

# Evaluation of the software SuperPro Designer through simulation of a biohydrogen production process

DIVISION OF BIOTECHNOLOGY | LUND UNIVERSITY  
ERIK BERGMAN | MASTER THESIS 2016



# Contents

<b>I. Introduction</b>	2
A. Background	2
B. Aim	2
<b>II. Modeling a process in SPD</b>	3
A. General workflow	3
B. Fermentation models	3
1. Kinetic growth	3
C. Mode of operation in SPD	4
D. Troubleshooting	4
1. User guides	4
2. Breakpoints	4
3. Unit operation equations	5
<b>III. Case study</b>	5
A. Introduction	5
B. Background	5
1. Microorganism	6
2. Initial pre-treatment	6
3. Initial dark fermentation	6
4. Initial downstream process	6
5. Hypothesized improvements	6
C. Replicating Ljunggren's process	6
1. Pre-treatment	7
2. Fermentation	8
3. Kinetics	8
4. Downstream process	9
5. Cases for cost analysis	9
6. Adjusting for additional costs	10
D. Economic results in SPD	10
1. Capital costs	10
2. Yearly costs	10
E. Feasibility of results	10
<b>IV. Discussion</b>	11
A. Knowledge gained	11
B. Limitations of SPD	11
1. Accessibility	11
2. CSTR models	11
<b>V. Possible improvements for the simulation</b>	12
A. Kinetic models	12
B. Modeling absorption	12
C. General notes	12
1. Recycling	12
2. Financial calculations	12
3. Potential of Dark Fermentation	12
<b>A. Appendix</b>	14

## Acknowledgments

Firstly, I would like to thank my examiner Olle Holst for offering me the opportunity to work on this thesis as well as allowing me to customize my work according to my own preferences.

I would like to thank my supervisor Carl Grey for continuously helping me with the creation of my thesis, for tiny details as well as large-scale decision making.

I would like to thank my good friend Boris Torbica for his good advice in thesis writing. Without your directions, the first few weeks of writing my thesis would have been considerably more difficult.

I would like to thank my father, Olle Bergman, for providing me with invaluable insight into the life of a young scientist. Having heard of the struggles of this life-changing phase beforehand has repeatedly put my mind at ease.

Lastly, I would like to thank my numerous friends and colleagues at the Guild of Chemical Engineering and Biotechnology. The good times I have had in your company have inspired me to keep working towards finishing my degree and I will forever remember my time at The Guild as among the greatest of my life.



## List of abbreviations

- AD - Anaerobic Digestion
- CIP - Cleaning in Place
- CSTR - Continuous Stirred-Tank Reactor
- DF - Dark Fermentation
- DSP - Downstream Process
- $OSM_{crit}$  - Critical Osmolarity
- OSM - Osmolarity
- SPD - SuperPro Designer

# Evaluation of the software SuperPro Designer through simulation of a biohydrogen production process

Erik Bergman<sup>1, a)</sup>

*Division of biotechnology, Department of chemistry*

(Dated: 18 March 2016)

## Abstract

A simulation in bioprocess technology was carried out in order to evaluate the accessibility and adequacy of the simulation software SuperPro Designer<sup>®</sup> used on an academic level. This was done by recreating an existing process and studying the results as well as observing the difficulties and limitations along the way. The study in question was a biohydrogen production plant consisting of three parts. Firstly, pre-treatment was simulated where potato peels were enzymatically treated to form a glucose solution. Secondly, fermentation was simulated where glucose was converted to a hydrogen and carbon dioxide stream as well as by-products in the form of lactic acid and acetic acid. These acids were then used as substrate and fed to an anaerobic digester where a methane and carbon dioxide mixture was formed. Thirdly, an absorption column was simulated for the purpose of separating the carbon dioxide from the hydrogen and methane.

At first, the process based on the simulation made by Ljunggren was thoroughly studied. Secondly, the software was studied in order to gain sufficient knowledge in how to create a similar plant. Thirdly, the simulation was created. Some compromises needed to be made in order to get accurate results such as a simplified kinetic model of the product formation of hydrogen. The pre-treatment did not manage to break even when comparing the cost of raw material to the outlet glucose. Neither did the fermentation part yield a profit, even after tweaking the process by several factors. The absorption column could not be accurately simulated due to limitations in the software. It was concluded that Dark Fermentation is difficult to make profitable at the current state. However, the knowledge gained from conducting the simulations resulted in a beginner's guide in SuperPro Designer<sup>®</sup> being written.

## I Introduction

### A Background

SuperPro Designer<sup>®</sup> (abbr. SPD) is a software piece which specializes in techno-economic calculations in process engineering.<sup>1</sup> The program is capable of setting up a batch process or a continuous process and provides data bases for chemicals, equipment and economical figures. After initializing the software and defining costs and revenues, the program is able to provide the user with cost estimation which takes into account capital costs, operating costs, material costs as well as administrative and auxiliary costs.

The software is currently being used in the Process and Plant Design course as part of the M.Sc. in Engineering in Biotechnology and Master Program in Biotechnology at Lund Faculty of Engineering. However, the software is usually not utilized fully due to several problems:

- An insufficient tutorial of the software.
- Lack of knowledge of how a batch or continuous process affect the results.

- Difficulty recycling streams.
- Difficulty to automatically regulate streams according to other conditions within the simulation.
- Difficulty troubleshooting.

By studying these issues and finding ways of facilitating the learning of the software, SPD could become a valuable tool in teaching process and plant design.

### B Aim

This thesis aims to recreate an existing bioprocess plant simulation created in another software. After completion, the accuracy and plausibility of the results will be studied. The accessibility and adequacy of SPD as an educational tool will be evaluated and methods of easing the learning curve of SPD in the view of a beginner will be suggested.

When choosing a study to replicate, the process needs to:

- Explore the problems previously described in the Background chapter.
- Utilize unit operations well-known in the chemical engineering and biotechnology industry.

---

<sup>a)</sup>Electronic mail: erik.bergman@biotech.lu.se

- Utilize and produce chemicals where the buying and selling prices can be easily obtained.
- Be suited for a master thesis, i.e. not too simple or too advanced.

## II Modeling a process in SPD

### A General workflow

A SuperPro Designer<sup>®</sup> simulation is centered around the flowchart of the process. After picking mode of operation (further described in II C), the user places equipment pieces in the workspace and connects them by using a connection tool, simulating pipelines.

SPD offers a database of chemicals with partially complete sets of physical properties. However, the user must pick those chemicals which are to be used in the process at hand. When doing this, it is advisory to check if the necessary physical parameters are filled in. The buying and selling prices of chemicals are occasionally filled in by default, but in most cases, it has to be done manually by the user.

SPD divides streams into one of three categories: Raw materials, waste and revenue. Raw materials are the inlet streams and need to have their buying prices filled in. Waste streams are outlet streams and need to have their waste disposal costs filled in. Revenue streams are outlet streams and need to have their selling prices filled in.

After initializing all unit procedures, the process starts and SuperPro solves all equations related. If the process has convergence demands, they are solved according to the number of allowable iteration attempts and accuracy, set by the user.

After the process is complete, the user may produce reports of equipment, flows and economics. The outcome of the economic reports are dependent on the capital costs, the operating costs, the buying and selling prices of chemicals as well as auxiliary costs.

In the case of a bottleneck in the process, SPD will automatically add parallel units which are not visible in the flowchart but appear in the equipment and economy reports. This is true for both batch and continuous processes.

These four steps summarize the work flow of SPD:

- Define chemicals and enter the necessary physical properties if they are missing.
- Construct the process.
- Enter the buying and selling prices of streams as well as classifying them as raw material, waste or revenue.
- Generate economic reports.

Out of these four, construction of the process is by far the most time-consuming. By following the built-in guides and by studying the provided example files, however, the user can gain a lot of knowledge in how to create a realistic simulation.

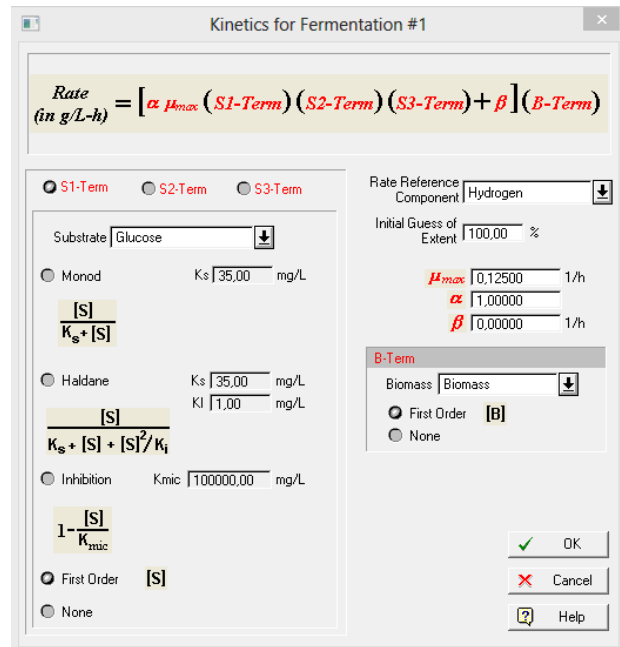


FIG. 1. A screenshot of the kinetic fermentation graphical interface.

### B Fermentation models

When setting up a reactor in SPD, the user first enters the chemical balance of the reaction to take place. This requires the amounts of substance to be equal on the reactant and product sides, and thus, all molar weights need to be defined beforehand. The user then enters the parameters which define nature of the reaction. SPD offers three models for this:

- Stoichiometric. In this mode, the time dependence is only set by temperature.
- Equilibrium. This is a variation of the stoichiometric reaction, but with equilibrium constants determining the extent of the reactions.
- Kinetic. This mode involves entering kinetic parameters into a selection of pre-defined models. A screenshot of the interface for kinetic fermentation is displayed in Figure 1.

The kinetic model is relevant for this experiment in particular.

#### 1. Kinetic growth

When working with SPD, the volumetric productivity  $q_C$  [g/(l\*h)] of component C is:

$$q_C = (\alpha * \mu_{max} * S_1 * S_2 * S_3 + \beta) * X$$

$\mu_{max}$  is the maximal growth of the biomass [h<sup>-1</sup>]. The three factors S are variables representing the possible growth models offered in SPD. If only one model is required, the remaining two S factors may be set to 1. X is the concentration of the biomass [g/l].

