^5 tonnes/ yr.

The number of equipment required to perform a procedure in the model is

dependent on the selection of maximum batch size, since this creates a limit on the maximum volume of an equipment. The assumed maximum batch size for all storage tanks and reactors used in the models can be found in appendix C. These were based on the inputs used in the continuous model. Variation in equipment size of two different maximum SSF reactor sizes were used, 1200 m^3 and 3975 m^3, to better understand the impact on scheduling, equipment and operating costs. As mentioned before, the reason for selecting these two equipment sizes was that 1200 m^3 was selected for the continuous model and 3975 m^3 was used by The National Renewable Energy Laboratory (NREL) in their report Process design and economics for biochemical conversion of lignocellulosic biomass to ethanol [7].

In this thesis, variations in equipment size for the SSF reactor were tested since the size of the reactor affects the amount of equipment required to operate in parallel. Decreased number of parallel SSF reactors are likely to affect the scheduling, especially for Case C and Case D since these cases were based on that all parallel equipment operates with staggered starting times.

The result of variation in equipment size is available in table 4.7. In all cases increased reactor size gave decreased number of equipment, reduced equipment and annual operating costs and increased time between starts of consecutive SSF procedures for Case C and Case D. The reason for this was that the number of staggered equipment had to be lower since fewer parallel equipment were required. If the same number of staggered equipment were to be used auxiliary equipment would be required.

The reason for decreased operating cost was likely due to decreased annual facility dependent. The reason that the facility dependent cost decreased was dependent on the definition used in the model. In this case the facility dependent cost was defined as a capital investment parameter. As the equipment cost decreases it is likely that the capital investment decreases, consequently leading to decreased facility dependent and operating costs.

Table 4.7: Comparison between two different bioreactor systems with different SSF reactor size, 1200 m^3 and 3795 m^3 for Case A, Case B, Case C and Case D. The first value represents the value corresponding to 1200 m^3 (denoted S) and the second value 3795 m^3 (denoted L).

Case	No. of equipment [pcs]		No. of staggered equipment [pcs]		Bottleneck equipment		Min. time utilization [%]		Equipment cost [M€]		Annual operating cost [M€/ yr.]	
	S	L	S	L	S	L	S	L	S	L	S	L
A, 90 hr	61	50	0		R-102		28		7.1	6.4	10.4	9.3
A, 96 hr	61	51	0		R-102		28		7.3	6.6	10.4	9.5
A, 100 hr	61	50	0		R-102		26	25	7.1	6.4	10.1	9.2
B, 90 hr	41	29	3		SFR-110		90		4.7	3.9	8.1	7.0
B, 96 hr	41	29	3		SFR-110		96		4.7	3.9	8.2	7.0
B, 100 hr	41	29	3		SFR-110		100		4.7	3.9	8.2	7.1
C, 90 hr	37	26	16	6	SFR-110		94		4.2	3.2	7.8	6.5
C, 96 hr	37	26	16	6	SFR-110		100		4.2	3.2	7.9	6.5
C, 100 hr	37	26	16	6	SFR-110		104		4.2	3.2	7.9	6.6
D, 90 hr	37	26	16	6	SFR-110		94		4.1	3.2	8.0	6.7
D, 96 hr	37	26	16+1	6+1	SFR-110		100		4.1	3.2	8.1	6.8
D, 100 hr	37	26	16+1	6+1	SFR-110		104		4.1	3.2	8.1	6.8

4.5 Final discussion

There are still several things that could make the model more accurate, but at this point data for more accurate predictions are not available. There are also a few concerns regarding the implementation of the centrifuge.

Regarding economic evaluation of the process a few assumptions were made. For example, operating cost could be decreased if things like heat integration, water recycling loops and on-site production of enzyme were implemented. This was not included directly, but the cost of water and electricity was assumed to be zero. The heat of reactions were assumed to be zero, because data was unavailable. This assumption will likely decrease the demand for cooling and heating agents. It is likely that the demand for cooling agent would increase since yeast propagation in aerobic environment is an exothermic process, hence cooling is required to ensure that the maximum temperature is not exceeded. The same assumption was made for all models including the model for the continuous process. The risk with making this assumption is that the result will be underestimated.

Concerning the implementation of the centrifuge used in the model a question arises regarding if it is actually necessity. The main use of the centrifuge was to remove liquid, which makes transportation more demanding. The centrifuge seems to be unnecessary since water was later added to the streams entering the SSF procedure to make transportation easier.

5. Conclusion and Suggestions for Future Work

The conclusions of this thesis are:

- Based on the result of the models created it seems like the most beneficial way of operating the bioreactor system, from annual operating cost and equipment cost perspective, is to operate all parallel equipment with staggered starting times.

  To make sure that this is the most economically sustainable option, it is suggested that the bioreactor section in the continuous model be substituted with the fed-batch model, which will allow evaluating the entire plant based on net present value and initial rate of return.

