TECHNISCHE HOCHSCHULE NÜRNBERG
GEORG SIMON OHM

Fakultät Angewandte Chemie

Process Design: Adipic Acid from Glucose via Rennovia Process

Master thesis

Author:

Olaya Aranguren

Bachelor in Chemical Engineering

University of Zaragoza, Spain

Tutor:

Prof. Dr. Brüggemann

Technishe Hochschule Nürnberg Georg Simon Ohm

Nürnberg 30.05.2018

Prüfungsrechtliche Erklärung

Ich versichere, dass wir die Arbeit selbständig verfasst, nicht anderweitig für Prüfungszwecke vorgelegt, alle benutzten Quellen und Hilfsmittel angegeben sowie wörtliche und sinngemäße Zitate als solche gekennzeichnet habe.

Plagiarism Declaration in Accordance with Examination Rules

I herewith declare that I have worked on this thesis independently. Furthermore, it was not submitted to any other examining committee. All sources and aids used in this thesis, including literal and analogous citations, have been identified.

Nürnberg, 30.05.2018

Unterschrift / Signature

Keywords

Adipic acid

Aspen Plus® simulation

Azeotropic distillation

Bio-based

Biorenewable

Carbon

Chemical

Crystallization

Distillation

DTmin

HINT software

Hydrodeoxygenation

Oxidation

Pinch method

Pinch point

Process

Renewable resource/feedstock

Glucaric acid

Glucose

Sustainability

Rennovia Inc.

Abstract

Among recently proposed production routes for mass chemicals from renewable resources the preparation of oxidized C6 chemicals, such as adipic acid, from glucose seems particularly attractive: On the one hand the natural C6 chain including functionality is preserved. On the other hand, linear C6 chemicals that are currently produced from mineral oil, require high efforts and inefficiencies if produced from alternative resources, such as natural gas.

From patent literature it can be concluded that Rennovia Inc. owns a leading technology for manufacturing adipic acid from glucose. In a previous project a Aspen Plus® Simulation for the two-step synthesis of adipic acid was built upon the Rennovia patent. The aim of this project is to complement the previous one, particularly regarding separation and purification of adipic acid (Chapter 3.3.1), recovery of acetic acid (Chapter 3.3.2), and an overall optimization of heat integration (Chapter 3.3.3).

Separation of adipic acid seems feasible by crystallization, conserving a high process yield of 98.1 % respect the previous one (99.4 %). Moreover, a conceptual process design of adipic acid separation including solvent (acetic acid) recovery is presented. However, high capital cost must be invested for the construction of the new sections of the process plant.

Used symbols and abbreviations

Chapter 4.1:

$Y_{k,i}$	-	Yield of substance i from substance k
$\dot{n}_{i,t}$	kmol/s	Molar flow of substance i at the time t
v_i	-	Stoichiometric coefficient of substance i

Chapter 4.2 and Appendix:

A	m^2	Area
π	-	Pi number
r	m	Radio
P	atm	Pressure
v	L	Volume
f-Factor	$kg^{0.5}m^{1.5}s^{-1}$	f-Factor
u	ms^{-1}	Gas velocity

Table of contents

1 Introduction and motivation

Nowadays, there is an important focus on replacing today's fossil-based economy with a more sustainable, biomass-based economy. In order to achieve this environmentally friendly goal, the target will be the development of new bio-refinery systems. These systems should process bio-based raw materials with high efficiency and cost-effectiveness to a wide variety of biofuel-based products and should allow successful integration into existing infrastructure in order to reduce costs.

Bio-based chemicals and polymers have recently gained strength due to the rise in oil prices and consumer demand. Renewable resources are becoming more important in the industry, including bio-based chemicals and polymers area. For that reason, it is becoming an attractive area for investment [1].

It is certain that humankind’s activities are the responsible for exhaustion of planet resources and pollution; nevertheless, chemical industry contributes to the mentioned problems as well as to the way of solving them.

This focus on achieving a biomass-based economy has emerged from different reasons. For example, the following topics and developments have gained especially in significance [2]:

- The pressure on companies to reduce pollution or create environmentally friendly processes has increased due to this new emphasis on environmental issues.
- Globalization has changed: now solid polymers rather than petrochemical feedstocks are exported from Middle East.
- There has been discovered wide reserves of shale gas in the United States and other countries that have changed the prediction of exhaustion.
- Important problems as climate change and sustainability have become a driving force for the investigation of new processes that come from renewable resources or produce less or no carbon dioxide.

In the first place, most of the problems have arisen from building of excess capacity (which has led to strong competition) and low prices. Another important reason is that nowadays lot of new countries have joined the industry world, which means that bigger amount of sources is needed. In addition, there has been much stricter government legislation whose purpose is to care for the environment and not to deplete the raw materials.

Some restructuring of the manufacturing of chemicals are carried out worldwide, mainly in areas such as United States, Western Europe and Japan. However, Middle East and Southeast Asia are starting acting the same way.

In the meantime, some things have not changed. The organic chemicals industry is still based on seven basic raw materials all deriving from petroleum and natural gas: olefins-ethylene (propylene and the C_4 olefins; which are butadiene, isobutene, 1- and 2-butenes), aromatics-benzene (toluene and the xylenes; which are *orto*, *meta* and *para*) and one alkane (methane) [2].

In petrochemical manufacturing industry, the most common feedstocks are naphtha and light gas oil. Both of them are produced from oil refining processes and individual gases such as ethane, propane and butane, which come from natural gas liquids. Natural gas liquids are composed by a complex mixture of hydrocarbons and exist under the ground in a liquid state along with methane. This mixture of natural gas liquids and methane is labelled as natural gas [3].

Pushed by environmental issues, there has been a huge improvement in bio-based production routes from renewable raw materials to commercial goods in the last years. Specifically, organic acids production has improved and has become a competitive field, due to their multiple uses, such as commodity chemicals or polymer building blocks.

Organic acids are part of biotechnological goods. First time that acetic and citric acids were produced was in 1823 and 1913 respectively [4]. Since that moment the amount of production has increased continuously owing to bigger demand, and more applications have been discovered which leads to different types of organic acids of biosynthetic origin. In addition to food and feed uses, organic acids are produced as bi-functional monomers. For example, di-carboxylic acids are used for the production of polyamides with advanced material properties, while acids with additional keto- or hydroxyl-groups are used as building blocks for polyesters [4].

Figure 1. European adipic acid prices [5].

From all of the organic acids, one of the most important acid to emphasize on is the adipic acid. Adipic acid, also known as hexanedioic acid (C6H10O4), is the most important commercial aliphatic dicarboxylic acid. The worldwide production of adipic acid was estimated for 2011 as

3.3 million of tons (the prize had increased during the previous years, at it is shown in Figure 1) [6]. It is found as odorless, colorless crystals with an acidic taste. Almost 90 percent of adipic acid produced is used in the production of nylon 66, which was first produced in 1930s by W.H. Carothers of DuPont. The nylon, which has a protein-like structure, is further processed into fibers for applications in carpeting, automobile tire cord, and clothing. Adipic acid is also used to manufacture plasticizers and lubricant components [6].

In addition to the production of nylon-6,6 polyamide, adipic acid is also used in order to produce polyester polyols, lubricant components as well as polyurethanes as a reactant to form plasticizers. Other purposes of the adipic acid can be using it as a food ingredient in desserts, or other kind of foods that require acidulation.

Currently, several industrial-scale chemical plants have been built with the purpose of producing adipic acid. Most of it is obtained from benzene. First of all benzene is reduced to cyclohexane. After that, cyclohexane is converted by two successive oxidation steps into a mixture of cyclohexanone and cyclohexanol. Later this mixture reacts with air, adipic acid and nitric acids in the presence of vanadium catalyst.

Adipic acid can also be made by hydrocyanation of butadiene. Later the hydroisomerization to adiponitrile takes place, which is hydrolyzed. N_2, NO, NO_2 and N_2O are formed during the oxidation processes and the principal byproduct is nitrous oxide. There emissions of NOx chemicals are an important issue to concern about from an environmental point of view, because they promote global warming and ozone exhaustion. Actually, 10% of the total N_2O emissions to the atmosphere are caused by the production of adipic acid [7].

One of the targets that matters about chemical production of adipic acid is the reduction of nitrous oxide emissions to the atmosphere, in order to achieve a more sustainable process. For example this would be achieved by N_2O-decomposition in industrial conditions. Another alternative for adipic acid production could also be the direct oxidation of cyclohexene with aqueous 30% hydrogen peroxide in organic solvent- and halide-free conditions [8].

However, the feedstocks for adipic acid synthesis come from limited non-renewable fossil fuels and are very hazardous for the environment, whereas adipic acid is not very toxic. For example, benzene is a chemical that leads to important diseases as cancer or leukemia [8].

Nowadays and in a close future, clean technologies and industrial biotechnology are the

ways of achieving economic and environmentally friendly developments. It involves also the sustainable production of chemicals with energy-efficient processes and high purity outputs from bio-renewable sources.

On this issue, two new markets have been built: on one hand, the provision of bio-renewables by green biotechnology, and on the other hand, their processing by white biotechnology. Despite this huge progress, oil-based chemistry is still heading the economic competition, as white biotechnology is ecologically friendly just if the markets deal with the corresponding costs. In the picture below it is shown the energy production classified by markets. While oil-fired power generation has previously been a key contributor to power supply, its relative importance has diminished over the past 40 years, favoring natural gas, coal, and (in some regions) nuclear [9].

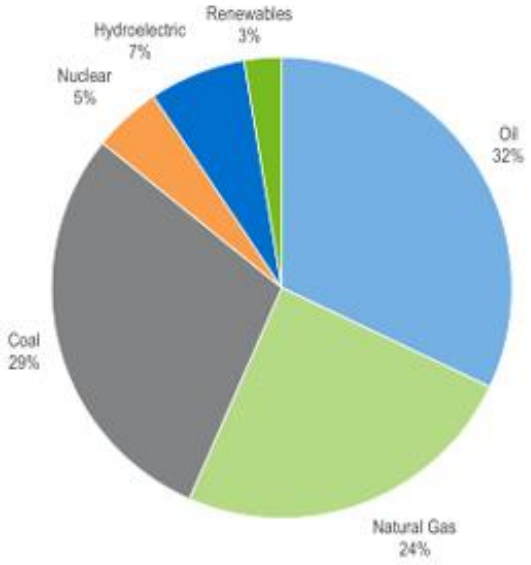


Figure 2. Primary energy production by source [9].

In the field of adipic acid, companies such as Rennovia Inc. and Verdezyne announced the commercial production based on renewable carbon sources on 2013/2014 and 2014/2015 respectively. However, those ideas have been patented but not commercialized yet in an industrial scale. For that reason, the purpose of this master thesis will be the Aspen plus simulation of some processing ideas of adipic acid announced by Rennovia, in order to check the viability of the process.

2 Literature overview

Rennovia Inc. is a specialty chemical company that focuses on the development of processes for the production of chemicals from renewable feedstocks, which was founded in 2009.