$\alpha$  and  $\beta$  are experimentally determined coefficients which are by default set to 1 and 0, respectively. These two constants can be used if the user wishes to express the formation of a product rather than the formation of biomass, according to the Luedeking-Piret model. This model states that  $\alpha$  determines the scale of growth-dependent product formation and  $\beta$  determines the scale of growth-independent product formation.<sup>2</sup>

Depending on the nature of the biomass, the user may combine up to three growth models multiplicatively. The models at disposal are displayed in Figure 1.

## C Mode of operation in SPD

When starting a new project in SPD, the user needs to specify whether the process operates batch-wise or continuously. This is important due to some differences. A batch process:

- Requires scheduling information.
- Requires process holdup time.
- Requires sequences of unit operations for each piece of equipment.
- Allows for graphing of certain parameters such as temperature or concentration over a given time span.

As mentioned above, batch processes use series of unit operations for each piece of equipment. As an example, a batch reactor will need to be heated, then loaded with one or more components, then react, then be emptied, then be cleaned. Operations in SPD are capitalized (PULL IN, HEAT, FILTER etc.). The operations used in this simulation are described in Appendix VII.

By exploring the available options for batch processes, the *Batch Sheet* was discovered. The Batch Sheet of a unit is a large document containing all properties of the unit at every point in time. The user may sort out information in order to customize a spreadsheet containing valuable pieces of information, such as the temperature of a reactor at five minute intervals for five hours. A graph showing a successful batch culture of SPD Dark Fermentation is displayed in Figure 2.

On the other hand, a continuous process:

- Only lets the user specify the steady state conditions
- Can be used to achieve steady state in recycled processes

Recycling in a continuous process is handled by connecting an outlet stream to the inlet of the process and setting a global convergence criterion on a *tear stream*, a phrase denoting the closing point of a loop. In order for converge to be met, two conditions need to be met:

- Components cannot accumulate within the system.

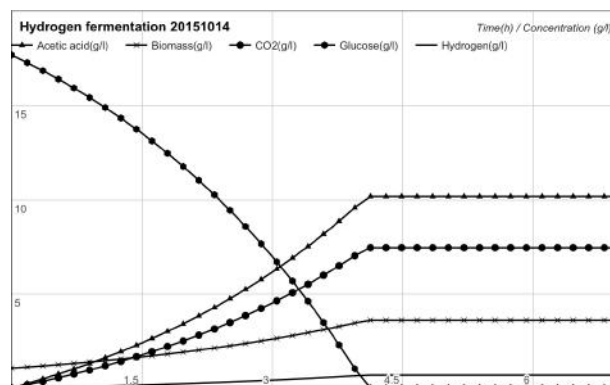


FIG. 2. A graph showing a successful attempt at batch-wise Dark Fermentation in SPD.

- Regulatory systems need to be incorporated which modify stream flows according to other parameters within the system.

If convergence is reached for the loop, the process settles at steady state.

## D Troubleshooting

### 1. User guides

When the user starts the program, the first steps may be unclear. However, the software offers a number of tutorials in the form of increasingly complete example files with a supplementary written guide. Using these tools, the user may learn the appropriate order of actions in order to create a practical simulation.

Apart from this, Intelligen Inc. offers a series of tutorials on Youtube in which a few examples of simulations are created in real-time along with narration. By following these steps, the user may create a starting point from which the process can be refined.

While working with the process, the user may hover the cursor over any part of the interface or the workspace and the help index will appear and offer an explanation. This works for unit operations in the flow chart as well as options and tools in the user interface.

### 2. Breakpoints

If complications or errors show up while working on the process, the user may set breakpoints in certain unit operations. By doing this, the process calculations are paused at that certain breakpoint, allowing the user to review the current condition of the setup, possibly finding the errors. Figure 3 displays the breakpoint interface of a reactor with multiple unit operations.



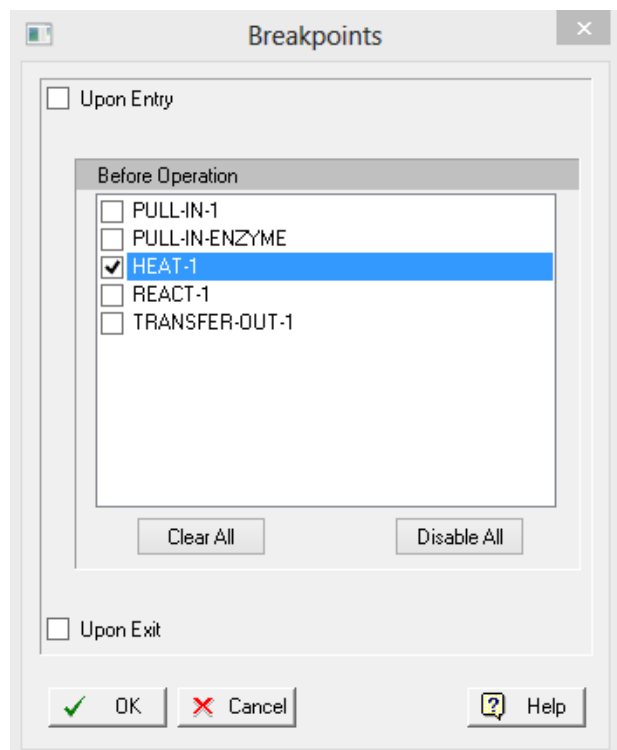


FIG. 3. A screen capture of the breakpoint interface of a reactor. In this case, the process will pause in between pulling in enzyme and heating.

### 3. Unit operation equations

While not entirely apparent, the equations which define the unit operations of SPD are very transparent. By browsing the Help Index and entering the name of a specific unit operation, the user may access its modeling calculations. By studying these models, the user may gain knowledge in which physical and chemical properties that affect the outcome of the unit operation. This is also useful since these models can be applied in external software if SPD is not appropriate. A figure displaying the modeling calculations guide of a kinetic fermentor is displayed in Figure 4.

## III Case study

### A Introduction

One industry which is currently being explored<sup>3</sup> is biological hydrogen production. As demand for alternatives to fossil fuel increases, more focus has recently been put into research regarding hydrogen as a fuel. From an environmental and economical perspective, the production of the gaseous chemical should optimally:

- Leave a small carbon footprint.
- Use renewable raw materials.
- Be economically viable.

$$C_A = \frac{N_A}{V} \quad \text{eq. (A.19)}$$

In the case of no feed stream (fed batch options are not selected) and constant volume:

$$dC_A = r_A dt \quad \text{eq. (A.20)}$$

The reaction rate  $r_A$  of component A is given by:

$$r_A = \sum_{j=1}^q r_{Aj} \quad \text{eq. (A.21)}$$

where  $r_{Aj}$  is the reaction rate of component A due to reaction j and q is the overall number of reactions. The reaction rate for reaction j is given by the following equation:

$$r_{Aj} = \frac{v_{Aj}}{v_{kj}} r_{kj} \quad \text{eq. (A.22)}$$

FIG. 4. A screen capture of the details surrounding the modeling calculations of a kinetic fermentation in SPD.

- Be producible large-scale.

As of today, by far the most common way of producing hydrogen is through the use of steam reforming.<sup>3</sup> This is, however, not a sustainable solution since the technique relies on natural gas. In order to get a zero or almost-zero carbon footprint from the production, biohydrogen is a better alternative. One technique of producing hydrogen through the use of microorganisms is called Dark Fermentation (abbr. DF).

This report aims to disclose the techno-economic details behind a biohydrogen production simulation created as a doctoral dissertation by Mattias Ljunggren in 2011. The work was created in Aspen Plus<sup>®</sup>, but this time, the process will be created in SuperPro Designer<sup>®</sup> instead.

## B Background

The 2011 process by M. Ljunggren aims to study the economic effects of a series of case studies for biological hydrogen production. The maximal volumetric productivity of H<sub>2</sub> was found to be 45.8 mmol/l/h, producing 11.0 kg H<sub>2</sub> per hour with a raw material demand of 13 400 kg/h.

The process consists of three parts:

- A pre-treatment where carbohydrates are treated enzymatically in order to convert polysaccharides to monosaccharides used as substrate.
- An fermentation process where hydrogen is formed in a bioreactor as well as a secondary methane product formed in an anaerobic digester.
- A downstream process where hydrogen and methane are separated from unwanted components.

## 1. Microorganism

The microorganism used for production of hydrogen is *Caldicellulosiruptor saccharolyticus*, an organism which is thermophilic<sup>4</sup> and is a promising strain in the field of biohydrogen since it is believed to achieve close to the theoretical maximum yield in dark fermentation.<sup>4,5</sup>. Despite its good yield, there are some difficulties surrounding the organism. Firstly, there is an abundance of by-products in the form of acetic acid, lactic acid and carbon dioxide. As these components build up osmotic pressure, inhibition of the hydrogen production takes place. Secondly, the bacterium is product inhibited and thus, the hydrogen needs to be sparged or the process must be terminated before inhibition occurs in order to maximize productivity. Thirdly, the strain is thermophilic and heating is needed in order to maintain the optimal operating temperature of 70°C. However, its thermophilic nature may also serve useful since contamination of other species is less likely.

Attempts have been made to genetically modify *C. saccharolyticus*.<sup>6</sup> However, the extremophilic nature of the species has proven to make genetic engineering difficult due to the lack of native plasmids used as vectors.<sup>6</sup>

## 2. Initial pre-treatment

In order for the biomass to grow, it needs a carbon source. Since pure glucose is expensive to obtain, it is preferable to resort to carbohydrates in more complex forms. For the studied process in particular, potato peels were used. These were then treated enzymatically, producing a syrup which was run through a rotary vacuum filter in order to remove impurities. A water stream was used to flush away the filter cake.

The dry weight of potato peels consists of 39% cellulose and 34% starch. For this process, all starch was treated enzymatically while all cellulose was flushed away in the filtration step.

## 3. Initial dark fermentation

After gaining an adequate glucose concentration through the pre-treatment, it was transferred to a bioreactor along with inoculum and other nutrients. The reactor was heated to 70°C and was periodically sparged in order to extract the hydrogen from the reactor.