- It is not only the lowest annual operating and equipment costs that determines the most promising scheduling of the process. Process flexibility, the possibility to adapt to unplanned events, is another parameter that should be considered. Operating all parallel equipment out of phase reduces the idle time, which makes the process less flexible.

  It might be better to focus on determining the most beneficial time between the start of two reactors operating out of phase. This is probably complicated and requires knowledge regarding the time frame within which it is likely that the optimal time for SSF reaction lies. It is therefore proposed that future work focuses on defining such time frame and make a statistical analysis to determine the most beneficial scheduling. Before such statistical analysis can be performed, it is recommended that more accurate estimations of time required for transfer of material and CIP be established. The reason for this is that variations are likely to affect the scheduling.

- Variation in reactor size may change the number of parallel reactors required. For Case C and Case D this gives that the time between the start of two SSF reactors varies unless auxiliary equipment are used. The positive effect of operating many reactors with staggered starting time is that material are drawn from yeast storage more frequently, which gives that the number or the volume of storage units required decreases.

It can be concluded that to be able to optimize scheduling, more information regarding available reactor sizes and their dimensions are required. As the result suggests selection of equipment size is of great interest during scheduling. Future work should therefore focus on getting in contact with companies producing different types of equipment to ensure that scheduling is optimized for equipment that are available on the market.

- Creating a batch model rather than a continuous gives the opportunity to include more parameters to the model. However, this will not automatically make the model better. It is essential that high quality inputs are available to avoid GIGO (garbage in garbage out).

  One interesting thing for future work could be to investigate the possibility to increase the quality of the input to the model by using the conversions achieved for each feed operation, instead of using zero as conversion for some of the reactions, in the SSF procedure generated by the kinetic model. This could probably be achieved using the tool which allows SPD to inter-operate with Excel since conversions from the kinetic model can be transferred to Excel as well.

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A. Data From Demo

Table A.1 shows the parameters used as input and output in the demo.

Table A.1: Data from demo

Parameter	Unit	Value
Pretreated biomass added	kg/batch	3144
Density pre-treated Biomass	kg/m^3	1000
Enzyme stock concentration	units/ml	150
Required enzymes	units	12009955
Enzymes	l/batch	80
Water	l/batch	1576
Yeast	kg/batch	24 (Cell/WIS = 0.02 g/g)
Temperature	^{o}C	35
pH		5
Aeration rate	VVM	Not specified
Agitation	rpm	400
Residence time	hr	96
Max volume	l	10000
Pressure	atm	Not specified
WIS	%	38.2

B. Data From Continuous Model

Table B.1: Comparison between the composition of the streams from the bioreactor section of the continuous model and the semi-batch model.

Component	Unit	Semi-batch	Continuous	Diff.
Acetic-acid	kg/s	0.28	0.28	0.00
Ash	kg/s	1.35	1.34	0.01
Biomass	kg/s	0.02	0.02	0.00
Cellulose	kg/s	1.17	1.17	0.01
Ethanol	kg/s	2.20	2.17	0.02
Extractives	kg/s	0.13	0.13	0.00
Furfural	kg/s	0.02	0.02	0.00
Glucose	kg/s	0.42	0.42	0.00
Glycerol	kg/s	0.14	0.13	0.00
Hemicellulose	kg/s	0.81	0.80	0.00
HMF	kg/s	0.01	0.01	0.00
Lignin	kg/s	3.16	3.15	0.02
Protein	kg/s	1.59	1.58	0.01
Sodium hydroxide	kg/s	0.00	0.2	-0.2
Soluble lignin	kg/s	0.06	0.06	0.00
Sulfuric acid	kg/s	0.05	0.05	0.00
Water	kg/s	33.89	39.76	-5.87
Xylitol	kg/s	0.11	0.11	0.00
Yeast	kg/s	0.15	0.17	-0.02

C. Inputs to SuperPro Designer

A Yeast propagation section

- Heat of reaction is not included, hence assumed to be zero.
- Conversion of glucose to yeast matter is 97 % and conversion of xylose to yeast matter is 95 %.
- Air supply is calculated such that 1 VVM is supplied to each reactor.
- Maximum working volume for bioreactor 1-5 are 0.08, 0.76, 7.57, 75.71 and 757.08 m^3 respectively.
- Working to vessel volume ratio is 90 %.
- Height to diameter is 3
- Equipment specification are calculated in design mode
- Specific power consumption of agitation is 0.5 kW/m^3.
- The material of construction for all equipment were selected to 304SS, since according to the report by NREL stainless steel is most likely more cost-effective compered to carbon steel. Carbon steel would have to be designed thicker for corrosion allowance and it tends become a contamination source [7].
- Venting is such that that the following component are included: Acetic-acid, Carbon dioxide, Ethanol, HMF, Nitrogen, Oxygen and Water.

Table C.1: Description of each procedure in the yeast propagation section of the bioreactor model.