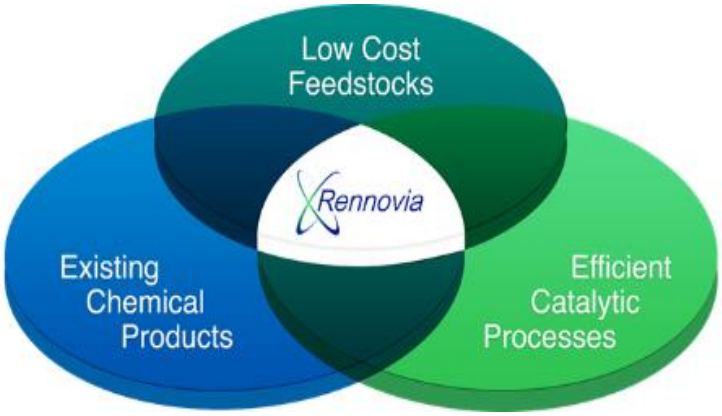


Figure 3. Rennovia logo.

The company works on production of chemical products such as glucaric acid, adipic acid, hexamethylenediamine and 1,6-hexanediol. All of these biobased chemicals are obtained from renewable feedstocks [10].

Global adipic acid market volume is approximately $6 billion per year, predicted to grow at 3 to 4 % CAGR (Compound annual growth rate) to 2022 [11].

There are many advantages associated to bringing petrochemical process efficiencies to biobased chemicals production, such as:

- Feedstock efficiency: maximize retention of mass, maximize use of functionality and minimize by-products.
- Catalytic conversion: high process yields, capital-efficient continuous processes and proven scalability.
- Isolation and purification: existing, scalable unit operations, concentrated process streams, and capital and energy efficient.

Despite adipic acid production has been mainly obtained from cyclohexane and phenol, new environmental concerns, stricter laws and changes in the hydrocarbon market have led to environmentally friendlier pathways of adipic acid production based on renewable resources such as the examples given in Figure 4 below. Among them is the production of adipic acid from glucose and fatty acids by fermentation and oxidation + hydrodeoxygenation [11]:

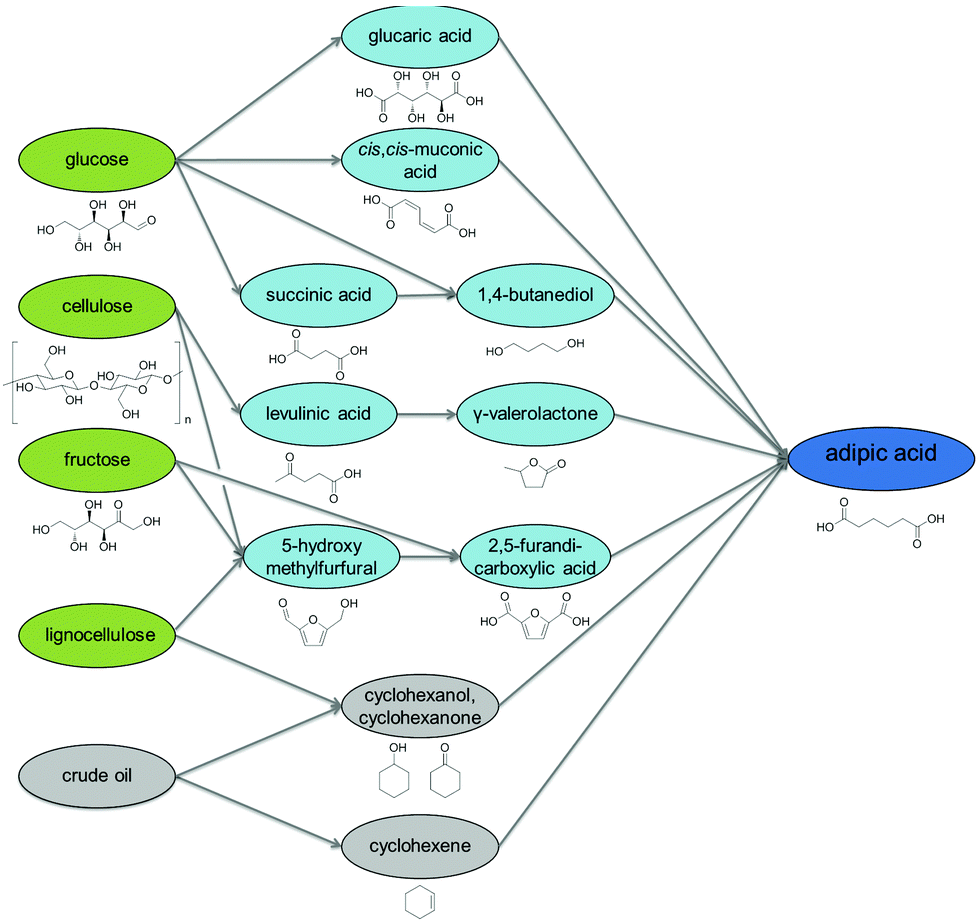


Figure 4. Outline of the production routes to adipic acid, showing biobased feedstocks (green), biobased platform chemicals (light blue), and existing petrobased routes (grey) [11].

2.1 Rennovia process vs. Conventional process

Rennovia is using innovative technology to adapt catalytic processes that have previously proven to be compatible, efficient and scalable in the refining and chemical industries. There are two main challenges related to the commercialization of industrial chemicals from renewable raw materials. On the one hand there is an important economic challenge due to the competitively inexpensive fossil feedstocks. In fact, sustainable technologies used for the conversion of biorenewable feedstocks prove to be potentially more profitable and economic than traditional petroleum-based chemical processes. On the other hand, there is a technical challenge which focus on operating at high process efficiencies in order to compete to existing petroleum-based raw materials [12].

Conventional Adipic Acid Production Technology.

Nowadays, petroleum-based adipic acid production is mainly obtained from benzene, by means of a multistep process, as it is shown in Figure 5 below. However, there are several issues to concern about involved in this process. Besides the high process complexity, it requires high energy consumption. Moreover, it has to deal with the production of nitroux oxide (N_2O) as by-product, which increasses the costs and process complexity due to abatement requirements. Nitrous oxide is a potent greenhouse gas (GHG) which contributes to global warming over 300 times than CO_2 [13].

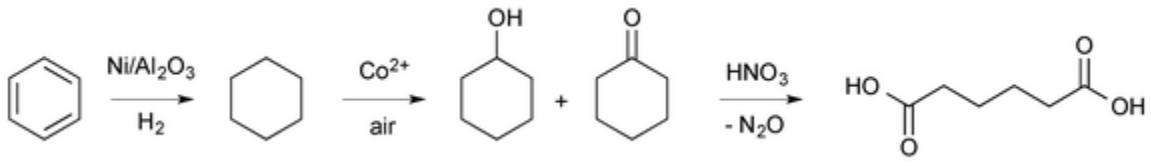


Figure 5. Conventional adipic acid production from benzene.

Figure 5 shows the current production of adipic acid. In the first step, the oil-derived benzene is hydrogenated to cyclohexane in presence of Ni/Al_2O_3 catalyst. After the hydrogenation step, cyclohexane is oxidized by air over a cobalt catalyst in order to obtain a mixture of cyclohexanol and cyclohexanone. This mixture is commonly known as KA-oil (ketone-alcohol oil). The conversion of cyclohexane in this reaction is usually very low (4-8%) because it is inversely dependent on selectivity. For that reason, it requires continuous distillation and recycling of cyclohexane. Finally, oxidation of KA-oil takes place with nitric acid. Afterwards, the desirable adipic acid is obtained, as well as a huge amount of undesirable nitrous oxide that requires abatement [14].

Fermentation-Based Adipic Acid Production Technology.

Fermentation is a metabolic process commonly used in the industry which can produce alcohols, organic acids or gases from carbohydrates, by the activity of enzymes of microbial origin. The metabolic activity of the microbes take place in a bioreactor [15].

One of the main advantages of adipic acid production by fermentation would be the variety of carbon sources, such us glucose, sucrose, etc. However, there are still some problems concerning about this process. There are some limitations due to the product toxicity or inhibition. For that reason, this process requires attention to the contamination and the need to maintain a sterile fermentation environment.

Other disadvantage would be the complexity of isolation and purification of adipic acid obtained from heterogeneous fermentation due to its non-volatile property, which adds costs and complexity to the process.

Regarding to economical of evaluation, the low carbon efficiency is also of paramount importance, with a yield below 92 % [13].

Rennovia's Bio-Based Adipic Acid Production Technology

Rennovia's proposal of an innovative and more environmentally friendly process to produce adipic acid from renewable feedstocks involves heterogeneous catalysis instead of fermentation. As it has been mentioned at the beginning of this chapter, this process includes the following advantages:

- Feedstock efficiency: maximize retention of mass, maximize use of functionality and minimize by-products.
- Catalytic conversion: high process yields, capital efficient continuous processes and proven scalability.
- Isolation and purification: existing, scalable unit operations, concentrated process streams, and capital and energy efficiency.

In addition, comparing to the previous detailed technologies for adipic acid production, biocatalytic synthesis of adipic acid from glucose avoids two of the main problems that concern about industrial adipic acid production: generation of nitrous oxide as by-product of a nitric acid catalyzed oxidation and use of carcinogenic benzene and benzene-derived chemicals as raw materials [16].

This innovative process involves two catalytic steps. The first one requires an oxygenation reactor where the aerobic oxidation of glucose to glucaric acid takes place. The second step feeds the glucaric acid into a hydrodeoxygenation reactor in order to obtain adipic acid. The reactions that take place are shown in the Figure 5 below:

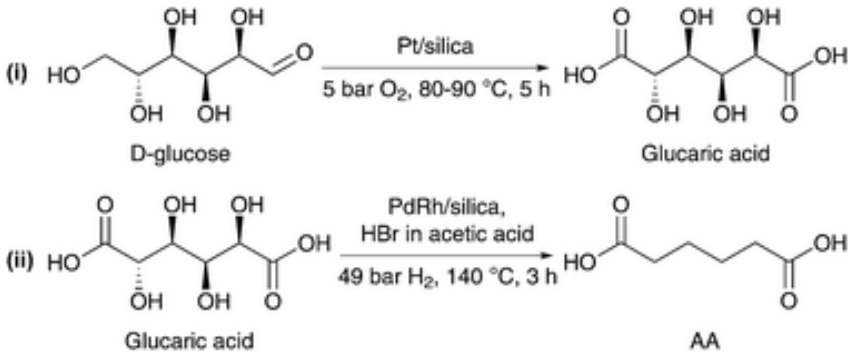


Figure 6. Two-step process for the conversion of glucose to adipic acid [17].

- Step 1: Selective oxidation of glucose to glucaric acid.

  In this step the problem about generation of nitrous oxide as by-product of a nitric acid catalyzed oxidation is avoided, because glucaric acid is currently produced at small commercial scale from glucose oxidation in presence of nitric acid. It is also profitable despite the additional costs caused by the difficulty of handling nitric acid and the low selectivity of the reaction. Moreover, glucaric acid is isolated from the reaction mixture via salt formation and reacidification, which increases the cost and complexity of scalability.