Along with the gaseous products from the DF step, several organic acids were formed. These should not go to waste and were therefore transferred to another reactor where the acids were degraded to form methane. The methane was then mixed with the H<sub>2</sub>/CO<sub>2</sub> mixture from the DF step.

## 4. Initial downstream process

The downstream unit operations were mutually called gas upgrading. This step was necessary in order to re-

TABLE I. Summary of inlet streams<sup>7</sup>

Stream	Buying price (USD/1000 kg)
Potato peels	3.00
Process water	0.180
Alpha-amylase	6000
Glucos-amylase	6000
Nutrients for H <sub>2</sub> production	9000
Inoculum for H <sub>2</sub> production	0
Inoculum for acetate production	0
Inoculum for CH <sub>4</sub> production	0

move the large amounts of carbon dioxide from the DF and AD steps. Firstly, the process utilized an absorption step where a diethanolamine solution was mixed with the gas stream, absorbing the Carbon Dioxide into the liquid stream. After absorption was complete, the diethanolamine solution was washed in a desorption column to be re-utilized for further absorption. The remaining stream exiting the adsorption column consisted almost exclusively of carbon dioxide.

In Ljunggren's dissertation, the capital cost and operating cost of the downstream process was roughly a third of the total capital cost and operating cost.

## 5. Hypothesized improvements

Looking at the initial process setup, a few improvements could possibly be made in order to increase profitability:

- More efficient utilization of the raw material, also using the cellulose in the potato peels.
- A less costly setup of the pre-treatment, using a single reactor rather than two for multiple enzymatic reactions.
- A more osmotolerant strain used in DF, allowing higher concentration of by-products.
- A strain allowing higher volumetric production of hydrogen.
- More efficient recycling of materials.
- A scale-up of the process.

## C Replicating Ljunggren's process

This process was divided into three separate simulations: Pre-treatment, fermentation and downstream process. Throughout the three divisions, the input streams can be viewed in Table I and the output streams can be viewed in Table II. A graphic of the pre-treatment can be viewed in figure 5. A graphic of the fermentation can be viewed in figure 6.

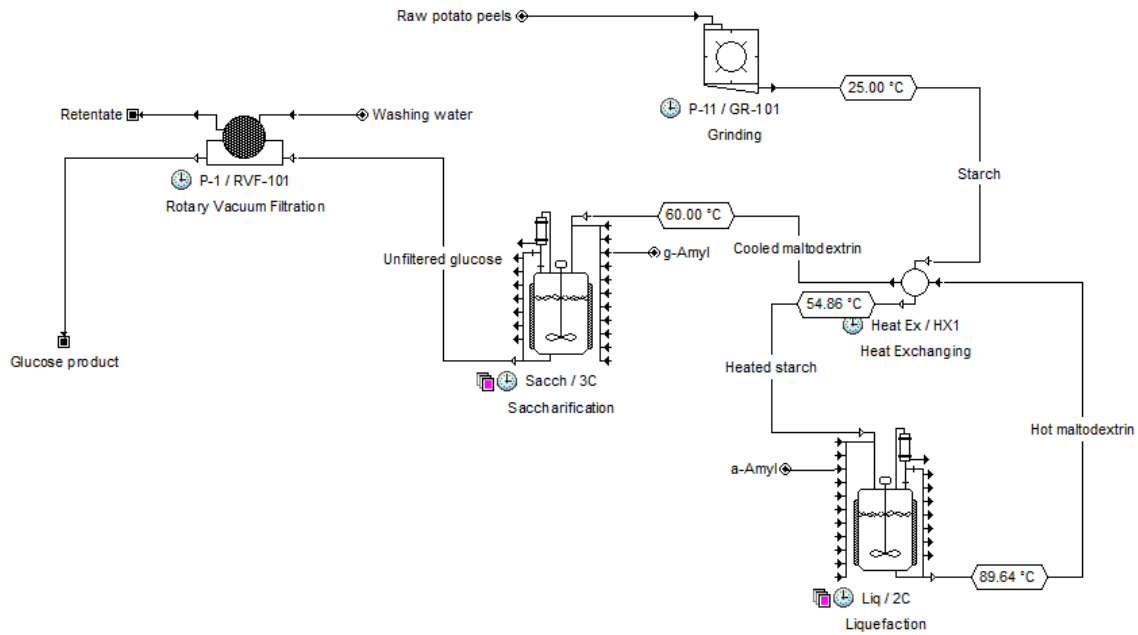


FIG. 5. A flowchart showing the pre-treatment.

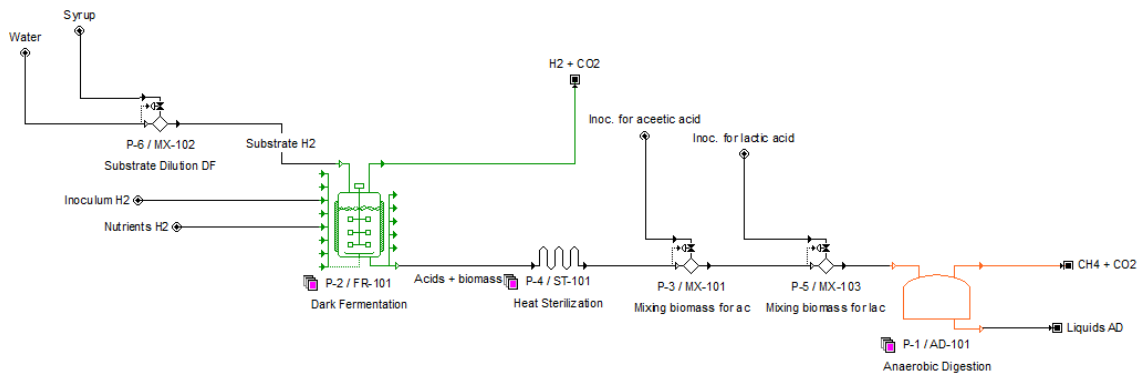


FIG. 6. A flowchart showing the fermentation steps.

TABLE II. Summary of outlet streams<sup>7</sup>

Stream	Selling price (USD/1000 kg)
Hydrogen	41200
Methane	3860
DF liquid	0
Filtration retentate	0

## 1. Pre-treatment

Pre-treatment was set up as a batch process and was divided into the following unit operations:

- Raw material storage.
- Grinding.
- Heat exchange between liquefaction inlet and outlet.
- Liquefaction.
- Saccharification.

- Rotary Vacuum Filtration.

The storage was simulated using an arbitrary storage container in SPD. Its only unit operations were PULL IN, STORE and TRANSFER OUT. For the grinding process, the GRIND operation was used as well as Cleaning in Place (abbr. CIP).

The ground potato peels were then heated in a countercurrent heat exchanger. The HEAT EXCHANGE operation was conditioned to have an outlet cooled stream temperature of 60°C and energy balances were calculated in accordance. Heat exchangers in SPD can easily be customized in order to scale the heat exchanger appropriately. In the case where two streams make contact in order to exchange heat, the scaling calculations can be based on:

- A target temperature difference between the two streams.
- A target temperature for either of the two streams.
- A target temperature *decrease* or *increase* for either of the two streams.



FIG. 7. A screenshot of the user interface of a custom heat exchanger unit in SPD.

A screenshot of the heat exchanger graphical interface can be viewed in Figure 7.

After heat exchange, the first reactor operation took place. Two PULL IN operations were utilized to load the ground peels and the Alpha-amylase<sup>8</sup>, respectively. After loading the reactor, it was heated with steam using HEAT to achieve 90°C.

After the first enzymatic step, another enzymatic process took place in order to further hydrolyze oligosaccharides to pure glucose. This was done using two PULL IN operations: One for the streams having gone through liquefaction, and one gluco-amylase stream conditioned to optimally match the oligosaccharide concentration in the above mentioned material stream. This condition was set by utilizing the settings available in the PULL IN operation. Specifically, the magnitude of the input gluco-amylase stream was automatically scaled in order to reach a certain mass/mass ratio inside the reactor. The reaction took place at 60°C.

After the second enzymatic step, the glucose solution went through a rotary vacuum filter in order to remove impurities. This filter utilized FILTER as well as CIP operations. The FILTER operation of a rotary vacuum filter does not incorporate any of the physical properties of the materials that pass through the unit. Instead, the user must make an assumption of the fractions of materials that pass through the filter. For example, the user may set that 100% of water passes through the filter, but only 1% of biomass does. However, there exist other filter units in SPD which incorporate density, particle size and shape of the entering components.

## 2. Fermentation

In order to let the simulation of fermentation be independent of the results of the pre-treatment, the fermentation was simulated in a separate SPD document. The mode of operation of the following fermentation step was

changed to a Continuous Stirred-Tank Reactor (abbr. CSTR) rather than a batch culture. Unlike the pre-treatment where all unit operations needed to be picked and initialized, this mode allows the user to only adjust the settings of the steady state process. Using a CSTR is also advantageous since continuous growth is more fitting when substrate inhibition is an issue, and the productivity is growth-dependent. It is also preferable to keep the process at a continuously high cell density which is only possible by using a continuous process.

The substrate stream consisted of two separate streams: A process water stream in the scale similar to that of Ljunggren’s work, and a stream of syrup consisting of 82% glucose and 18% water. Repeatedly adjusting these two streams to obtain certain compositions to the reactor inlet proved to be cumbersome. However, a new unit operation was discovered: Feedback regulatory systems. A feedback regulatory system was used in order to achieve the target substrate concentrations where an automatic water stream diluted the syrup accordingly. The substrate then entered the reactor along with streams of inoculum of *C. saccharolyticus* and nutrients (yeast extract).

## 3. Kinetics

The specific growth rate of the DF step in Ljunggren’s work was as follows:

$$\mu = \mu_{max} * \frac{G}{G+K_G} * I_{OSM} * I_{H_2}$$

$$I_{OSM} = 1 - \left(\frac{OSM}{OSM_{crit}}\right)^{n_{OSM}}$$

$$I_{H_2} = 1 - \left(\frac{H_{2aq}}{H_{2aq,crit}}\right)^{n_{H_2}}$$

$\mu$  is the specific growth rate [ $h^{-1}$ ],  $\mu_{max}$  is the maximum growth rate (0.280  $h^{-1}$ ),  $G$  is the substrate concentration [mol/l] and  $K_s$  is the half velocity constant in the Monod expression (0.0480 mmol/l).