Procedure/ equipment	Operation	**Description**
Bioreac. 1/ SFR-106	Transfer in hydrolysate	For 1440 min, 0.0099 % of the content from hydrolysate storage.
	Pull in yeast	For 1440 min to reach mass ration of 0.418.
	Batch stoich. ferment	24h, at 32 ^{o}C, 1.013 bar, aeration rate 1VVM.
	Transfer out	To bioreac. 2 for 30 min.
	CIP	For 60 min. Pre rinse, Caustic clean, rinse, disinfect, cooling.
Bioreac. 2/ SFR-107	Transfer in hydrolysate	For 1440 min, 0.09 % of the remaining content from hydrolysate storage.
	Transfer in	From bioreac. 1 for 30 min.
	Batch stoich. ferment	24h, at 32 ^{o}C, 1.013 bar, aeration rate 1VVM.
	Transfer out	To bioreac. 3 for 30 min.
	CIP	For 60 min. Pre rinse, Caustic clean, rinse, disinfect, cooling.
Bioreac. 3/ SFR-108	Transfer in hydrolysate	For 1440 min, 0.903 % of the remaining content from hydrolysate storage.
	Transfer in	From bioreac. 2 for 30 min.
	Batch stoich. ferment	24h, at 32 ^{o}C, 1.013 bar, aeration rate 1VVM.
	Transfer out	To bioreac. 4 for 30 min.
	CIP	For 60 min. Pre rinse, Caustic clean, rinse, disinfect, cooling.
Bioreac. 4/ SFR-109	Transfer in hydrolysate	For 1440 min, 9.091 % of the remaining content from hydrolysate storage.
	Transfer in	From bioreac. 3 for 30 min.
	Batch stoich. ferment	24h, at 32 ^{o}C, 1.013 bar, aeration rate 1VVM.
	Transfer out	To bioreac. 5 for 30 min.
	CIP	For 60 min. Pre rinse, Caustic clean, rinse, disinfect, cooling.
Bioreac. 5/ SFR-110	Transfer in hydrolysate	For 1440 min, 100 % of the remaining content from hydrolysate storage.
	Transfer in	From bioreac. 4 for 30 min.
	Batch stoich. ferment	24h, at 32 ^{o}C, 1.013 bar, aeration rate 1VVM.
	Transfer out	To centrifuge for 30 min.
	CIP	For 60 min. Pre rinse, Caustic clean, rinse, disinfect, cooling.

B Ethanol fermentation section

- Heat of reaction is not included, hence assumed to be zero
- Maximum working volume is 1200 m^3.
- Working to vessel volume ratio is 80 %
- Height to diameter is 3
- Equipment specification are calculated in design mode
- Specific power consumption of agitation is 0.05 kW/m^3
- The material of construction for all equipment were selected to 304SS, since according to the report by NREL stainless steel is most likely more cost-effective compered to carbon steel. Carbon steel would have to be designed thicker for corrosion allowance and it tends become a contamination source [7].
- Venting is such that that the following component are included: Acetic-acid, Carbon dioxide, Ethanol, HMF, Nitrogen, Oxygen and Water.

Table C.2: Description of each procedure in the ethanol fermentation section of the bioreactor model.

Feed/ Time	Operation	**Description**
1/ t=0 h	Pull in	30 min mixture of slurry, yeast, enzyme and water.
	Batch stoich. react.	Hydrolysis of cellulose and hemicellulose. 4 hours at 32 ^{o} C, P=1.013.
	Batch stoich. ferment	. 4 hours at 32 ^{o} C, P=1.013 and anaerobic conditions.
2/ t=4 h	Pull in	30 min mixture of slurry and water.
	Batch stoich. react.	Hydrolysis of cellulose and hemicellulose. 8 hours at 32 ^{o} C, P=1.013.
	Batch stoich. ferment	8 hours at 32 ^{o} C, P=1.013 and anaerobic conditions.
3/ t=12 h	Pull in	30 min mixture of slurry, yeast and water.
	Batch stoich. react.	Hydrolysis of cellulose and hemicellulose. 12 hours at 32 ^{o} C, P=1.013.
	Batch stoich. ferment	12 hours at 32 ^{o} C, P=1.013 and anaerobic conditions.
4/ t=24 h	Pull in	30 min mixture of slurry, yeast and water.
	Batch stoich. react.	Hydrolysis of cellulose and hemicellulose. 24 hours at 32 ^{o} C, P=1.013.
	Batch stoich. ferment	24 hours at 32 ^{o} C, P=1.013 and anaerobic conditions.
5/ t=48 h	Pull in	30 min mixture of slurry, yeast and water.
	Batch stoich. react.	Hydrolysis of cellulose and hemicellulose. 24 hours at 32 ^{o} C, P=1.013.
	Batch stoich. ferment	24 hours at 32 ^{o} C, P=1.013 and anaerobic conditions.
6/ t=72	Pull in	30 min mixture of slurry, yeast and water.
	Batch stoich. react.	Hydrolysis of cellulose and hemicellulose. 24 hours at 32 ^{o} C, P=1.013.
	Batch stoich. ferment	24 hours at 32 ^{o} C, P=1.013 and anaerobic conditions.
	Transfer out	30 min to prod. storage.
	CIP	For 60 min. Pre rinse, Caustic clean, rinse, disinfect, cooling.