  For those reasons Rennovia's process would be the best option due to ease of operation, low costs and flexibility for product isolation and purification. However, some of technical targets must be fulfilled in order to implement successfully this process, such us high catalyst selectivity and activity, long-term catalyst stability and proper reactor design in order to operate successfully at the required conditions for favorable process economics [12]. For this, Rennovia has already tested the catalysts in a fixed bed reactor over 1000 hours of operation. The selectivity for glucaric acid and its intermediates amounted to more than 70% [13].

- Step 2: Selective hydrodeoxygenation of glucaric acid to adipic acid.

  In the second step glucaric acid is converted to adipic acid by the reduction of the C2-C5 secondary alcohol groups with hydrogen without reducing the C1 and C6 carboxylic acids or cleaving C-C bonds (see Figure 6). Direct catalytic reduction of alcohols to alkanes is not a very common reaction. However, it has become important due to its application on bio-oils of fatty acid derivatives conversion into hydrocarbon fuels.

The conventional hydrotreating constists in a petroleum refining unit operation for removing sulfur and nitrogen from crude oil, in order to obtain transportation fuels. One of the problems related to most of the employed systems is the fragmentation of the carbon chain owing to the use of catalyst or reaction conditions. This is can be suitable for fuel production, but counterproductive for adipic acid conversion from glucaric acid.

Selective hydrodeoxygenation of C-OH bonds is a highly desirable reaction for bio-based feedstocks conversion to specialty chemicals that are not obtained in petrochemicals production. For making this reaction possible is necessary the development of the catalytic transformation scalability. Rennovia claims to solve this challenge with the dehydration of each alcohol in order to produce an intermediate oleofin and after that the catalytic hydrogenation. [12].

Rennovia has already proved long term pilot operation of adipic acid production from glucose via two step catalytic processes like the ones mentioned before, as well as pilot-scale operation of all unit operations involved in the process [18].

The pilot-scale operation was announced in 2014 and created in cooperation with Johnson Matthey group. The division is a global supplier of catalysts, licensed technologies and other services to the petrochemical, syngas, oil refining and gas processing industries. The successful mini-plant is located at the Johnson Matthey Technologies R&D Center in Stockton, England. The mini-plant is designed to allow direct scale-up for the production of 135,000 tons/year of adipic acid. Moreover, Rennovia foresees the first commercial-scale bio-based adipic production plant in 2018, also in collaboration with Johnson Matthey group [19].

3 Process simulation and methods

3.1 Basis of the simulation

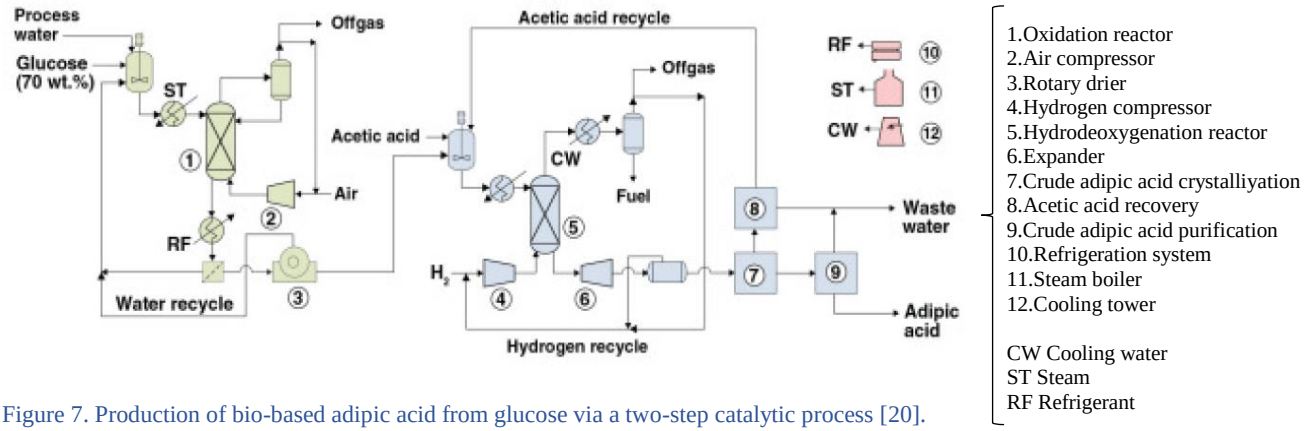


Figure 7. Production of bio-based adipic acid from glucose via a two-step catalytic process [20].

The process shown in the picture above was used as reference for a previous project of a simulation in Aspen Plus® [21], where production of adipic acid from glucose via a two-step catalytic process takes place. The purpose of this master project will be the improvement of the existing chemical plant simulation, which be explained below. A patent from Rennovia [22] was used in order to find useful data for the simulation, but some parameters were estimated due to the lack of information, such us pump efficiency or heat transfer coefficient for heat exchangers. All of data for different chemicals were used from storage data in Aspen Plus®, except data for glucaric acid. The missing parameters were estimated using the method UNIFAC in CHEMCAD.

The general process can be divided into two sub-processes. The first sub-process corresponds to the oxidation of glucose in glucaric acid and its purification (which is shown in green in the diagram). The second sub-process shows the hydrogenation of the glucaric acid and the subsequent separation of glucaric acid (shown in blue in the diagram).

Glucaric acid synthesis. The raw material is a glucose solution, which is mixed with recycled water at the beginning of the process. Then is heated and fed to the oxidation reactor. Oxygen is supplied to the reaction by feeding compressed air to the bottom of the reactor. The overhead from the reactor is bought to a knock-out drum, from which a liquid stream is removed and recycled to the reactor. The reactor's bottom product is cooled and filtered. The glucaric acid is obtained as a solid and brought to rotary dryers where water is removed [20].

Adipic acid synthesis. Glucaric acid obtained in the first part of the process is dissolved in acetic acid. Later, the mixture is heated and fed to the hydrodeoxygenation reactor, where glucaric acid and hydrogen react at high pressure conditions. From the top of the reactor it is obtained a hydrogen-rich stream, which is partially condensed. The condensed part (light byproducts) is burned as fuel, and the gaseous stream is recycled to the hydrogen compressor. The product obtained from the bottom of the reactor is expanded in a turbo generator, producing electricity. Later, this product is directed to a knock-out drum, where a hydrogen-rich stream and a liquid stream are separated. The hydrogen-rich gaseous phase is recycled to the hydrogen compressor, and the liquid phase (composed mainly by acetic acid, adipic acid and water) is bought to a crystallizer. After the crystallizer, the product is fed to a rotary dryer to obtain adipic acid. The evaporated acetic acid and the mother liquor from the filter are fed together to an extractive distillation system. In this way, acetic acid is separated from water and recycled to the hydeodeoxygenation feed mixer. Crude adipic acid obtained from the rotary dryer must be dissolved in water and subjected to further crystallization, filtering and drying in order to achieve fiber-grade purity [20].

3.2 Description of the simulation

The previous simulation was carried on according to a Rennovia's patent research, but mainly according to the patent US 9,434,709 B2 [22]. Below it is shown in the following tables the explanation of the different streams and unit operations involved in the process:

Table 1. Naming of streams (YY for numbering).

Streams' Nomenclature	Description	Explanation
YY-FEED	Supply of reactants	Coming from the left
YY-S	Main stream	Ascending numbering towards product
YY-R	Recycle streams	E.g. RG-YY for the gas recirculation in the second sub-process and RYY for the water recycling in the first sub-process
YY-P	Purge streams	Removed to the right
YY-GAS	Gas stream	Recirculation in the first sub-process
YY-H2	Hydrogen feed streams	Starting from FEED-H2 via 2 compressor stages, a heat exchanger and a mixing point to the reactor RHYD

YY-AIR	Air supply streams	Starting from FEED-AIR via a compressor stage and a heat exchanger
YY-HD	Inlet heating/cooling medium	Steam/Water
YY-KD	Outlet heating/cooling medium	Steam/Water
YY-Q	Heat integration flows	Use of the heat of reaction
YY-KDQ & YY-HDQ	Heating/cooling medium by means of WT-Q	Use of the heat of reaction
YY-KDQR	Heating/cooling medium from reactors	Use of the heat of reaction
YY-QOUT	Output	Heat output
YY-AA	Product	Adipic acid
YY-MTBE	Methyl *tert*-butyl ether	Used for azeotropic distillation (see Chapter 3.3.2)

Table 2. Unit Operations' Nomenclature (X refers to the section of the simulation YY for numbering). Section 1 is the first sub-process and section 2 the second.

Unit Operations' Nomenclature	Description	Explanation
G-XYY	Phase separator	Gas-liquid separation
K-XYY	Compressor	For gas streams
M-XYY	Mixer	Streams' merging
P-XYY	Pump	Streams' impulse
R-XYY	Reactors	R-101: oxidation reactor & R-201: hydrodeoxigenation reactor
S-XYY	Splitter	Streams' separator
T-XYY	"Black box" separation	Separation of products (glucaric acid, adipic acid , H_2O)
V-XYY	Valve	To decreasse pressure
W-XYY	Heat exchanger	Heating or cooling of streams

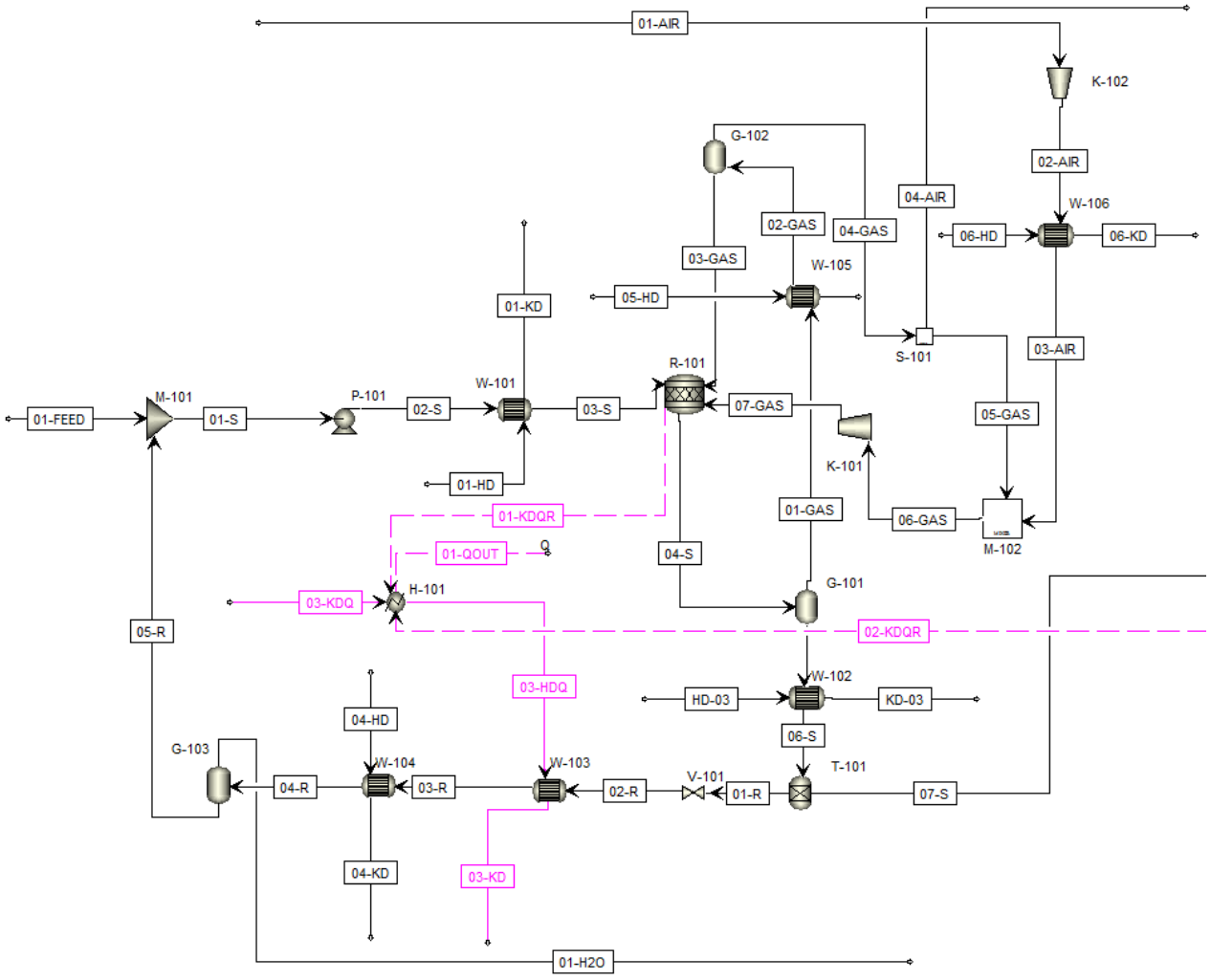


Figure 8. First sub-process for adipic acid production from glucose.