$OSM$  is the osmolarity, consisting of acetate, lactate and glucose [mol/l] and  $OSM_{crit}$  is a constant denoting the point where inhibition has reached its critical point and no product is formed anymore (0.28 mol/l at average).  $n_{OSM}$  is an empirically determined constant which affects the sharpness of inhibition as a function of osmolarity.  $I_{H_2}$  and its variables and constants denote the respective properties for dissolved hydrogen, with  $H_{2aq,crit}$  at an average of 2.20 mmol/l.

When dealing with kinetic models for fermentation, SPD offers five models for constructing a function for product formation (see Figure 1). These are Monod, Haldande and critical inhibition kinetics as well as first order and zeroth order formation. These can be combined to detail the function. However, the software does not allow the addition of an exponent in order to specify the velocity of e.g. inhibition.

In Ljunggren’s experiments, these exponents ( $n_{OSM}$  and  $I_{H_2}$ ) were found to be in the range of 3 to 15, depending on glucose concentration and stripping rate. This led to a production rate which would quickly reach zero as  $OSM_{crit}$  was approached. The mode of operation for

the simulation was changed to a CSTR with low glucose concentration and continuous venting of the reactor, and thus the sudden inhibition could be neglected.

The DF reactor was equipped with two outlet ports, one yielding the product and one containing a water solution of cell mass, acetic acid and lactic acid. The liquid stream was sterilized at 140°C and was then mixed with two inoculum streams. The inocula were assumed to carry the kinetic properties of *Clostridium formicoaceticum* and *Methanosarcina mazei* consuming lactic acid and acetic acid, respectively.<sup>9,10</sup> The stream entered an anaerobic digestion unit sized 8800 m<sup>3</sup>. The following reaction summarizes the formation of hydrogen and methane:<sup>10,11</sup>:



In this case, Monod kinetics could easily be applied for the second reaction, using parameters from earlier studies.<sup>9</sup>

#### 4. Downstream process

The downstream process was separated into another simulation. The gas inlet of an absorption column was fed with a stream consisting of a molar ratio of 2:1 of hydrogen and carbon dioxide, respectively. This was the case for the stream leading out of the DF in the previous process division. The liquid inlet of the column was fed with a diethanolamine solution. Thermodynamic properties of the two inlet streams were added. However, the software did not allow reactions to take place within the column and thus, the process was unable to converge since diffusion was the sole driving force for removing carbon dioxide. A graph of the attempted absorption can be viewed in figure 8.

Attempts were made to use a continuous reactor as a placeholder for an absorption column. This was done by using two inlet streams of diethanolamine solution and CO<sub>2</sub>/H<sub>2</sub> mixture. However, cost estimations could not be made accurately when simulating incorrect equipment.

Attempts were made to use an adsorption column rather than an absorption column. However, this unit operation required information regarding the packing of the column. Since the absorption does not employ packing beds, this compromise could not be used to accurately describe the process.

After browsing through all potential replacements for the absorption column, it was concluded that none were adequate for the process. For this reason, economic evaluation of the downstream process was disregarded and an alternative solution is described in chapter III C 6.

#### 5. Cases for cost analysis

Four studies were made in order to get a figure of the capital and operating cost of the fermentation:

1. A case where no streams were recirculated. This case was the most similar to Ljunggren's study.

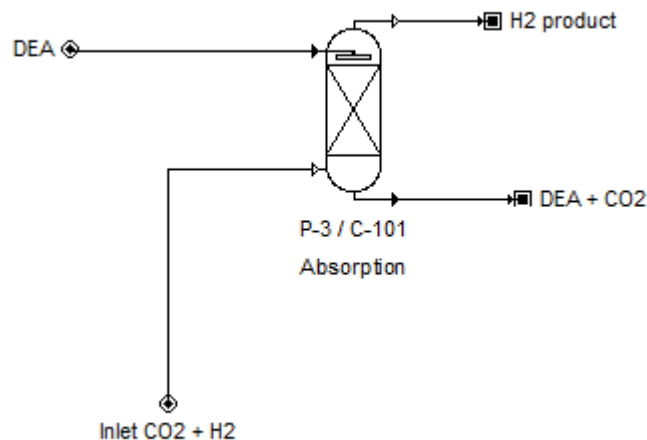


FIG. 8. A graph of the attempted absorption simulation.

2. A case where water and nutrients were recirculated.
3. A case where water and nutrients were recirculated, and the substrate concentration was increased by a factor of 6. This was done with a maintained dilution rate in the fermentor.
4. A case where the above conditions were met, as well as setting a condition where the syrup feed and equipment were scaled up to achieve 1000 kg of hydrogen product per hour.

For cost analysis of the case where water and nutrients were recycled, the raw material cost of those components were set to zero. The case where the glucose concentration was increased assumed that no substrate inhibition took place, which is often the case for a CSTR. In the case where the process was scaled up, the Process Throughput window was used to set a target throughput of 1000 kg of hydrogen per hour, where the syrup-water regulatory system was automatically adjusted to provide the DF unit with required amount of glucose. The scale-up was calculated by entering the *Process Throughput* settings which can be viewed in Figure 9.

After each case study, an Economic Evaluation was generated using the built-in function in SPD. Relevant data was compiled and entered into a spreadsheet.

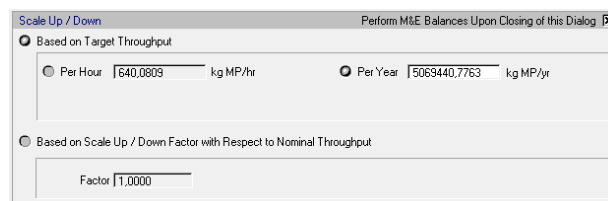


FIG. 9. A screen capture of the scale-up settings. "MP" denotes "Main Product".

TABLE III. Summary of operating costs for pre-treatment

	Cost (k\$/year)	%
Raw materials	343.7	0.7400
Facility	24 180	51.75
Salaries	18 080	38.69
Misc.	4 125	8.830
<b>Total</b>	<b>46 730</b>	<b>100</b>

## 6. Adjusting for additional costs

The only product exiting the pre-treatment was a concentrated glucose syrup stream. The selling price of syrup is 0.45 USD/kg in accordance to the market standard.<sup>12</sup> An economic analysis revealed that the glucose syrup could potentially be sold for 45 700 000 USD per year while the total operating cost of the pre-treatment is 46 730 000 USD per year. The operating costs can be viewed in Table III. After concluding that the operating cost of the pre-treatment would exceed buying raw syrup for the fermentation, it was decided that the pre-treatment should be discarded for the techno-economic evaluation.

It should be noted that after a conclusion was made, it was discovered that the high salary costs of the pre-treatment was a result of slow pumping into the enzymatic reactors. The longer process time resulted in more working hours, affecting the labor dependent cost. After this was adjusted, the salary cost was significantly decreased. However, these results were still insufficient in making the pre-treatment profitable.

A continuous absorption tower was set up in SPD in order to replicate that of Ljunggren’s work. However, the application lacked the ability to simulate chemical reactions within the tower and failed to create a cost estimation. The absorption is vital in order to achieve adequate product concentration in the outlet streams from DF and AD. In order to address this, an adjusted operating cost was introduced. Using data from the original study, it was assumed that absorption accounted for a 50% increase in operation cost not related to purchase of substrate or nutrients.

## D Economic results in SPD

After carrying out simulation of Ljunggren’s work in SPD, the following figures were obtained. For full figures, see Appendix C.

### 1. Capital costs

A summary of the capital costs needed for the DF and AD steps are displayed in Table IV. The only considerable differences in capital costs were observed in cases 1-3 compared to case 4.

For cases 1-3, the throughput was within the capacities of all three unit operations, and thus, only one of each unit was needed. For case 4, however, several units

TABLE IV. Summary of capital costs

	Case 1-3 (k\$)	Case 4 (k\$)
DF total cost	1 889	13 374
AD total cost	5 340	70 750
Sterilizer total cost	698	5 610
Unlisted equipment cost	1 982	22 430
<b>Total</b>	<b>9 090</b>	<b>112 200</b>

TABLE V. Summary of unit count

	Case 1-3	Case 4
DF unit count	1	3
AD unit count	1	10
Sterilizer unit count	1	6

needed to be used parallel. A summary of the number of units used can be viewed in Table V.

### 2. Yearly costs

An overview of the yearly costs and incomes are displayed in Table VI. All case studies were found to be an economic loss. The table also displays the loss in relation to the mass of purchased substrate.

## E Feasibility of results

The study was divided into three parts: pre-treatment, fermentation and absorption. The pre-treatment produced results indicating that the entire setup was an economic loss. Specifically, the selling price of the glucose in the product stream did not exceed the buying price of potato peels and enzymes needed. There are several possible reasons for this. Firstly, only half of the carbohydrates in the raw material were treated enzymatically since all cellulose exited the process as waste. Secondly, the equipment used for degradation of carbohydrate were highly expensive and multiple reactors needed to work parallel.

The DF step produced a hydrogen stream with a  $H_2/CO_2$  quotient which is usual for *C. saccharolyticus*. However, the product flow was comparatively low in relation to the amount of substrate and water needed. In a set of case studies, assumptions were made in which the process was made more economically viable, such as a speculative assumption where the hydrogen productivity of *C. saccharolyticus* was increased manifold. Despite these changes, the process was unable to break even. This is in accordance to recent studies showing that speculative Dark Fermentation plants have difficulty yielding an economic profit.<sup>13,14</sup>

The downstream process did not yield reliable results since the absorption was meant to be reaction based, but SPD only allowed for diffusion based absorption. In order to address this, the operational cost of the fermentation was modified to account for the cost of absorption.

TABLE VI. The distribution of annual costs for different case studies.

Case	Adj. operating cost (k\$/year) <sup>a</sup>	Revenues (k\$/year)	Results (k\$/year)	Results/Mass of syrup (\$/kg)
Case 1	42280	6548	-35730	-5.145
Case 2	31720	6548	-25170	-3.624
Case 3	76200	43070	-33130	-0.7079
Case 4	720600	601600	-119000	-0.1836

<sup>a</sup> For details on the adjusted operating cost, see III C 6

## IV Discussion

### A Knowledge gained

SuperPro Designer<sup>®</sup> has proved to be a useful tool used for economic analysis of large-scale processes. The author of this thesis has acquired knowledge in the following fields:

- Effectively utilizing the user interface.
- Utilizing methods for regulating streams according to local and/or global constraints.
- Distinguishing an array of similar unit operations from one another and using the appropriate pieces where suited.
- Recycling of streams in a continuous process.
- Troubleshooting using simulation breakpoints and user guides.
- Extracting data from unit operations into external formats such as spreadsheets.