Table C.3: Yield and conversion for cellulose hydrolysis and fermentation of glucose to ethanol.

Reaction and time	Yield [kg/kg]	Conversion [%]
Hydrolysis cellulose at t = 90 hr	85.51	76.97
Fermentation Glucose to Ethanol at t = 90 hr	46.56	91.04
Hydrolysis cellulose at t = 96 hr	86.88	78.20
Hydrolysis cellulose at t = 100 hr	87.73	78.96
Fermentation Glucose to Ethanol at t = 100 hr	46.56	91.04

Table C.4: Conversion for remaining reactions in the SSF reactor.

Reaction and time	Conversion [%]
Hemicellulose hydrolysis	0.01
Glucose to glycerol	0.74
Xylose to ethanol	0.01
Xylose to xylitol	14
Xylose to glycerol	20.20

C Storage section

- Heat of reaction is not included, hence assumed to be zero.
- Maximum working volume is 1000 m^3 for product storage. The remaining storage units have a maximum working volume of 1800 m^3.
- Working to vessel volume ratio is 90 %.
- Height to diameter is 3
- Equipment specification are calculated in design mode.
- The material of construction for all equipment were selected to 304SS, since according to the report by NREL stainless steel is most likely more cost-effective compered to carbon steel. Carbon steel would have to be designed thicker for corrosion allowance and it tends become a contamination source [7].

Table C.5: Description for each procedure and each case in the storage section of the bioreactor model.

Procedure/ equipment	Case	**Description**
Slurry/ V-102	A	Store continuously, τ = 97.5 hours, adiabatic conditions, P= 1.013 bar.
	B	Store continuously, τ = 25.5 hours, adiabatic conditions, P= 1.013 bar.
	C	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
	C large	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
	D	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
	D large	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
Product/ V-103	A	Store continuously, τ = 26.25 hours, adiabatic conditions, P= 1.013 bar.
	B	Store continuously, τ = 26.25 hours, adiabatic conditions, P= 1.013 bar.
	C	Store continuously, τ = 26.25 hours, adiabatic conditions, P= 1.013 bar.
	C large	Store continuously, τ = 26.25 hours, adiabatic conditions, P= 1.013 bar.
	D	Store continuously, τ = 26.25 hours, adiabatic conditions, P= 1.013 bar.
	D large	Store continuously, τ = 26.25 hours, adiabatic conditions, P= 1.013 bar.
Hydrolysate/ V-105	A	Store continuously, τ = 97.5 hours, at 35 ^{o}C, P=1.013 bar.
	B	Store continuously, τ = 25.5 hours, at 35 ^{o}C, P=1.013 bar.
	C	Store continuously, τ = 25.5 hours, at 35 ^{o}C, P=1.013 bar.
	C large	Store continuously, τ = 25.5 hours, at 35 ^{o}C, P=1.013 bar.
	D	Store continuously, τ = 12.75 hours, at 35 ^{o}C, P=1.013 bar.
	D large	Store continuously, τ = 12.75 hours, at 35 ^{o}C, P=1.013 bar.
Yeast/ V-106	A	Store continuously, τ = 97.5 hours, adiabatic conditions, P=1.013 bar.
	B	Store continuously, τ = 25.5 hours, adiabatic conditions, P= 1.013 bar.
	C	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
	C large	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
	D	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.
	D large	Store continuously, τ = 5.74 hours, adiabatic conditions, P= 1.013 bar.

D Main section

Table C.6: Description of each procedure in the main section of the bioreactor model.

Procedure/ equipment	**Description**
Centrifuge/ DC-102	Centrifuge to remove solids, min d_p=1 micron, density 1030kg/m^3, sedimentation efficiency 30 %.
Fan/ P-6	Pumping air with a pressure increase of 0.02 bar.
Design Spec (conc.)	Control concentration of yeast at 0.332 %. using hydrolysate as the manipulated stream.
CO_2-Scrubber	Adding water such that mass ratio between water. added and CO_2 in the vent gases are 1.3. Component. split remove all CO_2, nitrogen and oxygen.

E Economic parameters

Parameters used to estimate capital investments in SPD:

- Total equipment purchase cost (PC):
  $PC = listedequipmentcost + unlistedequipmentcost$
  $unlistedequipmentpurchasescost 0.00 \times PC$
- Working capital: Estimate to cover expenses for 30 days of labour, raw material, utilities and waste treatment.
- Start-up and validation cost estimate as 5 % DFC.