In the 01-FEED stream, the starting material glucose is contained as an aqueous solution (ωGlucose = 0.7) and is fed to the process from the left. In M-101 it is mixed with recycled water. As a result, a glucose solution is achieved with a mass fraction of about 0.27. This dilution was carried out since, according to US Pat. No. 9,434,709 B2 [22], a 10% glucose solution is required. In this case, the mass fraction of the glucose solution was not adjusted as set out in the patent to 10%, because on the one hand no reasons for such a dilution are recognizable and on the other hand, a higher concentration of glucose solution leads to less energy being needed for the heating of the reaction mixture. Subsequently, the solution is preheated in the heat exchanger W-101, wherein the heat exchanger is used only for starting the reactor. In the simulation, the heating cost of the heat exchanger was taken into account by continuously supplying the heat exchanger with a small amount of heating steam (10 kg/h).

The glucose solution is fed to the reactor R-101 and oxidized to glucaric acid with oxygen, which is supplied from the stream 01-air by means of compressed air to 5 bar. The reactor sump (05-S), which contains predominantly water, glucaric acid and glucose, is subsequently cooled by the heat exchanger W-102. The flows 01-GAS to 07-GAS characterize the gas recirculation. About 04-AIR, some gas is discharged from the process to prevent unwanted accumulation. After the W-102, the T-101 device separates the glucaric acid from water and glucose. T-101 is considered a black box because the exact separation is not listed in the patent.

In stream 07-S, the pure, anhydrous glucaric acid is fed to the next process section. With the streams 01-R to 05-R, the return of water and glucose is ensured. The colored streams (pink) in Figures 8 and 9 show the heat integration of the manufacturing process of adipic acid. Heat integration takes place via the heat exchanger W-103 from the heat quantities generated by the oxidation and hydrogenation in the reactors R-101 and R-201. For this purpose, the heat flows 01-KDQR and 02-KDQR, which are fed into the heat exchanger H-101, as heating current 03-HDQ supplied to the W-103. The purpose of the heat exchanger W-103 is to pre-heat the return flow 02-R so that the heating steam used in the W-104 can be reduced. In order to prevent accumulation of water, G-103 discharges water from the circulation overhead by the action of heat.

The output currents are thus summarized for the first sub-process: discharge of gas or water (with dissolved glucose) in 04-AIR or 01-H2O and the product flow 07-S.

The next part of the process involves the hydrogenation of glucaric acid to adipic acid in the R-201 reactor (see Figure 9).

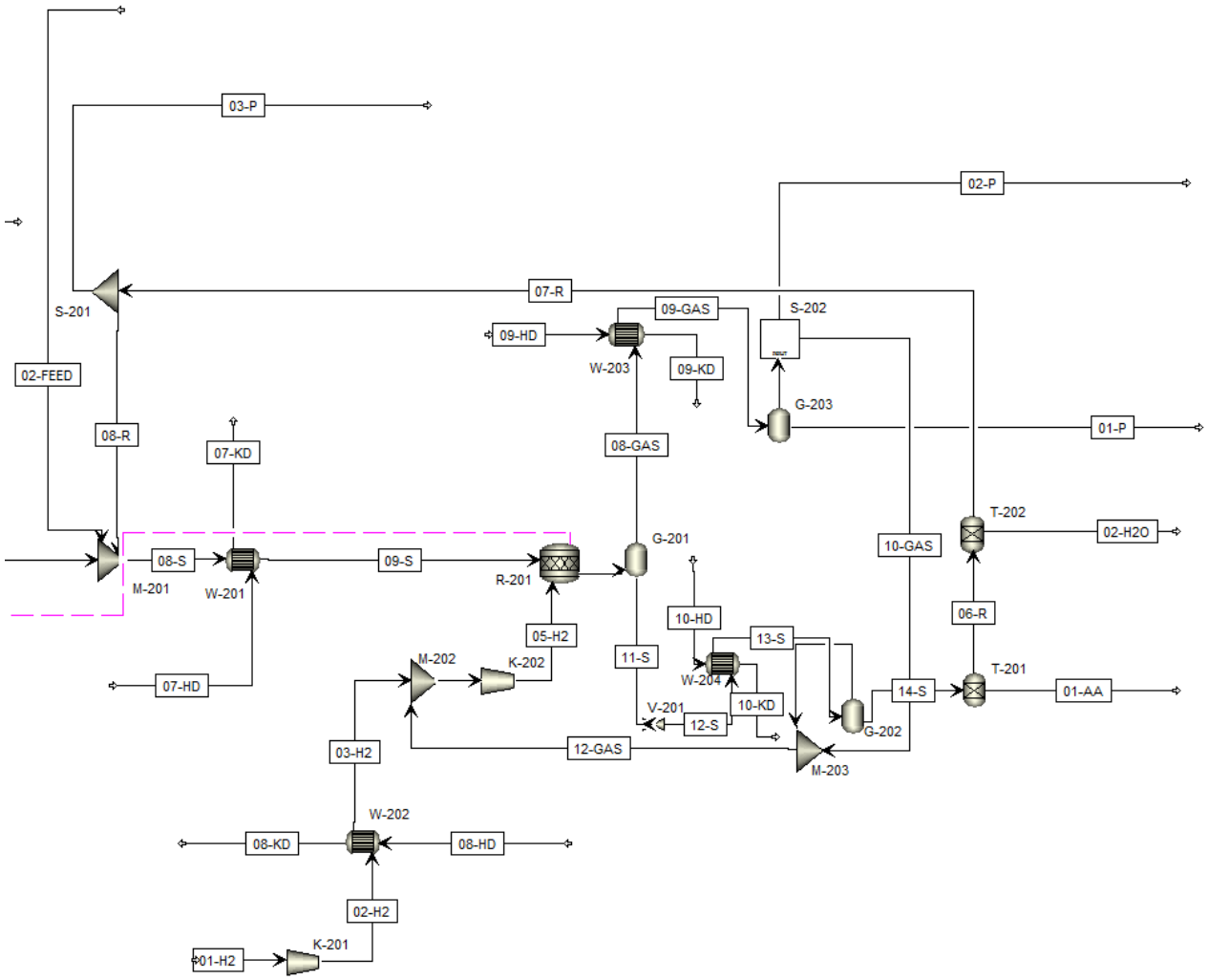


Figure 9. Second sub-process for acipic adic production from glucose.

The glucaric acid recovered from the first process section is fed via stream 07-S and mixed with acetic acid from 02-FEED and with the recycle stream 08-R in M-201. In the stream 08-S, glucaric acid has a mass fraction of about 8%. The heat exchanger W-201 is intended to preheat the glucaric acid solution, but like the W-101, it is only used when starting the reactor. Here a low, continuous heating steam flow of 10 kg/h is assumed as well. The preheated stream 09-S is fed to the reactor R-201.

Compressed hydrogen at 30 bar is fed into the process via the 01-H2 stream. In order to reach the desired pressure of 49 bar in the R-201 reactor, two compressor stages K-201 and K-202 are compressed under intercooling with W-202 (streams 02-H2 to 05-H2). In R-201, the glucaric acid is hydrogenated to adipic acid at 160 °C.

In G-201 (analogous to G-101 in the first sub-process), the separation of gaseous components into stream 08-GAS takes place, since this can not be mapped in the RSTOIC reactor model.

The reactor sump 11-S is expanded via the valve V-201 and then cooled down to 50 ºC. in the heat exchanger W-204. From the cooled stream 13-S, the residual gaseous hydrogen is removed in the G-202 (stream 11-GAS) and fed back via 12-GAS.

The obtained adipic acid is separated from the liquid stream 14-S with T-201. Again, T-201 represents an ideal and unrealistic separation. The mentioned patent by way of example that separation by solvent extraction or crystallization would be possible [22].

The same happens with T-202. Here the acetic acid is separated from water. 4 moles of water arise per mole of adipic acid. A discharge of water is important for a good yield of adipic acid. The recovered acetic acid is recycled via the stream 07-R or 08-R and can therefore be used again as a solvent for the glucaric acid. About S-201 and 03-P, some acetic acid is released from the process, again to prevent accumulation.

Gas streams 08-GAS to 12-GAS provide the recirculation loop of unused hydrogen in the hydrogenation reaction. 08-GAS is cooled down from 160 °C to 30 °C above the heat exchanger W-203. In G-203, the liquid fraction is removed as "fuel" (flow 01-P) analogously to Figure 7. The gas stream is split in the S-202, whereby a small proportion is discharged as purge gas in the stream 02-P. Through streams 10-GAS and 12-GAS, the recycled hydrogen in M-202 is mixed with freshly fed and pre compressed hydrogen from 03-H2.

The output streams are thus combined for the second sub-process: discharge of gas or water into 02-P or 02-H2O, "fuel" in 01-P, acetic acid purge stream 03-P and the product stream of adipic acid (01-AA).

3.3 Simulation improvements

3.3.1 T-201: Crystallization and purification of adipic acid.

One of the improvements that have been carried out is related to the crystallization process, which in the previous simulation plant corresponds to T-201 unit operation. As is has been mentioned in the previous chapter, the crystallization was conceived as a black box, involving any method of separation due to the lack of information presented in the patent.

However, while doing a research about the patents assigned to Rennovia Inc., no details have been found on how to carry out the crystallization. For this reason, the crystallization method of adipic acid used in the conventional process for obtaining adipic acid from cyclohexane has been

taken into account. The technology used is described in the patent US 3,096,369, which was assigned to Stamicarbon N.V. in 1957. This patent mentions that the invention is applicable to the crystallization of adipic acid from varying types of solutions. Thus, solutions of acipic acid in water or organic solvents, e.g., cyclohexanol, may be treated according to the invention [23].