When working with SPD, mastering these skills will greatly streamline and improve the quality of the simulation. If given an adequate introduction to the software, the intuitive graphic interface of SPD can serve as a great tool for teaching plant design from a techno-economic perspective.

Utilizing the knowledge gained while writing this master thesis, another document has been created, titled "Simulation of fermentation using SuperPro Designer". This guide has been provided to students in the Process and Plant Design course mentioned in the background and aims to ease the first steps in creating a simulation. See Appendix B.

### B Limitations of SPD

#### 1. Accessibility

As a beginner attempting to use SPD for the first time, the amount of options at the user's disposal may be overwhelming. As seen in Figure 10, many of these options are displayed in the form of abstract icons where the user may disregard a majority and still be able to create an adequate process. However, the built-in user guide offers a brief description of all these options.

SPD creates backup files in the same folder as the main file every 15 minutes. However, only two of these files can be stored at the same time and the user will need to manually save the file in order to keep older copies of a project.

When working with the flow chart, some features are missing that could significantly improve the user experience. SPD offers no Undo command which means that changes are permanent unless a backup file is saved.

When initializing the process, all parameters are entered through text boxes in pre-designated locations inside various dialogues. When doing repetitive work, this task may become cumbersome. By implementing a system where all design parameters are stored in a spreadsheet or a database, the user could easily export data to be easily implemented in another part of the process or another process altogether.

If the process isn't correctly initialized or if convergence demands are not met, the process terminates and displays an error message. In many cases, these error messages fail to convey the message of what changes must be done in order to get a working simulation.

#### 2. CSTR models

Continuous reactors in SPD do not allow for the usage of the PULL IN operation described in Appendix A. This means that all available streams entering the reactor must be known beforehand, and thus, given biomass concentration and flow must be specified. In reality, inoculum in a CSTR is only needed at start-up and not after the reactor has reached steady state. In order to avoid an error message in SPD, a continuous stream of biomass needs to enter the reactor which is not representative of the reality.

When working with CSTR, the substrate concentration is usually set to a level where substrate inhibition has an insignificant impact on the productivity. The dilution rate  $D$  [ $\text{h}^{-1}$ ] of the reactor is set to match the maximal growth of the biomass, avoiding wash-out. SPD does not warn the user if wash-out occurs, which may result in large amounts of substrate in the outlet liquid stream.

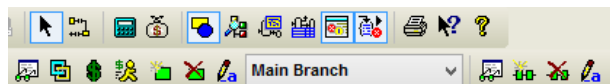


FIG. 10. A screen capture of the user interface of the flow chart.

## V Possible improvements for the simulation

### A Kinetic models

When the DF step was set up, one bold assumption was made: First order kinetics. This would suggest that neither the products nor by-products affect the productivity of hydrogen. At first, the base case assumed to have realistic properties and cases 3 and 4 (see III C 5) would increase the substrate level to beyond saturation. However, the volumetric productivity resulting from case 1 turned out to exceed the maximum ever recorded experimentally as of 2014<sup>6</sup>.

For the DF step, the hydrogen productivity was assumed to be first-order, and no regard was made towards the inhibition of by-products or hydrogen. However, calculations revealed that for case 1 and 2, the critical H<sub>2</sub> concentration was exceeded by a factor of 9. For case 3 and 4, the critical osmotic pressure was exceeded by a factor of 6. In order to get an accurate figure, the reaction could be simulated using another software piece such as Aspen Plus® or MATLAB® where the full kinetic model is incorporated.

Contact was made with a representative from Intelligen Inc. regarding the issue of limited reaction models. The representative revealed that the developers are currently working on a new version of the program which allows for custom reaction kinetics. When this feature is released, it may be possible to create a more realistic model of the DF.

### B Modeling absorption

A lot of work needs to be done in order to get an accurate model of the absorption step to work in SPD since the absorption column unit available in the software does not support the use of reactions taking place inside the tower. The absorption of CO<sub>2</sub> using diethanolamine is a complex one, depending on several substeps and varying pressure and temperature conditions.<sup>15</sup> For this reason, a batch reactor could be a more accurate type of vessel where a series of unit operations can simulate the sequence of events that would take place inside an absorber. With the possibility of the introduction of user-made reaction coefficients in a future version of SPD, it may be possible to create an adequate absorption simulation in the future.

### C General notes

#### 1. Recycling

While working on this project, recycling of materials has simply been handled by setting the cost of the selected materials to zero. However, SPD is able to handle recycling<sup>16</sup> by connecting a stream to a preceding unit

operation and adding a condition of the mass fraction or flow that should be recycled. For this to work, two conditions need to be met: No mass is allowed to accumulate within the process, and regulatory systems need to be used in order to auto-adjust streams. With knowledge in recycling, a future process may be created where a more accurate model is created.

#### 2. Financial calculations

The financial calculations inside SPD take into account costs beyond direct costs related to production. These costs include administrative costs, insurance, taxes and contractor fees. These figures are all based on construction of a plant in the U.S. under the condition that a loan is required for the start up. In reality, the plant may be localized in another location under different circumstances. In a future study, these supplementary costs could be more carefully entered.

Components exiting the process which cannot be sold are treated as waste. In reality, there is an additional cost of handling these waste streams which has not been accounted for in this simulation.

The purchase costs of equipment in SPD are pre-defined depending in built-in models. These models could be further studied in order to get more accurate capital cost figures.

#### 3. Potential of Dark Fermentation

As of today, hydrogen production using *C. saccharolyticus* faces the following issues:

- Substrate inhibition. Though this has been disregarded in the SPD simulation, substrate is in reality inhibitory to the H<sub>2</sub> productivity.
- Product inhibition. Dissolved hydrogen as well as by-products such as acetate will need to be exited quickly enough for the chemicals not to impede productivity considerably.
- Wash-out. A potential productivity increase through adjusting the flow through the reactor is limited by the maximal growth of the organism (appr. 0.3 h<sup>-1</sup>). This was not an issue in this simulation since the reaction followed first-order kinetics.

*C. saccharolyticus* is among the best possible strains for biohydrogen production<sup>5,17-19</sup> and rather than exploring different species, attempts should be made to improve the potency of *C. saccharolyticus*. While the yield of hydrogen per glucose is most likely optimized<sup>4,5</sup>, the productivity could potentially be improved if more inhibition tolerant strains were to be developed.

<sup>1</sup>IntelligenInc, "Superpro overview," (2010).

<sup>2</sup>S. O. Enfors and L. Hggstrm, *Bioprocess technology fundamentals and applications* (The Royal Institute of Technology, Stockholm, 2000).

- <sup>3</sup>J. M. Ogden, Annual Review of Energy and the Environment **24** (1999).
- <sup>4</sup>H. J. G. van de Werken, M. R. A. Verhaart, A. L. VanFossen, K. Willquist, D. L. Lewis, J. D. Nichols, H. P. Goorissen, E. F. Mongodin, K. E. Nelson, E. W. J. van Niel, A. J. M. Stams, D. E. Ward, W. M. de Vos, J. van der Oost, R. M. Kelly, and S. W. M. Kengen, Applied and Environmental Microbiology **74**, 6720 (2008).
- <sup>5</sup>K. Willquist, A. A. Zeidan, and E. W. van Niel, Microbial Cell Factories **9**, 9.
- <sup>6</sup>S. S. Pawar, *Caldocellulosiruptor saccharolyticus: an ideal hydrogen producer?*, Ph.D. thesis, Lund University, Faculty of Engineering (2014).
- <sup>7</sup>M. Ljunggren and G. Zacchi, *Techno-economic analysis of a two-step biological process producing hydrogen and methane*, Ph.D. thesis, Lund University, Faculty of Engineering (2010).
- <sup>8</sup>S. J. SWANSON, A. EMERY, and H. C. LIM, Biotechnology and Bioengineering **19**, 1715 (1977).
- <sup>9</sup>Shang-Tianyang, I.-C. Tang, and M. R. Okos<sup>2</sup>, Applied and Environmental Microbiology **53**, 823 (1986).
- <sup>10</sup>J. Silverstein, "Anaerobic digestion processes," (2010).
- <sup>11</sup>S.-T. Yang and I.-C. Tang, Applied Microbiology and Biotechnology **35**, 119 (1991).
- <sup>12</sup>H. Focus, "Glucose syrup,".
- <sup>13</sup>P. Sathyaprakasan and G. Kannan, International Journal of Environmental Science and Development **6**, 352 (2015).
- <sup>14</sup>J. X. W. Hay, T. Y. Wu, and J. C. Juan, Biofuels, Bioprod. Bioref. **7**, 334 (2013).
- <sup>15</sup>M. Haji-Sulaiman, M. K. Aroua, and A. Benamor, CHEMICAL ENGINEERING RESEARCH AND DESIGN **76**, 961 (1998).
- <sup>16</sup>IntelligenInc, "Superpro designer - algal oil production," (2015).
- <sup>17</sup>A. A. M. Bielen, M. R. A. Verhaart, J. van der Oost, and S. W. M. Kengen, Life **3**, 52.
- <sup>18</sup>E. van Niel, M. Buddeb, G. de Haasb, F. van der Walb, P. Claassenb, and A. Stamsa, International Journal of Hydrogen Energy **27**, 1391 (2002).
- <sup>19</sup>J. V. Zurawski, S. E. Blumer-Schuetten, J. M. Conway, and R. M. Kelly, Microbial BioEnergy **38**, 177 (2014).
- <sup>20</sup>S. Mohan, G. Mohanakrishna, S. Raghavulu, and P. Sarma, International Journal of Hydrogen Energy **32** (2007).
- <sup>21</sup>T. de Vrije, A. E. Mars, M. A. W. Budde, M. H. Lai, C. Dijkema, P. de Waard, and P. A. M. Claassen, Applied Microbiology and Biotechnology **74**, 13581367 (2007).
- <sup>22</sup>I. Inc., "Superpro designer user guide," (2015).