Parameters used to estimate operating cost in SPD:

- Maintenance included, use equipment specific multipliers.
- Depreciation included, use contribution for each equipment's undepreciated purchase cost.
- Equipment usage or equipment availability
- Laboratory, quality, quality assurance cost: Estimate as 10 % of all labour cost.

D. Image of Continuous Model in SuperPro Designer

In Figure D.1 to Figure D.3 are visual representations of the continuous model of the biorefinary shown.

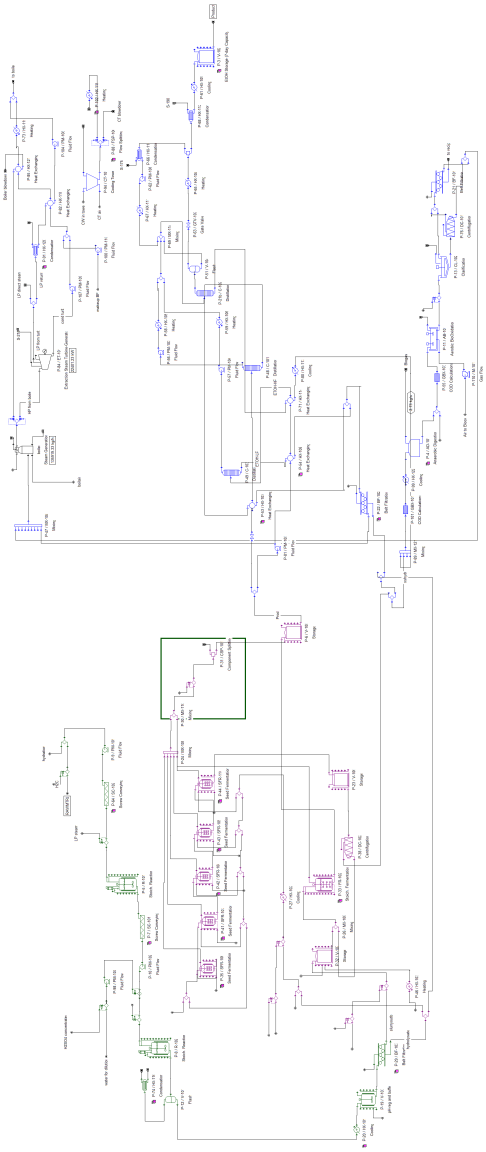

Figure D.1: The continuous SPD model of the biorefinery

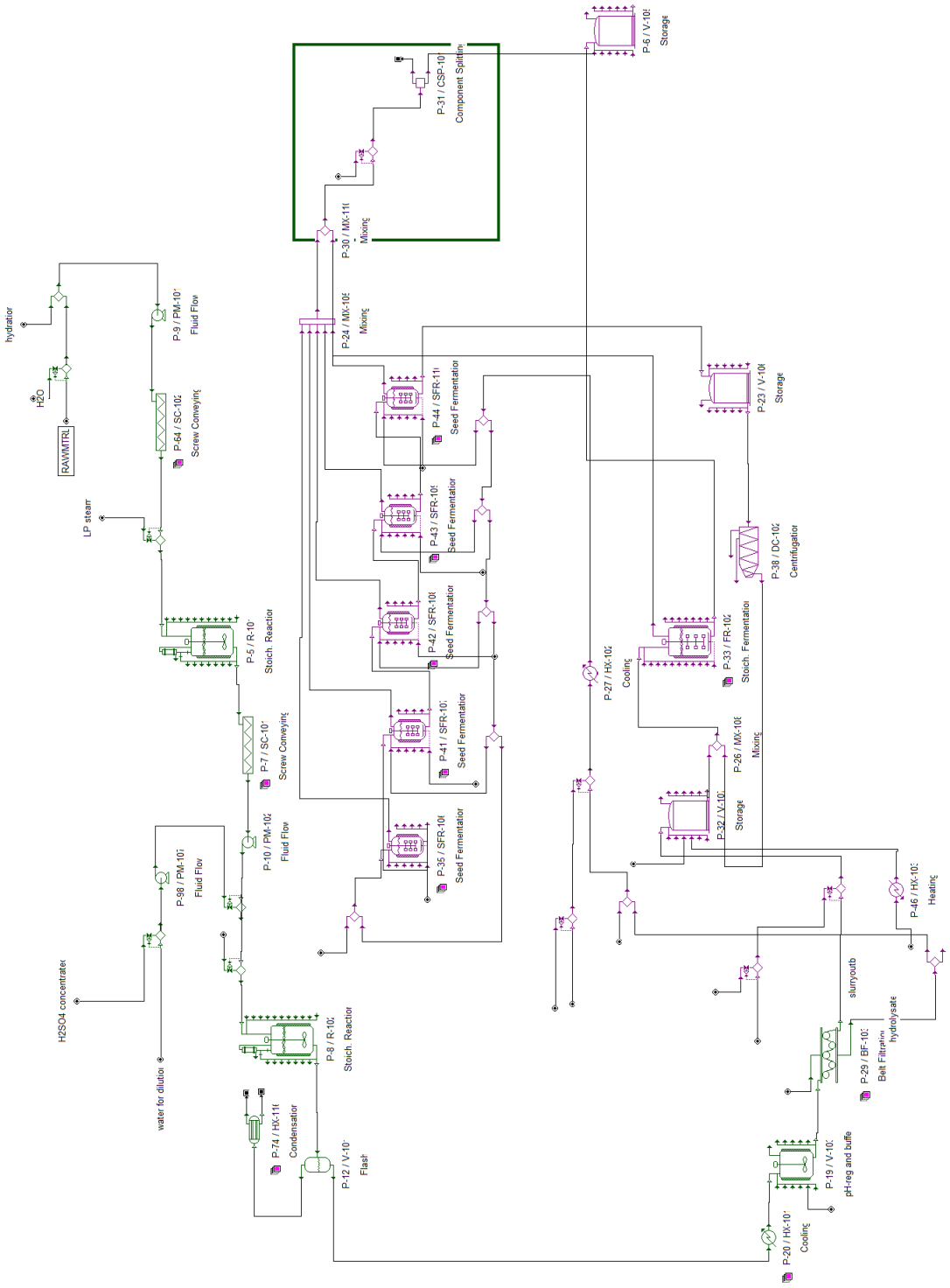

Figure D.2: The continuous SPD model of the pre-treatment and reactor section of the biorefinery

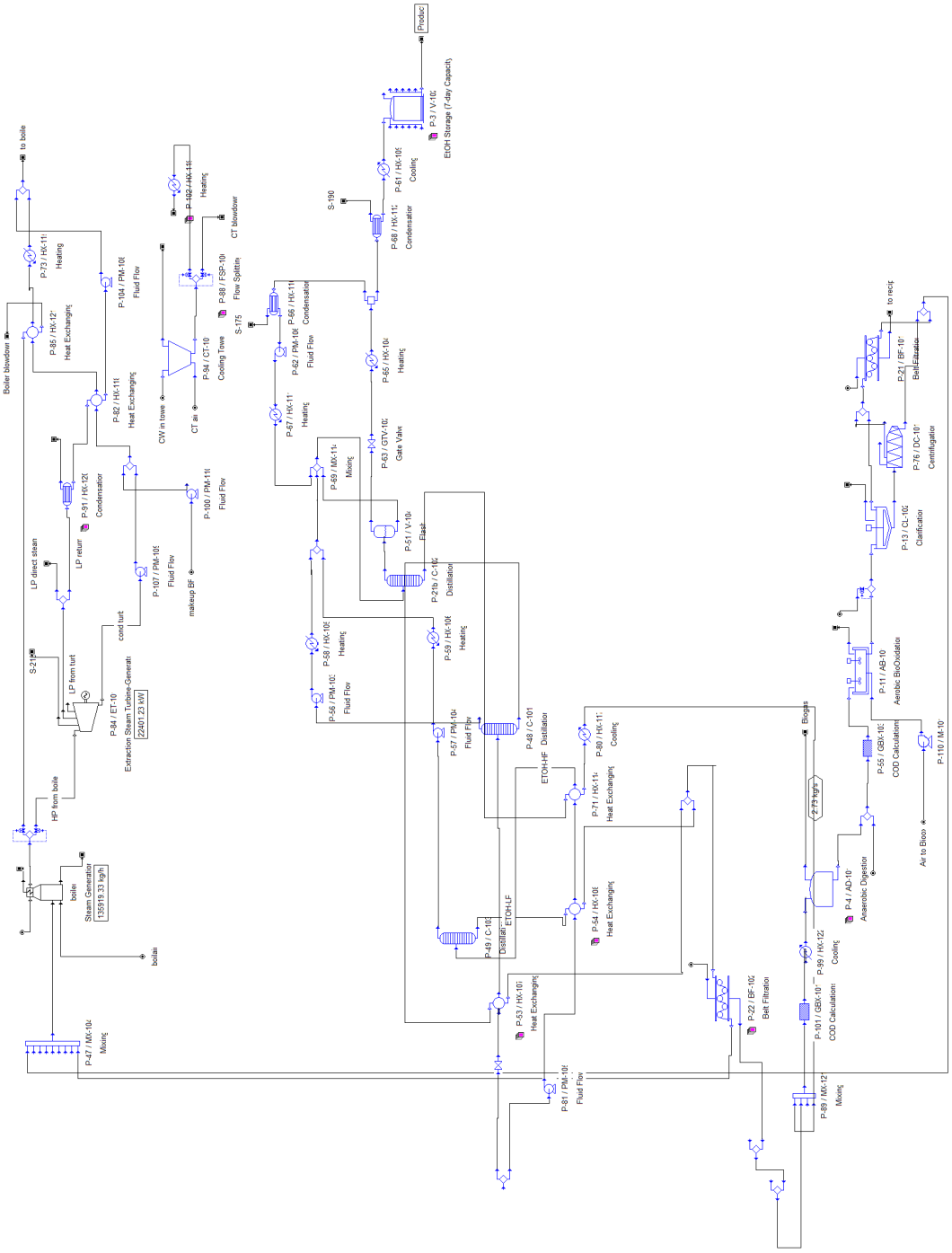

Figure D.3: The continuous SPD model of the downstream section of the biorefinery