Before describing the technology, there should be remarked some facts concerning about crystallization. There are four types of crystallization [24]:

- Evaporation of solvent.
- Temperature change of the solution.
- Chemical reaction (precipitation).
- Precipitation with a compound decreasing the solubility (the presence of other compounds can affect the solubility of the product).

In this case, the second method of crystallization is used because there is no reaction involved in this step of the process. The solubility decreases with the decrease of temperature, so it is called cooling crystallization. Specifically, the principles are equally applicable to batch crystallization (alternating different cooling temperatures), even though the crystallization was studied in a continuous system [25].

It should be also mentioned that size of crystals increases, the higher the temperature at which the crystals are formed. For that reason, at higher temperatures the rate of growth of the crystals increases whereas the rate of nucleus formation decreases, so that bigger crystals are formed. However, the purity of the crystals decreases with the increase of the crystals growth rate [22].

Another issue that should be considered in order to understand the process offered by the patent is that the beginning of crystallization is favored in presence of other crystals. The first step of the formation of crystals is called nucleation. Nucleation entails an energy barrier that needs to be surpassed, which means that supersaturation is not enough to start crystallization. A solution will be supersaturated when the concentration of one or more compounds is higher than the allowed for the equilibrium solubility at the given conditions. Any solution can be supersaturated by cooling it (see Figure 10 below). If seed crystals are added to the solution, new crystals will appear and start growing as there is no energy barrier for growth [26].

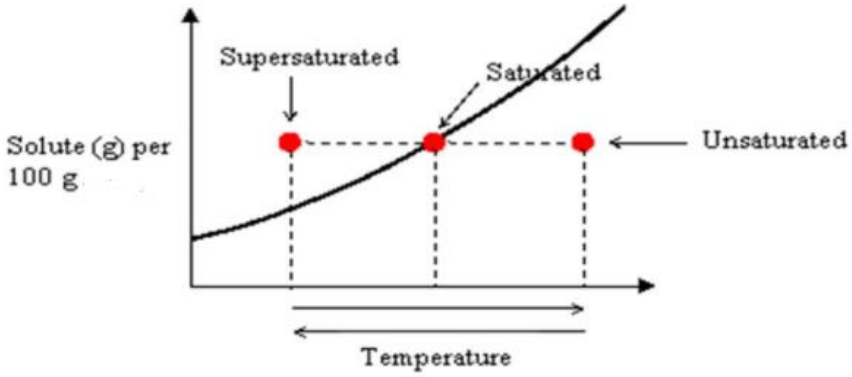


Figure 10. Solubility curve [27].

When the solution is not supersaturated enough for forming nuclei spontaneously, it is said that the solution remains in the metastable zone. The width of the metastable zone varies depending on the compound´s properties and the given conditions, like cooling rate [26]. For example, pure water is frozen at -42 ° C, instead of its melting temperature of 0 ° C, if there are no nucleators for ice formation [28].

Once that the basis of the crystallization have already been explained, some critical points about the crystallization of adipic acid carried out in one conventional crystallizer will be discussed, because it usually involves several problems, such us:

- During crystallization, a milky product is obtained which contains crystal particles of such small dimensions that are difficult to separate from the mother liquor, what generates a loss of product.
- Crusts of crystals are deposited on the cooling surface, which leads to a reduction of heat transfer and, consequently, a reduction of crystal growth rate. Thus, it is necessary to interrupt the process several times in order to clean the crystallizer, unless the crystallizer has already a system that allows crystal deposits removal. Anyway, that system would increase the complexity of apparatus and decrease the ease of operation. For that reason the invention offers a batch operation method of crystallization [23].
- The by-product organic acids are significantly effective in annulling adipic acid crystals nucleation, as well as in decreasing the crystal growth rate. For that reason it is possible to cool the solution about 10 °C under the saturation conditions without appreciating any change. No nucleation is evident and supersaturation is released only very slowly on existing crystal surfaces [25].

The purpose of the invention is to deal with the problems mentioned above. The first step of the invention is cooling an adipic acid solution until a crystal suspension is obtained. Part of this cool crystal suspension is recycled, separating previously the obtained crystals and using the recycled part for cooling the new adipic acid solution at a temperature below 30 °C by mixing them. That mixture is then cooled again to the desired temperature between 5 and 25 °C. By using this recycling technique, the previously mentioned problem about the nucleation energy barrier is avoided. This means that no new crystals appear and the existing ones will grow after passing through both of the crystallizers. However, during the process those crystals will collide, breaking into pieces and creating new smaller and less pure crystals. Moreover, the multi-stage direct cooling of the adipic acid solution offers the advantage of crystallization at higher temperature, which favors the formation of bigger crystals [23].

Figures 11 and 12 show a preferred method of crystallizing the acid from aqueous solution offered in the patent and the changes of the simulated process:

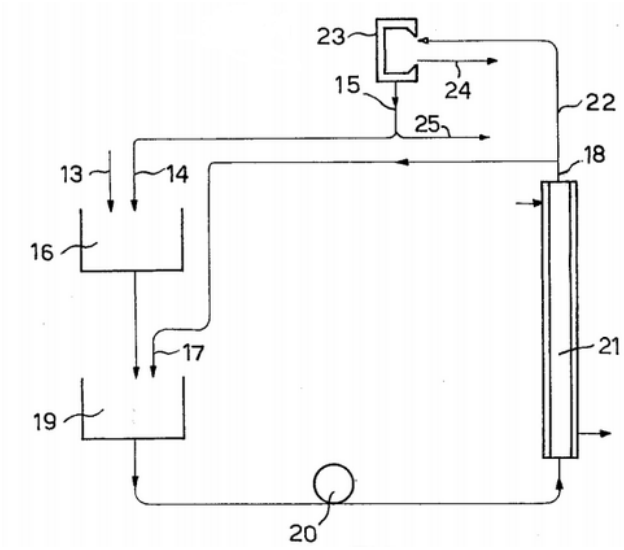


Figure 11. Crystallization process for adipic acid from aqueous solution presented according to the patent US 3,096,369 [23].

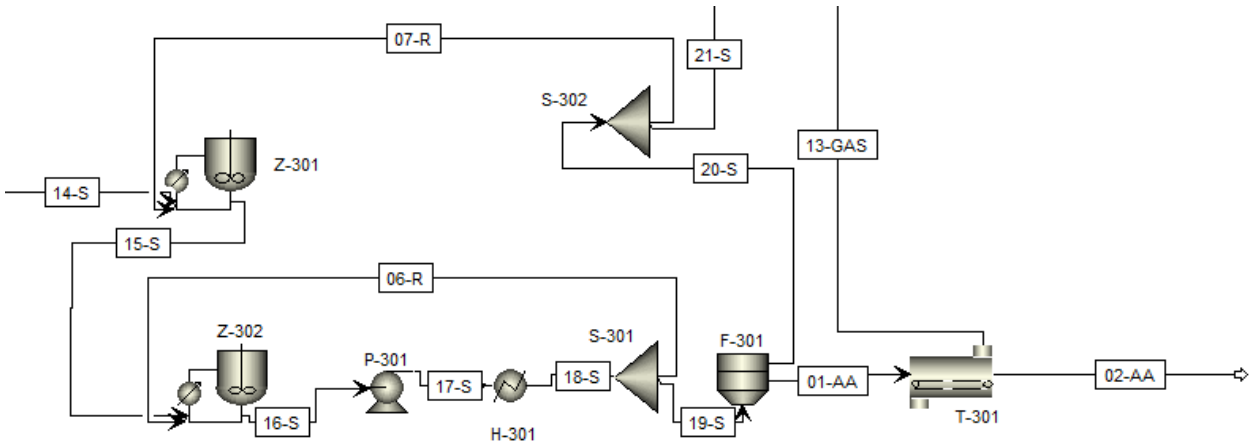


Figure 12. Crystallization process from the new simulation.

According to the process, the adipic acid solution resulting from the process (14-S) is fed into the first crystallizer (Z-301) together with a recycled portion of previously cooled mother liquor (07-R), where first crystallization takes place at 25 °C. The new suspension (15-S) is fed into the second crystallizer (Z-302) with another recycled crystal suspension (06-R), where crystallization takes place at 15 °C. The new crystal suspension (16-S) is driven by a pump (P-301) and cooled (H-301) at a temperature of 12.5 °C. A portion of the cooled suspension (19-S) is fed to the centrifuge (F-301) where adipic acid crystals and mother liquor are separated. Bigger crystals will be obtained as output and smaller crystals will be recycled. Finally, the resulting adipic acid crystals are fed to a rotary dryer (T-301) where the steam is removed (13-GAS) and dried crystals are obtained (02-AA).

It should be noted that the use of centrifuge as solids separator instead of hydrocyclone or other commonly used separator is mentioned in the patent [23], as well as in other scientific articles about adipic acid production [29]. Both equipments are used in order to separate heavy and light particles by using centrifugal force. However, hydrocyclones are passive separators capable of applying big amounts of centrifugal force, while centrifuges are dynamic, spinning separators that are able to apply even bigger centrifugal force. Centrifuges obtain more accurate size of product, but the cost is higher and they need better control of the rotary machine [30].

The division of the particles takes place due to their centrifugal settling method, which works thanks to the movement of particles in fluid. Fine or light particles might not be able to settle when a liquid is passed through a centrifuge, which means that they will be taken out with the liquid. On the other hand, larger particles are separated by throwing them out from the liquid [31].

Table 3. New Unit Operations replacing T-201 (X refers to the section of the simulation YY for numbering). Section 3 is the crystallization process.

Unit Operations' Nomenclature	Description	Explanation
F-301	Centrifuge	Selective separation of bigger crystals
H-301	Heater/Cooler	Heating or cooling streams
P-301	Pump	Streams' impulse
S-301 & S-302	Splitter	Streams' separator
T-301	Rotary dryer	Drying of crystals by removing water
Z-301 & Z-302	Crystallizer	Cooling crystallization medium

3.3.2 T-202: Water removal.

The second improvement of the simulation works as a substitute of T-202 unit operation. As it is explained in Chapter 3.2, T-202 is conceived as a "black box", which means that the compounds are ideally separated, but that is not realistic. However, after the Rennovia patent research it has been concluded that there is not public information about the wastewater removal.

The aim of this section is to separate the water from the solution, which contains water, glucaric acid, acetic acid and adipic acid. This process present the problem of separating water from acetic acid, due to the proximity of the respective boiling points, which are 118 ºC for acetic acid and 100 ºC for water. The simulation improvement offers the possibility of separating acetic acid from water by the use of azeotropic distillation system [32], which will be added after a previous cleaning distillation column whose purpose is separating all of the remaining compounds (glucaric acid, adipic acid and adipic acid) from the acetic acid-wastewater mixture.

Azeotropic distillation process separates close boiling compounds in presence of an added liquid that forms an azeotrope with one of both of the compounds. The azeotrope former alters the relative volatility in order to make a greater separation on each plate, which makes the separation possible with fewer plates. The system consists of a multiple rectification column. It has been discovered that certain organic compounds increase effectively the relative volatility between acetic acid and water, such us methyl propionate, benzyl acetate, isopropyl acetate, butyl ether, etc. [32].