## A Appendix

TABLE VII. Descriptions of unit operations in a batch process

<b>Unit operation</b>	<b>Description</b>
PULL IN	The unit pulls in a certain amount of material from a certain stream. The specified amount can be dependent on a certain criterion such as reaching a set concentration or volume level. When creating a raw material stream, the flow of the stream does not need to be specified and can rather be set using the PULL IN operation of the first unit of the process.
PULL OUT	Depending on the next step in the process, a certain amount of material exits the unit. Using PULL IN in combination with PULL OUT is a good routine.
TRANSFER IN	This operation is similar to PULL IN. However, the amount pulled in is per default all available mass in the inlet stream. This operation is preferable when used in between units, as the user cannot know for sure the amount that exits the previous step.
TRANSFER OUT	This operation is similar to PULL IN. However, it requires information regarding the mass or percentage of total mass that should exit the unit. Using TRANSFER IN in combination with TRANSFER OUT is a good routine.
STORE	The material is assumed to stay in the unit for a set period of time.
GRIND	The material in the unit is ground, requiring labor and energy as well as affecting scheduling.
HEAT EXCHANGE	The temperatures of two streams entering the unit are partially or completely equalized, depending on the entered heat transfer coefficient. The user may specify if either of the two outlet streams should reach a target temperature.
HEAT	The temperature of the unit is increased, affecting the material inside. The user may specify which energy source to use, such as electricity or steam.
FILTER	The stream entering the unit is filtered depending on separation coefficients entered in the specifications of the unit. Since particle size is
CIP	The unit is cleaned, requiring labor and energy as well as affecting scheduling.

# Simulation of fermentation using SuperPro Designer

for KBT042

## Introduction

SuperPro Designer is a software tool used to simulate industrial scale processes in chemical engineering. This guide aims to teach users the basic concepts in creating and running a biotech simulation and briefly mentions the necessary steps needed to do so. It is important that you recognise two terms that will be used frequently throughout this guide:

**Unit** – A piece of equipment in SuperPro Designer. A reactor, an extractor or a heater are a few examples.

**Unit operation** – An action carried out by a unit. Filtering, storing or fermenting are a few examples.

## 1. Choosing mode of operation

When the program starts, you will be asked to choose your mode of operation, i.e. a batch process or a continuous process. It is important that you have made sure which one is relevant for your process, since scheduling and, as a result, the operating costs will be highly affected. These are some examples of differences between the two modes:

### Batch process

- Requires scheduling information.
- Requires sequences of unit operations for each piece of equipment.
- Allows for graphing of certain parameters such as temperature or concentration over a given time span using the *Profiles* tab of a unit operation.


### Continuous process

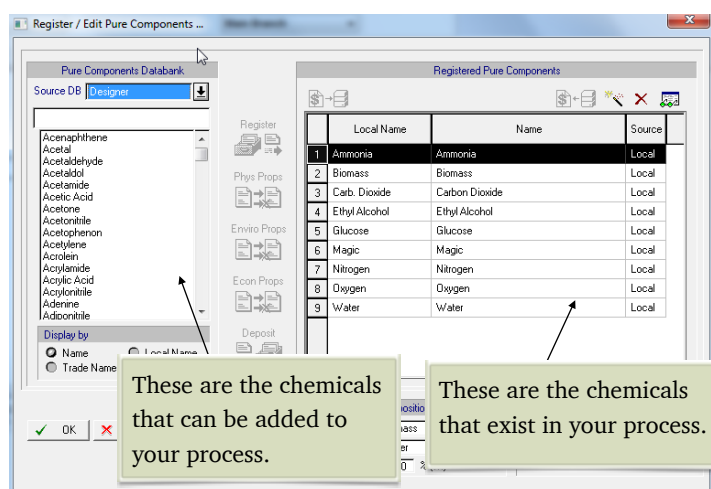
- Only lets the user specify the steady state conditions.
- Can be used to achieve steady state in recycled processes.

## 2. Defining chemicals

### Components

First off, know that SuperPro does not compute chemical reactions for you – all reactants, products and by-products must be known beforehand. Every single component taking place in your process is **entered into the component register**, which can be found in *Tasks* → *Pure Components* → *Register, Edit/View Properties*.

On the left side of the window, you will see the default database of chemicals present in SuperPro. Search for a chemical and double-click it to add it to the right column, which contains the components that will be present in your process. Once the chemical has appeared in the right column, double-click it again to view its properties. You can also create a new compound by pressing the wand  symbol.



### Mixtures

As well as compounds, there is also a register of mixtures. This may be relevant if you're dealing with rough components such as plant materials or foods. For example, you could define a cereal as a mixture containing 15% water, 60% carbohydrates and 25% protein. Mixtures are registered under *Tasks* → *Stock Mixtures* → *Register, Edit/View Properties*.


## 3. The flowchart

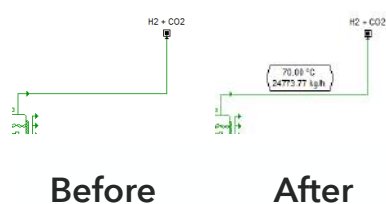
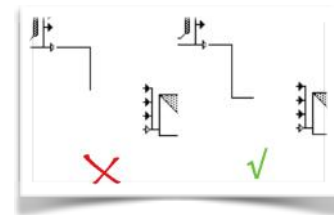
### Units

When you have picked your mode of operation and entered all chemicals, you can start constructing your process. Go to *Unit Procedures* in the menu bar and start browsing through the units at your disposal. Note that this menu contains both continuous and batch reactors no matter what mode of operation you have chosen. It is possible to mix modes of operation within one document but I advise you to stick to one or the other. That is, if you are running a batch process, do not use any continuous reactors and vice versa.

The proceeding workflow using units is described in chapters **4a** and **4b**, depending on your mode of operation.

### Dealing with streams

Streams are added with the connection  tool. Use the escape key to unselect the connection tool. The units that you are using have inlet and outlet ports marked by arrows – this is where you can add a connection. Note that streams can only be connected when they are aligned horizontally, and they can only be connected in in the direction of the flow and not backwards.



It is advised that you name all your streams by right-clicking and choosing *Edit tag name*. You can also display a summary of the properties of the stream by right-clicking and going to *Style* → *Edit Style* → *Highlight Info Tag* → *Info Tag*. In this window, you can enter what properties should be displayed. If you need to delete a

stream but want to preserve its contents, or if you want to duplicate a stream, you can right-click the stream and click *Copy Contents*. The composition of that stream can then be copied to another stream by right-clicking and clicking *Paste Contents*.

### Raw material streams

Streams at the beginning of the process are called raw material streams and can contain any number of chemicals or mixtures. Double-click the raw material stream in order to edit its contents in the same fashion as the Pure Components register. The composition and flows of a raw material stream can be defined by two methods:

1. Enter the mass composition of each component and then enter the total flowrate.
2. Only enter the mass composition of each component. Inlet streams can be connected to a unit operation which will automatically adjust the total flowrate according to a certain condition. For example, you can utilise the PULL IN operation of a reactor and specify that the inlet stream should contain the exact amount that will result in a reactor temperature of 37°C. This concept will be discussed further in the next chapter.

## 4a. Batch processes

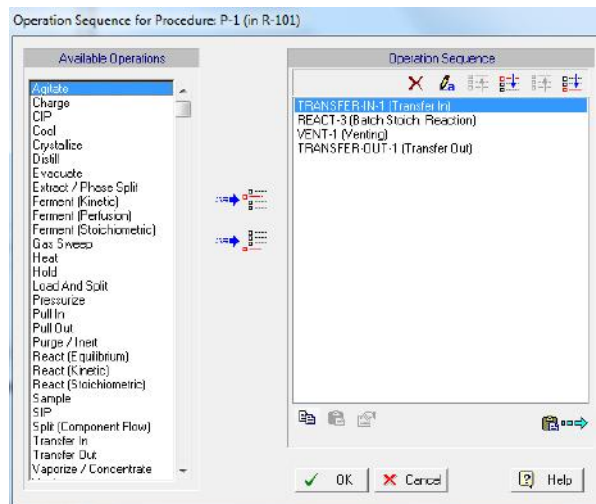
### Choosing your unit operations

SuperPro features a large array of reactors, downstream processing equipment and other accessories. However, the user will need to specify how each and every unit is operated.

## Appendix B

This is done by right-clicking the unit and choosing *Add/remove operations*, or simply double-clicking the unit.

Double-click the units that you want to move to the operation sequence. This may be harder than expected, since multiple of the operations at your disposal seem to serve the same purpose.



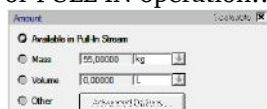
### TRANSFER IN vs CHARGE vs PULL IN

While all these operations involve material entering the unit, there are some subtle differences.

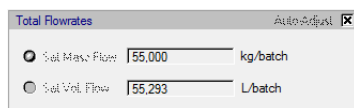
- TRANSFER IN is used for transferring material from one unit to another. The operation will simply transfer all available material that exits the previous unit.
- CHARGE is used for raw material streams (streams entering the process). You can set the operation to either charge everything from the inlet stream (makes the stream editable) or charge a definite amount (makes the stream un-editable).
- PULL IN is a more complex variant of CHARGE, also containing the *Advanced options* window. This window can be very useful if you want a certain component to reach a certain concentration, or if you want the reactor to reach a certain temperature.



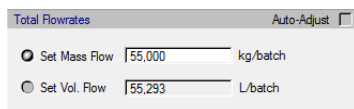
If a specific mass flow is picked within the CHARGE or PULL IN operation...



If it is not...



... then the stream flow cannot be edited.



... then the stream flow can be edited.

### TRANSFER OUT vs PULL OUT

The difference between these two operations is very subtle. TRANSFER OUT will simply take all available material and then transfer it to the next stream. PULL OUT, however, is more complex. It “listens” to the unit that comes after and makes sure that its criterions are met. For example, if a PULL OUT is followed by a PULL IN, then that PULL OUT operation will only transfer the amount requested by the PULL IN operation.