E. Variation in Operation Cost

Figure E.1 shows the different parameters that affect the annual operation cost. It contains the load that each of the parameters has on the operation cost for each of the four Case A- Case D for 96 hours SSF procedure time.

Case A, 96 hours

	€/yr	€/batch	€/kg MP	%
Materials	1,629,526	20,627	0.03	15.94
Facility-Dependent	7,127,505	90,222	0.12	69.71
Labor-Dependent	0	0	0.00	0.00
Laboratory / QC / QA	0	0	0.00	0.00
Consumables	0	0	0.00	0.00
Utilities	713,642	9,033	0.01	6.98
Waste Treatment / Disposal	753,374	9,536	0.01	7.37
Transportation	0	0	0.00	0.00
Miscellaneous	0	0	0.00	0.00
Other	0	0	0.00	0.00
Total Annual Operating Cost	10,224,047	129,418	0.17	100.00

Case B, 96 hours

	€/yr	€/batch	€/kg MP	%
Materials	1,725,531	5,676	0.03	21.12
Facility-Dependent	4,747,511	15,617	0.08	58.12
Labor-Dependent	0	0	0.00	0.00
Laboratory / QC / QA	0	0	0.00	0.00
Consumables	0	0	0.00	0.00
Utilities	821,977	2,704	0.01	10.06
Waste Treatment / Disposal	873,547	2,874	0.01	10.69
Transportation	0	0	0.00	0.00
Miscellaneous	0	0	0.00	0.00
Other	0	0	0.00	0.00
Total Annual Operating Cost	8,168,566	26,870	0.13	100.00

Case C, 96 hours

	€/yr	€/batch	€/kg MP	%
Materials	1,700,629	5,594	0.03	21.52
Facility-Dependent	4,200,640	13,818	0.07	53.15
Labor-Dependent	0	0	0.00	0.00
Laboratory / QC / QA	0	0	0.00	0.00
Consumables	0	0	0.00	0.00
Utilities	1,172,602	3,857	0.02	14.84
Waste Treatment / Disposal	829,923	2,730	0.01	10.50
Transportation	0	0	0.00	0.00
Miscellaneous	0	0	0.00	0.00
Other	0	0	0.00	0.00
Total Annual Operating Cost	7,903,794	25,999	0.13	100.00

Case D, 96 hours

	€/yr	€/batch	€/kg MP	%
Materials	1,852,477	3,042	0.03	22.94
Facility-Dependent	4,147,165	6,810	0.07	51.35
Labor-Dependent	0	0	0.00	0.00
Laboratory / QC / QA	0	0	0.00	0.00
Consumables	0	0	0.00	0.00
Utilities	1,244,553	2,044	0.02	15.41
Waste Treatment / Disposal	831,484	1,365	0.01	10.30
Transportation	0	0	0.00	0.00
Miscellaneous	0	0	0.00	0.00
Other	0	0	0.00	0.00
Total Annual Operating Cost	8,075,678	13,261	0.13	100.00

Figure E.1: Operation cost for Case A, Case B, Case C and Case D.

F. Variation in Reaction Time

For Case A, Case B, Case C Case D is the number of equipment required 61, 41, 37 and 37 respectively. These values are independent on if the procedure time in the SSF reactor.

Table F.1 shows the impact that variation in reaction times has on equipment size and number of units per equipment required to process 9.0×10^5 tonnes biomass slurry per year for Case A, Case B, Case C and Case D. In table F.1 is neither fans nor valves and mixers included.

Table F.1: Variation in reaction times impact on equipment size and number of units required per equipment for Case A, Case B, Case C and Case D.