The process used for the simulation is called hybrid extraction/distillation process. It has

proved to be more effective than other processes, such us multi-effect distillation or heterogeneous azeotropic distillation. It combines an extraction column and the azeotropic distillation process together. All of these unit operations will follow the previous cleaning distillation column that has been mention before, which separates the rest of the compounds from the acetic acid-wastewater mixture. The simulation will be carried out with methyl *tert*-butyl ether as entrainer [33].

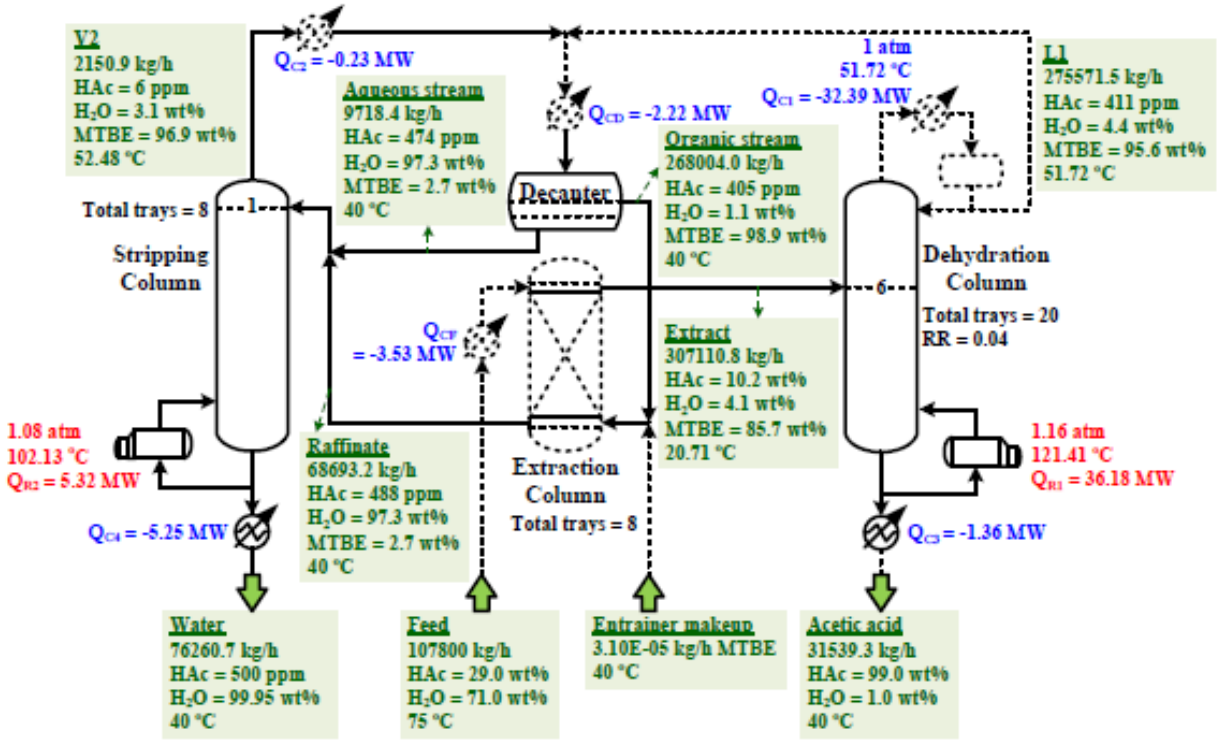


Figure 13. Simulation scheme of liquid-liquid extraction with methyl *tert*-butyl ether as entrainer used as reference [33].

However, while simulating the hybrid extraction/distillation process there were some difficulties due to the difference in the feed proportions to the system. In the adipic acid production plant, at this point the ratio of acetic acid to water is much higher than the suitable. As it can be notice in Figure 13, the feeding stream contains 29 wt% of acetic acid, while in the simulation plan the amount of acetic acid after the cleaning distillation column (23-S) is 95 wt%. That case was already tried in simulation but it was proven that a huge amount of MTBE was required to make the separation possible. Moreover, as there is so much MTBE in the system, all of it went through the bottom of the stripping column showed on the left part in Figure 14. For that reason, it was concluded that it is necessary to add another additional distillation column before the azeotropic distillation step, just to separate some acetic acid from water. The acetic acid will be recirculated to the beginning of the second sub-process (glucaric acid conversion to adipic acid) so the obtained amount

of acetic acid after the second distillation column (24-S) will be 40 wt%, which is closer to the proportions of acetic acid and water shown in Figure 14. The value of 40% was the optimal changing 2 parameters of the column: number of plates and reboiler duty.

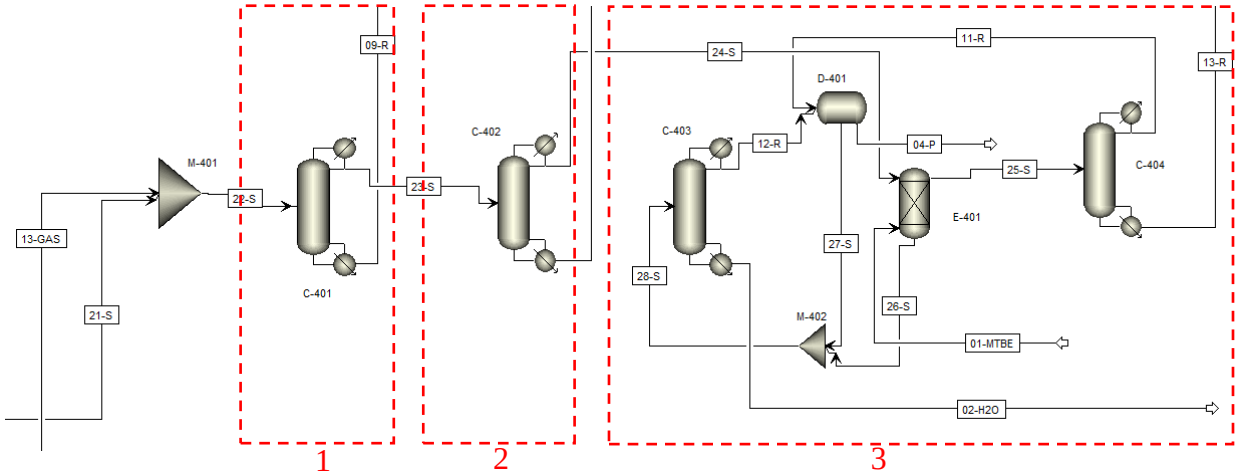


Figure 14. Water removal and acetic acid recovery process from the new simulation divided in 3 parts: 1- pre cleaning distillation column, 2- pre distillation column of acetic acid and water mixture, 3- azeotropic distillation.

The recycled streams from the crystallization process (21-S and 13-GAS) are mixed (M-401) and fed to the previous cleaning distillation column mentioned before (C-401). The mixture obtained from the bottom (09-R) is recycled to the beginning of the second sub-process (see Figure 9). The acetic acid-water mixture obtained from the top (23-S) is fed to a pre distillation column of acetic acid and water mixture (C-402). The condensate (10-R) consist mainly of acetic acid (99,9 wt%) but also a little bit of water (0.1 wt%), and is also recycled to the beginning of the second sub-process together with 09-R. The distillate obtained from C-402 (composed of 60 wt% acetic acid and 40 wt% water) is finally fed to the azeotropic distillation system described before. The stream 24-S is carried to the extraction column (E-401) where water and acetic acid are mixed with the entrainer MTBE, forming an azeotrope. From the top of E-401 emerges the extract stream rich in MTBE (25-S). That stream is carried to the dehydration column (C-404) where acetic acid is separated from the mixture and obtained through the bottom of the column (13-R). The acetic acid is recirculated to the beginning of the second sub-process and mixed with the rest of the recycled streams in S-201. The distillate obtained from the dehydration column (11-R) is carried to a decanter (D-401) where phase separation takes place. The organic stream rich in MTBE (04-P) will be purged. The feeding stream (01-MTBE), mainly composed by MTBE is fed to the bottom of the extraction column (E-401). The aqueous stream obtained from the decanter (27-S) will be mixed (M-402) with the raffinate stream obtained from the bottom of the extraction column (26-S). The

mixture (28-S) is fed to the stripping column (C-403) where the distillate (12-R) is carried to the decanter. Finally, the water is obtained from the bottom from the stripping column (02-H2O) and removed from the process.

It can be noticed that there is a small difference between Figures 13 and 14. The organic stream obtained from the decanter (04-P) should be recycled and fed into the bottom of the extraction column (E-401) together with the feeding stream of MTBE (01-MTBE), as it is shown in Figure 13. There was a problem about convergence during simulation. As it is necessary to add only a small amount of MTBE, the huge recycle of MTBE going through a closed circuit leads to numerical problems in solving the steady state: MTBE comes out from the bottom of the decanter, it enters through the bottom of the extraction column, it goes to the dehydration column, it gets out from the top of the dehydration column and goes back to the decanter.

For that reason, a pseudo-recycle is used. Instead of recycling the MTBE stream from the decanter, a purge outlet from simulation was used. In order to compensate, all the necessary MTBE is fed as "Entrainer make-up". The simulation was run several times and the result composition of the decanter outlet was copied as "Entrainer make-up" until similar result composition was obtained.

In reality, stream 04-P would be recycled and taken to the extraction column as it has been mentioned before.

Table 4. New Unit Operations replacing T-202 (X refers to the section of the simulation YY for numbering). Section 4 is the water removal process.

Unit Operations' Nomenclature	Description	Explanation
C-401, C-402, C-403 & C-404	Distillation column	Separation by volatility difference
D-401	Decanter	Liquid separation by density difference
E-401	Extraction column	Liquids separation by difference of solubility
M-401 & M-402	Mixer	Streams' merging

3.3.3 Heat exchange network optimization.

The cost of energy has increased the last years, and it is expected to continue increasing. For that reason, it is becoming extremely important for chemical engineers to optimize the use of energy. There are two suitable and commonly used methods for minimizing the use of energy: Heat Exchanger Network Synthesis (HENS) and Pinch Method. This chapter focuses on the second one

[34].

The main objective of pinch method is to identify the minimum target cost and heat exchanger network (HEN) capital cost targets of the process, as well as recognizing the pinch point [35]. In the following chapter, a free software for heat exchanger network design based on the pinch method are presented (HINT software) for the normal operation of the process. Both heat exchangers W-101 and W-201 do not work during normal operating conditions because the previous streams (02-S and 08-S) are already at the target temperatures due to the hot recycled streams.

Figure 15 shows the input data for HINT software obtained from Aspen Plus simulation for the operation of the process:

Stream	Description	Type	Heat type	T1 (K)	T2 (K)	H (kW)	mcp (kW/K)
1	W-102	Hot	Sensible	362.1	303.15	-16721.	283.6472
2	W-103	Cold	Sensible	303.15	372.15	16896.	244.8696
3	W-104	Cold	Latent	372.15	372.15	15161.	-
4	W-105	Hot	Sensible	362.991	313.15	-14216.	285.227
5	W-106	Hot	Sensible	432.265	303.15	-3831.	29.67122
6	W-202	Hot	Sensible	324.371	303.15	-243.	11.45092
7	W-203	Hot	Sensible	433.15	303.15	-3440.	26.46154
8	W-204	Hot	Sensible	433.15	323.15	-21894.	199.0364
9	H-301	Hot	Sensible	288.189	285.15	-852.	280.3554

Figure 15. Input data of every stream from different heat exchangers, obtained from Aspen Plus simulation.