## 4b. Continuous processes

Unlike a batch process, a continuous process doesn't need series of operations that take place one after another. This means that the only options available for units are its steady state conditions. In a continuous process, you can access unit operations simply by double-clicking the unit in question.

### Recycling

SuperPro Designer allows for recycling of materials. However, this may not be without difficulty. In order to get a working recycling loop to work, these conditions need to be met:

1. No material may accumulate inside the loop.
2. The loop needs some sort of regulatory system.

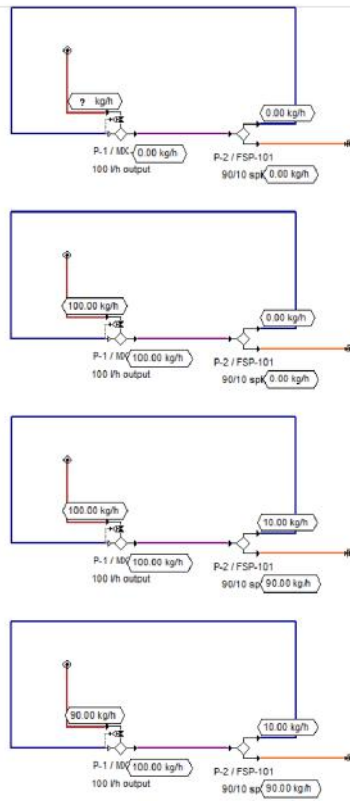
To give you a very basic example, here is a steady state loop which recycles water.

1. An **unknown stream** and an **empty main stream** enter a custom mixer. The custom mixer is set to always pump **out** 100 kg/h.

2. The mixer senses that the **main stream** is zero, and adjusts **the unknown stream** to 100 kg/h so that **the output** is 100 kg/h.

3. The 90/10 splitter is set to divide the **incoming stream** so that 10% goes **up** and 90% goes **down**.

4. This time, the **main stream** is 10 kg/h, and the custom mixer adjusts the **unknown stream** to 90 kg/h so that they add up to 100 kg/h once again.



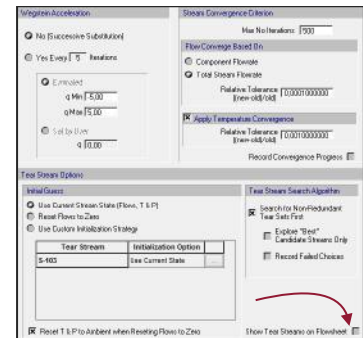
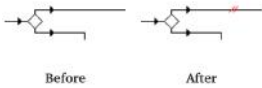
As you can see, we have met both criteria for a working recycle loop: The custom mixer made sure to adjust the flow entering the next unit using an unknown inlet stream. The



## Appendix B

splitter also made sure that part of the flow exited the loop, avoiding accumulation of material.

So what happens after step 4? If you right-click anywhere on the workspace and select *Recycle Loop & Tear Stream Options*, you will find a check box at the bottom right of the window saying “Show Tear Stream on Flowsheet”. After doing this, two red lines will appear on one of your streams. This is the so called **tear stream**. The tear stream fills two purposes:



1. To be the starting point of calculations inside a loop. In the previous example, the blue stream was the tear stream which is why the mixer was the first unit to be calculated. If the purple stream had been the tear stream, the process would have started before the splitter instead.
2. To check if steady state has been achieved. By default, SuperPro calculates the flow rate of the tear stream over and over and assumes that steady state is reached when two successive laps have a difference of less than 0.001%. If 500 laps are made without reaching this quotient, you will get an error message. These two numbers can be modified inside the loop options.

## 5. Fermentation

### The FERMENT operation

Perhaps the most complex part of your process is the product formation which takes place inside a batch or continuous reactor. It is important that you define the **time dependence** of your fermentation, which can be done in a number of ways. The ones discussed in this guide are **stoichiometric** and **kinetic** fermentation. Note that your fermentation likely needs **aeration** and **vent** streams, assigned to the top right and bottom left ports of the fermentor, respectively.

Firstly, let's have a look at the Operator's

These options let you specify whether or not power should be used to achieve a certain temperature before fermentation starts.

This is where you fill in the preparation time of the reaction and, more importantly, the duration of the reaction. Keep an eye out on this setting!

Thermal Mode

- Set Final Temp. 37.00 °C
- Adiabatic
- Set Duty
  - Heating 0.00 kcal/h
  - Cooling 57939.56 kcal/h

Heat Transfer

Agent: Chilled Water

Inlet Temp. 5.00 °C

Outlet Temp. 10.00 °C

Rate 11536.66 kg/h

Power Consumption (for Agitation, etc.)

Power Type: Std Power

- Set Specific Power 3.0000 kW/m<sup>3</sup>
- Set Total Power 24.7607 kW
- Set Power per Unit 24.7607 kW

Power Dissipation to Heat 100.00 %

Gas/Liquid Composites Available To Flood

Assume No Phase Change(s) in Reactor

Duration

Setup Time 0.00 min

Reaction Time

- Set by User 24.00 h
- Set by Master-Slave Relationship

Match the duration of this operation to the duration of another operation or string of operations.

Broth Aeration

Air Supply Stream: In #9: Air In

Aeration Rate

- Calculated to Achieve 0.500 VVM (STD)
- Use Available on Air Supply Stream

Secondary Air Supply Stream: Use Secondary Aeration

In #8: (none)

Secondary Aeration Rate

- Calculated to Achieve 0.000 VVM (STD)
- Use Available on Secondary Air Supply Stream

In this field, you may fill in the total power consumption not related to heating or cooling. I advise you to trust the default settings!

These are the options for air supply of the fermentation. If your process is anaerobic, turn this off!

## Appendix B


conditions of the fermentor unit. Note that if you are using a continuous reactor, some of these options will be missing since a continuous process is a simpler approach. At the top of the window, you will find a series of tabs (*Oper Cond's*, *Volumes*, *Fed Batch* etc.). A quick guide to the Operation Conditions is displayed in the above graph. If you are running a continuous process, the Duration setting is missing. However, it is important that you instead define the residence time which can be done under "Volumes". The number of tools at your hand may feel overwhelming at first, but we'll go through all tabs one by one and quickly explain whether they are important or not.

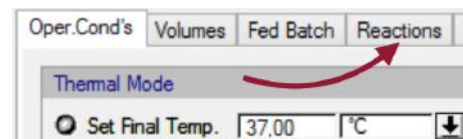
### Settings inside the FERMENT unit operation

Setting	Description	Relevance for this course
Oper.Cond's	As mentioned in the guide above, this is where the general conditions for the operation are set.	High
Volumes	This is where you enter the maximum and minimum working volume of the reactor. If the reactor reaches values above or below these values, you will get an error message. For a continuous process, this is also where you enter the holdup time.	Mid (High for a continuous process)
Fed batch	This is where you can specify if your reactor should be of semi-continuous nature. If you want to add substrate at a controlled rate, this tab may be relevant.	Mid
Reactions	This is where you define the reactions that take place inside your reactor. This will be discussed soon.	High
Vent/Emissions	This is where you define how venting is handled in your reactor. Gaseous by-products are very common, and you should make sure that they don't result in unwanted pressure increases.	High
Profiles	If you want a diagram of what goes on inside your batch reactor, this is where you enter what parameters you want to plot. After you have done this, you may right-click the reactor (or any other unit where Profiles is present) and choose <i>Dynamic Data Records</i> .	Mid
Labor, etc.	This tab lets the user define the number of people working on the unit operation as well as auxiliary costs. I advise you to trust the default settings.	Low
Description	This tab contains for setting for the way the unit operation is described if a Batch Sheet (see below) is created.	Low
Batch Sheet	A batch sheet is a report where the entire process is described in the form of a checklist.	Low
Scheduling	SuperPro Designer will try to optimize the way a batch process is scheduled. However, if you want to customize the scheduling, you can do it in this tab.	Mid


### Stoichiometric reaction

A stoichiometric reaction is independent of kinetic parameters which define the rate of product formation. This means that the chemical reaction takes place linearly over the course of the holdup time which is a rather poor approximation. If you choose to use this method, know that the only number determining the duration of the reaction is the Reaction time, which can be found under *Oper.Cond's* in a batch fermentor or under *Volumes* in a continuous fermentor.


When setting up your chemical balance, go to the *Reactions* tab and click the Stoichiometry  button.



In this window, you may balance your equation according to molar or mass coefficients. Note that **biomass needs to be incorporated** into your balance since it is forming inside your reactor. Since biomass isn't one single compound (although SuperPro inaccurately treats it as a molecule with molar weight 24.63 g/mol), it is advised to balance the reaction according to mass.

If multiple reactions take place inside the reactor, you may add more using the Insert or Add  buttons. Know that all reactions in a fermentor take place parallel, meaning at the same time.

### Kinetic reaction

A kinetic fermentation is dependent on kinetic constants which need to be known beforehand. Before editing the kinetics, the reaction formula needs to be entered. Firstly, go through the steps mentioned in **Stoichiometric reaction**. Next, go to the Kinetics window marked by the R  symbol. The kinetic equation that you will be working with reads as follows:

$$\text{Rate (in g/L-h)} = \left[ \alpha \mu_{\max} (S1\text{-Term}) (S2\text{-Term}) (S3\text{-Term}) + \beta \right] (B\text{-Term})$$

*Rate* denotes the volumetric productivity (measured in mass).

$\alpha$  is a constant denoting growth-dependent product formation.

$\beta$  is a constant denoting growth-independent product formation.

$\mu_{\max}$  is the maximum growth rate of the microorganism.

*B-term* is the concentration of biomass in the reactor.

## Appendix B

$S_1$ ,  $S_2$  and  $S_3$  are terms used to implement inhibition mechanics in the productivity.

As an example, if the standard Monod expression were used to define growth in SuperPro Designer, values would be entered as follows:

$$\mu = \mu_{\max} \frac{S}{K_s + S}$$

1. If the substrate used goes by the name Media, “Media” is entered as the substrate.
2. The *Rate* term in this case is the growth of biomass,  $\mu$ , and therefore “Biomass” is entered as Rate Reference Component.
3. The biomass which produces additional biomass is of course the same component, and for this reason, the B-term is entered as “Biomass” as well.
4.  $\mu_{\max}$  for the organism is 0.20 h<sup>-1</sup> for this substrate in particular.
5.  $\alpha$  and  $\beta$  are not present in the expression and are left at 1 and 0, respectively. This is usually the case if the Rate Reference Component is biomass.
6. The  $S_1$  term is assigned to follow Monod Kinetics while  $S_2$  and  $S_3$  are left at None, meaning that they have the value 1. The  $K_s$  constant in the Monod expression is 35 mg/L for this organism and this substrate in particular.