		90 hours	**96 hours**	**100 hours**
Case	Equipment name	$[m^3]/[No.]$	$[m^3]/[No.]$	$[m^3]/[No.]$
A	V-102	1600/ 7	1600/ 7	1700/ 7
	V-103	850/ 6	850/ 6	880/ 6
	V-105	1600/ 2	1600/ 2	1700/2
	V-106	230/ 1	230/ 1	240/ 1
	R-102	1200/ 17	1200/17	1200/17
	SFR-106	0.07/ 7	0.07/ 7	0.07/ 7
	SFR-107	0.7/ 5	0.7/ 5	0.7/5
	SFR-108	6.9/ 5	6.9/ 5	6.9/ 5
	SFR-109	69/ 5	69/ 5	69/ 5
	SFR-110	690/ 5	690/ 5	690/ 5
B	V-102	1500/ 2	1500/ 2	1500/ 2
	V-103	850/ 6	850/ 6	850/ 6
	V-105	860/ 1	860/ 1	860/ 1
	V-106	61/ 1	61/ 1	61/ 1
	R-102	1000/ 20	1000/ 20	1000/ 20
	SFR-106	0.06/ 2	0.06/ 2	0.06/ 2
	SFR-107	0.5/ 2	0.5/ 2	0.5/ 2
	SFR-108	4.3/ 2	4.3/ 2	4.3/ 2
	SFR-109	43/ 2	43/ 2	43/ 2
	SFR-110	430/ 2	430/ 2	430/ 2
C	V-102	670/ 1	670/ 1	670/ 1
	V-103	850/ 6	850/ 6	850/ 6
	V-105	190/ 1	190/ 1	190/ 1
	V-106	14/ 1	14/ 1	14/ 1

Case	**Equipment name**	$[m^3]/[No.]$	$[m^3]/[No.]$	$[m^3]/[No.]$
	R-102	1100/ 17	1100/ 17	1100/ 17
	SFR-106	0.06/ 2	0.06/ 2	0.06/ 2
	SFR-107	0.5/ 2	0.5/ 2	0.5/ 2
	SFR-108	4.3/ 2	4.3/ 2	4.3/ 2
	SFR-109	43/ 2	43/ 2	43/ 2
	SFR-110	430/ 2	430/ 2	430/ 2
D	V-102	670/ 1	670/ 1	670/ 1
	V-103	850/ 6	850/ 6	850/ 6
	V-105	190/ 1	190/ 1	190/ 1
	V-106	14/ 1	14/ 1	14/ 1
	R-102	1100/ 17	1100/ 17	1100/ 17
	SFR-106	0.06/ 2	0.06/ 2	0.06/ 2
	SFR-107	0.5/ 2	0.5/ 2	0.5/ 2
	SFR-108	4.4/ 2	4.4/ 2	4.4/ 2
	SFR-109	43/ 2	43/ 2	43/ 2
	SFR-110	430/ 2	430/ 2	430/ 2

G. Lessons Learned in SPD Programming

There are a lot of things in SuperPro Designer that are prespecified, and some of these prespecified parameters will create unreasonable results. In this appendix the reader is warned about things that need to be taken under consideration to prevent gaining unreasonable answers.

When creating a batch vessel procedure in a reactor and adding a batch stoichiometric fermentation operation the default value for power consumption (for agitation) is set to 3 kW/m^3. This can be compared to the default value of continuous stoichiometric fermentation procedure in a reactor where the value is 0.005 kW/m^3. In large reactors this difference in power consumption will give a significant impact on the power demand. This will in turn have a large impact on the annual utility cost of the process.

In SPD there are a lot of predefined economic parameters which are most suitable for pharmaceutical industry and are likely to give an overestimation of operation and equipment costs. Using these predefined values is not recommended for biofuel processes.

Adding equipment operating in staggered mode in SPD automatically increases the throughput of material in the process. In this project the flow rate of biomass slurry supplied from pre-treatment was set as a fixed value, hence the amount of material in the biomass slurry stream had to be adjusted each time more units operating with staggered start times were added.

Unexpected changes in the flow rate of biomass slurry created a lot of confusion in other situations as well, so my recommendation is to always make sure that the flow rate remains as intended when getting unexplained results.

For some reason when the decanter centrifuge, that was used in the model, was operating in batch mode the flow was only divided into two streams with the same composition. As a result, a lot of the yeast produced was wasted. By changing the operation mode to continuous two streams with different composition were obtained, hence the centrifuge was assumed to be a continuous procedure.

When dividing the model into sections in SPD, it is important to keep in

mind that the default values for capital investment and operating cost will be given to all new sections. These values should therefore be adjusted if these values are not suitable for the section.

SPD offers three models to account for the nature of the reaction, stoichiometry, equilibrium and kinetics. The Stoichiometric model expresses only the time dependence of temperature. In the equilibrium model the extent of the reactions is determined using equilibrium constants and the kinetic model require entering kinetic parameters into a selection of predefined models [12]. Earlier in the project, which this thesis is a part of, a kinetic model for the SSF reactions was constructed. Due to limitations in SPD this kinetic expression cannot be entered directly into the model. As a result of this limitation stoichiometries model was used. The disadvantage is that stoichiometries models may not be advanced enough to capture the behaviour of the reaction, hence not give a reliable estimation of the conversion which makes the model less reliable.

The cost of Biomass slurry and hydrolysate should not be based on the price for different components available in these streams, these streams were there for added as mixtures. This makes it possible for the user to specify the price of these streams.