The input data consist of supply and target temperatures (K), enthalpy of the stream (kW), and heat capacity flow rate (kW/K). The value of enthalpy is the difference of the streams properties, before and after going through the heat exchangers from the Aspen® Plus simulation´s results. The heat capacity flow rate is automatically calculated by the program. Each stream goes thought a different heat exchanger in Aspen Plus® simulation. Those heat exchangers have the nomenclature that is represented in the descriptions in Figure 15.

Figure 16 shows the Q (W) vs T(K) curves for each heat exchanger involved in the process, obtained from Aspen Plus® simulation.

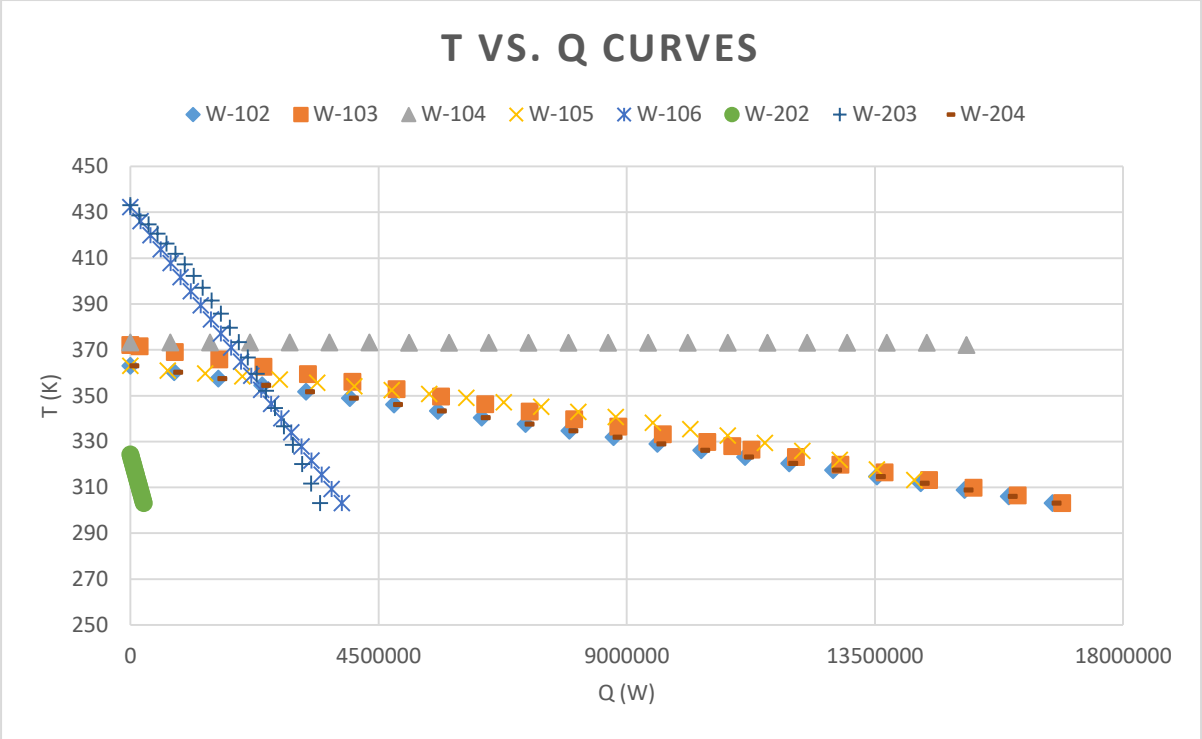


Figure 16. Q (W) vs. T (K) curves for each heat exchanger involved in the process.

As it can be observed, during the heating of the stream that goes through the heat exchanger W-104, there is almost no increment of temperature, while the value of Q increases considerably. That means that there is a phase change and the heat type of stream 3 will be latent, at it is shown in Figure 15.

Once that the data has been introduced, the next step is to calculate the *"*temperature approach*"*. In practice the hot stream can only be cooled to a temperature defined by the "temperature approach" of the heat exchanger. The temperature approach is the minimum allowable temperature difference (DTmin) in the stream temperature profiles, for the heat exchanger unit. The temperature level at which DTmin is observed in the process is referred to as "pinch point" or "pinch condition". The pinch defines the minimum driving force allowed in the exchanger unit [35].

HINT software offers the possibility of estimating the impact of the variation of DTmin in different parameters. The optimal DTmin will be the one that involves lower energy and capital costs. Figure 17 shows the total cost of the heat exchange network ($), for DTmin values between 1 and 50 K, according to HINT software:

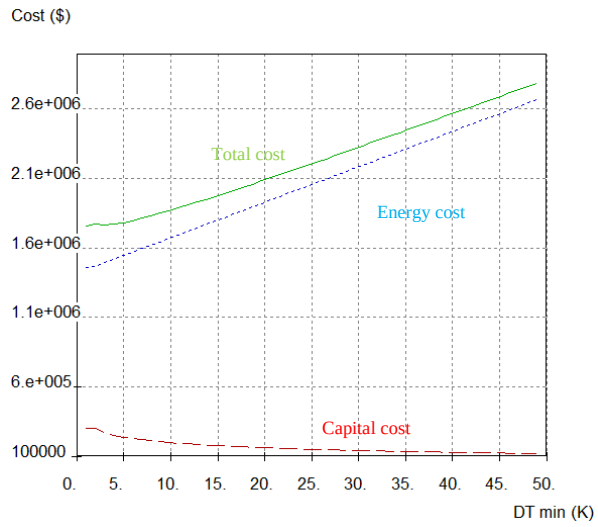


Figure 17. Cost target vs. DTmin.

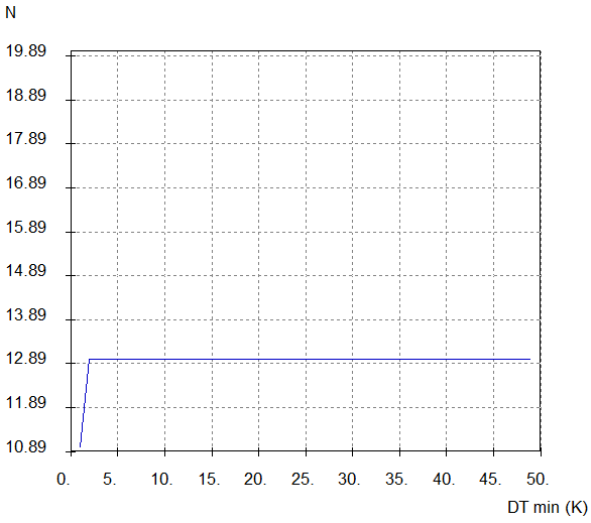


Figure 18. Number of heat exchangers vs. DTmin.

Figure 18 shows the minimum number of heat exchangers that are necessary for the start-up of the process plant for DTmin values between 1 and 50 K, according to HINT software. As it is shown in both figures, DTmin values of 10 K or less, lead to lower cost and require a smaller number of heat exchanges for the process. However, a very small DTmin value, perhaps 8 ºC, can lead to a very complicated network design with a large total area due to low driving forces [35]. For that reason, DTmin value chosen for pinch method will be 10 K.

Once that DTmin value has been chosen, the next step is to plot the "grid diagram", which is the graphical method of representing flow streams and recovery matches. Every stream has its initial and target temperatures, and the vertical line in the middle show the pinch temperature. In Figure 18 it is shown the grid diagram with the different matches between cold and hot streams. The line located in the middle of grid diagram refers to the "pinch point" or "pinch temperature", which is 298.15 K. Pinch technology defends that no heat should be transferred across the pinch point for an optimal design. The numbers above each stream represents initial and target temperatures. In the same way, the number above each heat exchanger means the temperature at which the stream leaves the heat exchanger.

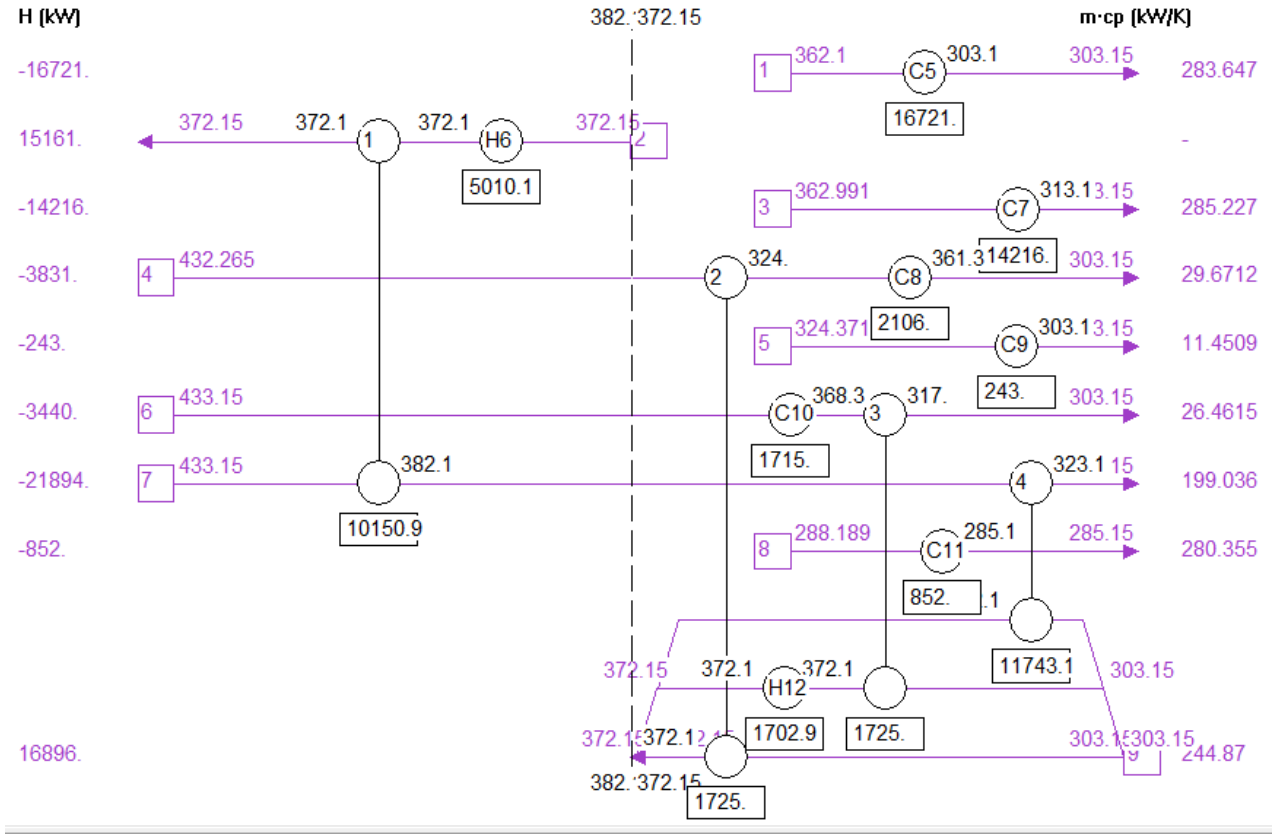


Figure 19. Grid diagram made by HINT software.