These three buttons let you define each and every one of the S terms.  $S_2$  and  $S_3$  are by default set to 1 (None).

This field represents the substrate which is consumed by the biomass, for example Glucose.

These 5 alternatives are the possible models that can be assigned to the S term currently chosen. As you can see in this example, the  $S_1$  term follows Monod kinetics.

This field represents the product which is formed. It is advised to fill in Biomass in this field.

Guess used for solving internal differential equations.

$\mu_{\max}$  is the maximum growth rate of the biomass. If you choose not to fill in Biomass as the Rate reference component (see the above box),  $\alpha$  and  $\beta$  need to be specified for the preferred component.

This field represents the biomass component which defines the productivity. First order or zeroth order production can also be chosen.

These two options are only present in a batch process. They can be used to specify scheduling of the fermentation, such as reaching a certain biomass concentration.

## 6. Finishing up your process

### Completing chemical properties

When viewing the list of chemical properties in *Pure components* (see chapter 2), you will find that they are sometimes not complete – for example, the melting point or vapour pressure of a chemical may be missing. However, these properties will not necessarily have an effect on the process. How do we know if this information is relevant or not?

1. In your flowchart, click a unit and press F1. This will open the user guide for that unit in particular.
2. Under “Operations”, search for the unit operation that you want to study, for example REACT or FILTER.
3. Look for the *Modeling calculations* of the unit operation. This section will tell you about all physical and chemical properties that define the outcome of the unit operation.
4. If a variable is present in the Modeling Calculations but not in the properties of your chemical, you are advised to fill it in.

Also check the economics tab for your raw materials and products. **Purchasing and selling prices are rarely filled in beforehand** – it is vital that you enter this! You can usually find prices in online chemical traders such as [www.alibaba.com](http://www.alibaba.com).

### Defining costs and revenues

When you have finished your process, SuperPro can help you create quite detailed reports on its profitability. However, you will need to define what components you are actually selling. To do this, go to *Tasks* → *Stream Classification*. In the Classification column, **mark your product stream as "Revenue"**. In this table, you can also set the selling or buying price of a certain stream by checking *Is Cost/Price Set By User* and then filling in a figure on the column to the right. Doing this will override any prices entered into the chemical database. In the bottom right corner, you may also define which is your main product, which will show up in your economic reports.

**Classification of Output Streams**

Stream Name	Classification	Is Cost/Price Set By User	Disposal Cost or Selling Price	Units	Cost/Price Ref. Amount	Mark as Hazardous
1 Vent	Emission	<input type="checkbox"/>	0,000000	\$/kg	(Total Stream)	<input type="checkbox"/>
2 Distillate	Revenue	<input type="checkbox"/>	2,000000	\$/kg	(Total Stream)	<input type="checkbox"/>
3 Condensate	Aqueous Waste	<input type="checkbox"/>	0,000000	\$/kg	(Total Stream)	<input type="checkbox"/>
4 Biomass waste	Solid Waste	<input type="checkbox"/>	0,000000	\$/kg	(Total Stream)	<input type="checkbox"/>

**Classification of Input Streams**

Stream Name	Classification	Purchase Price	Units
1 Inoculum	Raw Material	0,300000	\$/kg
2 Substrate	Raw Material	0,464000	\$/kg

**Main Product/Revenue**

Stream: Distillate

Flow Basis:

Total Stream Flow

Single Component in Stream

Ethyl Alcohol



Flow Ref. Units: /kg

Quick Ref. Symbol: MP

OK Cancel Help



### Results

Once your process is set up, you may let SuperPro have a go at simulating it. You do this by pressing Solve Balances.  Check if your outlet streams are desirable. If not, tweak your process until you get the compositions you want and then also solve the economic simulation.  Now you can browse through the various reports under the *Reports* menu to find economic evaluations, energy expenditure and more. A Gantt chart for a batch process can be found under *Charts*.

## Extras

### Improving your process

After completing your process and studying the results, you may get figures that seem unrealistic. There are a few ways of improving the process:

- **Check if your process operates under reasonable conditions.** For example, SuperPro will gladly calculate a distillation which reaches nearly azeotropic conditions without warning you that you will need a fortune in energy to do so.
- **Double check the buying and selling prices.** As mentioned before, some of these figures are missing by default and will need to be added. When researching prices, keep in mind that price ranges for a single chemical may be vast. For example, there is a considerable price difference between ethanol with the purity of 90% and 99%, respectively.
- **Don't be scared to discard parts of your process.** If parts of your process do nothing but increase the operating costs, then you might have to rethink if they are actually necessary. Is it worth the expense of the equipment needed to increase the purity of your product from 95% to 98%? If the pre-treatment of your raw material is unnecessarily expensive, why not skip it altogether and just buy raw substrate?
- **Scale it up!** If you have defined your main product in the *Stream Classification* window, you may go to *Tasks* → *Adjust Process Throughput* and set a target for each batch or hour. By increasing this figure, the process in its entirety will scale up which may increase profitability.

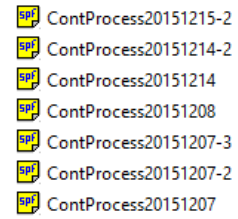
### Software precautions

As with any other software, SuperPro Designer has its drawbacks and limitations. These are some points to consider:



## Appendix B

- SuperPro is **not** familiar with the “undo” command. If you should make an error and want to revert it, you can look for a file in the same directory as your SuperPro document, but with the file extension “.sp~” or “.s~~”. These are backups which are created every 15 minutes and can be opened through SuperPro but cannot be edited and will need to be saved as new files. The backups are also auto-deleted after 15 minutes of using SuperPro. It is advised that you often use *Save As* and include the date of your current revision while working on your project.
- When editing data inside pop up windows, note that pressing the “x” mark will revert all changes. You will specifically have to press the “OK” button for any action to take place.
- Throughout the program, there are **a lot** of options at your disposal. However, keep in mind that many of these will have a negligible effect on your simulation, and are meant to be used when simulating larger, more complex processes.



### Final notes

Use SuperPro Designer as a tool to simplify your calculations in process design, but make sure to first and foremost **trust your own instincts as an experienced engineering student**. And more importantly, **experiment!** I learned to use this application simply by exploring the hundreds of options and tools available. Chances are you may discover a new useful tool that I haven't even heard of yet.

**Good luck!**

# Economic Evaluation Report for ContProcess20151217

december 17, 2015

## 1. EXECUTIVE SUMMARY (2015 prices)

Total Capital Investment	59,886,000 \$
Capital Investment Charged to This Project	59,886,000 \$
Operating Cost	22,351,000 \$/yr
Main Revenue	3,486,000 \$/yr
Other Revenues	3,062,681 \$/yr
Total Revenues	6,548,000 \$/yr
Cost Basis Annual Rate	84,605 kg MP/yr
Unit Production Cost	264.18 \$/kg MP
Net Unit Production Cost	264.18 \$/kg MP
Unit Production Revenue	77.40 \$/kg MP
Gross Margin	- 241.32 %
Return On Investment	- 17.50 %
Payback Time	N/A
IRR (After Taxes)	N/A
NPV (at 7.0% Interest)	- 131,069,000 \$

MP = Flow of Component 'Hydrogen' in Stream 'H2 + CO2'

## Economic Evaluation Report for ContProcess20151217

december 17, 2015

### 1. EXECUTIVE SUMMARY (2015 prices)

Total Capital Investment	59,441,000 \$
Capital Investment Charged to This Project	59,441,000 \$
Operating Cost	17,454,000 \$/yr
Main Revenue	3,486,000 \$/yr
Other Revenues	3,062,681 \$/yr
Total Revenues	6,548,000 \$/yr
Cost Basis Annual Rate	84,605 kg MP/yr
Unit Production Cost	206.30 \$/kg MP
Net Unit Production Cost	206.30 \$/kg MP
Unit Production Revenue	77.40 \$/kg MP
Gross Margin	- 166.54 %
Return On Investment	- 9.39 %
Payback Time	N/A
IRR (After Taxes)	N/A
NPV (at 7.0% Interest)	- 96,169,000 \$

MP = Flow of Component 'Hydrogen' in Stream 'H2 + CO2'

## Economic Evaluation Report for ContProcess20151217

december 17, 2015

### 1. EXECUTIVE SUMMARY (2015 prices)

Total Capital Investment	65,795,000 \$
Capital Investment Charged to This Project	65,795,000 \$
Operating Cost	42,235,000 \$/yr
Main Revenue	23,576,000 \$/yr
Other Revenues	19,499,304 \$/yr
Total Revenues	43,076,000 \$/yr
Cost Basis Annual Rate	572,241 kg MP/yr
Unit Production Cost	73.81 \$/kg MP
Net Unit Production Cost	73.81 \$/kg MP
Unit Production Revenue	75.28 \$/kg MP
Gross Margin	1.95 %
Return On Investment	9.43 %
Payback Time	10.61 years
IRR (After Taxes)	1.17 %
NPV (at 7.0% Interest)	- 20,171,000 \$

MP = Flow of Component 'Hydrogen' in Stream 'H2 + CO2'

## 1. EXECUTIVE SUMMARY (2015 prices)

Total Capital Investment	695,570,000 \$
Capital Investment Charged to This Project	695,570,000 \$
Operating Cost	521,514,000 \$/yr
Main Revenue	326,386,000 \$/yr
Other Revenues	275,233,152 \$/yr
Total Revenues	601,620,000 \$/yr
Cost Basis Annual Rate	7,922,001 kg MP/yr
Unit Production Cost	65.83 \$/kg MP
Net Unit Production Cost	65.83 \$/kg MP
Unit Production Revenue	75.94 \$/kg MP
Gross Margin	13.31 %
Return On Investment	15.48 %
Payback Time	6.46 years
IRR (After Taxes)	9.45 %
NPV (at 7.0% Interest)	100,505,000 \$

MP = Flow of Component 'Hydrogen' in Stream 'H2 + CO2'