As it is shown in Figure 19, for this process the requirements are 4 heat exchangers and 8 utilities (2 heaters and 6 coolers). In total, 12 heat exchangers would be needed, which agrees with Figure 18 about the minimum number of necessary heat exchangers involved.

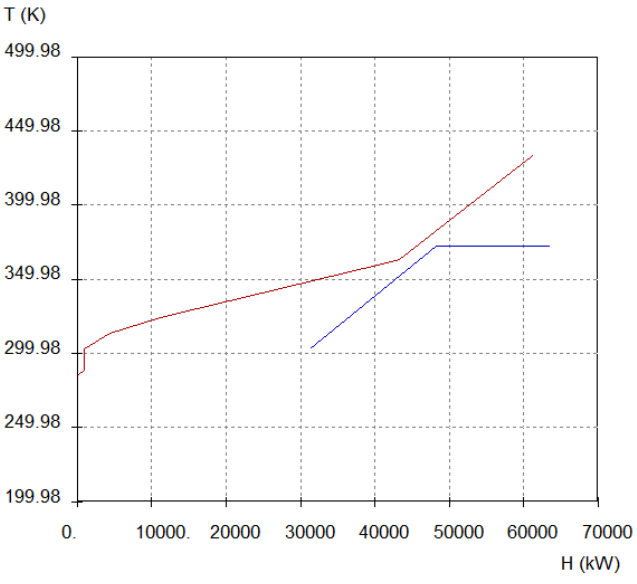


Figure 20. Composite curves of the process.

Composite curve shown in Figure 20 represents temperature (K) vs. enthalpy (kW). Line red refers to the hot composite curve and line blue to the cold composite curve. The point in which both lines get closer at vertical distance is DTmin (10 K). The horizontal distance between the end of hot and cold composite curves means the hot utility (QHmin) and the horizontal distance between the beginning of hot and cold composite curves means the cold utility (QCmin).

3.4 Assumptions

3.4.1 Assumptions from previous simulation.

Due to the lack of data for the pilot plant process, some assumptions were made in the previous simulation. Those assumptions are briefly explained in Table 5:

Table 5. Previous assumptions.

Nr.	Equipment	Assumptions
1	P-101 & P-301	Pump efficiency: 0.8 (isentropic), Diver efficiency: 0.8 (mechanical)
2	K-101, K-102, K-201 & K-202	Pump efficiency: 0.8 (isentropic), Diver efficiency: 0.8 (mechanical)
3	Pressure loss	0.05 bar per device
4	R-101 & R-201	No side reactions HBr as a cocatalyst and the solid catalysts are not considered in the simulation

It was assumed that the isentropic and mechanical efficiencies of the pump were both 0.8 because it is realistic and is often used for pumps. A deviation of this value does not have a significant effect on the process costs. The second pump P-301involved in the crystallization process would have bigger effect because the solution is carrying crystals.

For the compressors, isentropic and mechanical efficiencies of 0.8 were also assumed for the same reasons as for the pump. The difference here is that changing the assumed value to lower efficiencies would have a greater impact on the process costs, since the two compressors K-201 and K-202 should generate a pressure of 49 bar. For pressure losses incurred in the process, a pressure drop of 0.05 bar per unit was assumed. A greater loss of pressure in the process would lead to greater energy consumption of the pump or compressors.

For the material data model, the Wilson method was used, which calculates the thermodynamic correction factor for the calculation of the Fick diffusion coefficients.

The assumptions of R-101 and R-201 reactors are shown in the Figures 21 and 22:

Figure 21. Reaction of R-101 reactor, where operation conditions are 90 °C and 4,95 bar.

Figure 22. Reaction of R-201 reactor, where operation conditions are 160 °C and 49 bar.

The chosen valid phases for both reactors are Vapor-Liquid. The RSTOIC model was used for both and the corresponding reaction equations were deposited with the performance mentioned in the patent [22].

For the reactors it was further assumed that no side reactions take place because the exact course of the reaction with all the secondary reactions is not completely known.

As an additional assumption for the R-201 reactor, the direct addition of an HBr solution was dispensed with since HBr is not consumed and, therefore, does not play a significant role in the costs of the process. However, the initial use of HBr could be taken into account in estimating the cost of solid catalysts.

For the R-101 reactor, instead of the pure oxygen used in the patent, air with a composition of x (oxygen) = 0.2 and x (nitrogen) = 0.8 was used.

3.4.2 Assumptions from new simulation.

Table 6. New assumptions.

Nr.	Equipment	Assumptions
6	Z-301 & Z-302	Liquid phase only Not new crystals formed Solubility data
7	F-301, Z-301 & Z-302	PSD user
8	F-301	
9	T-301	

10	E-401	Amount of MTBE
11	W-XYY & H-XYY	Heat transfer coefficient
12	W-XYY & H-XYY	Cost estimation

For the crystallizers involved in the process, it was supposed that evaporation does not take place because the type of crystallization is cooling.

It was also assumed that during the crystallization process any new crystals appear. As it has been explained in Chapter 3.3.1, the by-product organic acids are significantly effective in annulling adipic acid crystals nucleation, as well as in decreasing the crystal growth rate. For that reason it is possible to cool the solution about 10 °C under the saturation conditions without appreciating any change. No nucleation is evident and supersaturation is released only very slowly on existing crystal surfaces, as it is explained in the patent US 2,813,122 [28]. For that reason, it is reasonable to think that no new crystals appear and the ones that are recycled grow, until they break and create small pieces that are again recycled to the process.

As most of the solution is acetic acid, the solubility data was taken from solubility of adipic acid in acetic acid + water mixtures [36].

The size of crystals, particle size distribution and morphology of the particles depend on crystal growth kinetics, temperature, supersaturation, seeding procedure, stirring speed and other parameters that are varied in crystallization [37]. For that reason and for the lack of crystal growth kinetic parameters for adipic acid, for crystallizer equipment as well as for the centrifuge, the particle size distribution used in simulation was the one that is given in Aspen Plus by default.

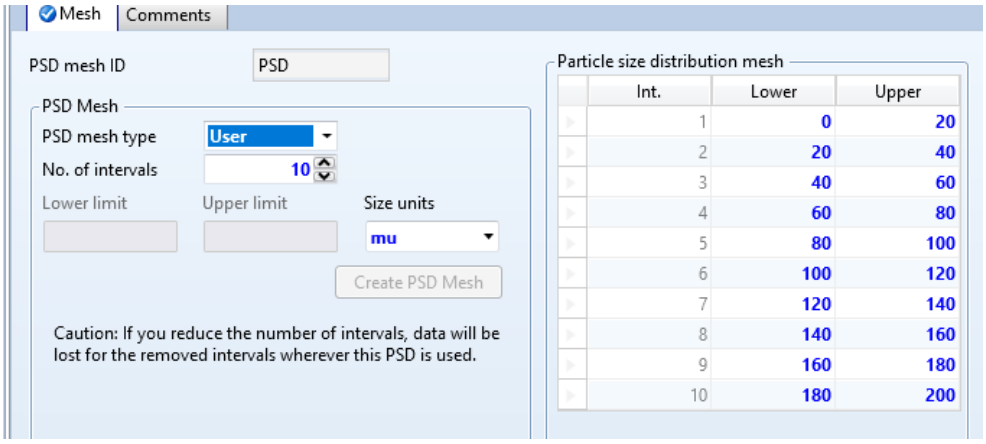


Figure 23. Particle size distribution given by Aspen Plus.

Figure 23 shows the particle size distribution mesh (Simulation → Setup → Solids → PSD

→ Modify the default particle size distribution). Moreover, during the design of the crystallizer PSD from inlet was chosen, as it is shown in Figure 24:

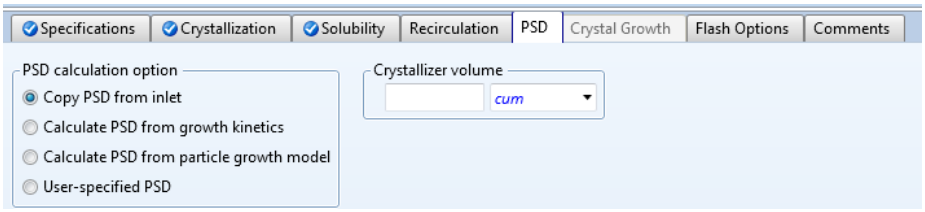


Figure 24. PSD for crystallizer´s design.

The parameters for the centrifuge´s design are shown in Figure 25. A fraction of 0,99 of solids to solid outlet was taken. It was also supposed that the whole output was solid load.

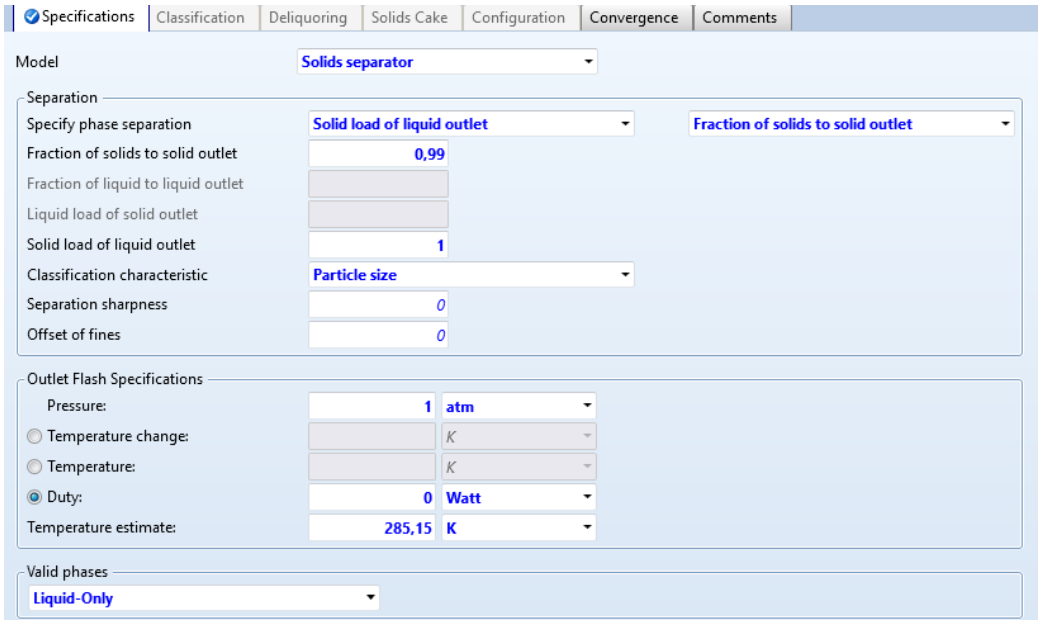


Figure 25. Parameters for centrifuge´s design.

Figure 26 shows the chosen parameters for the dryer:

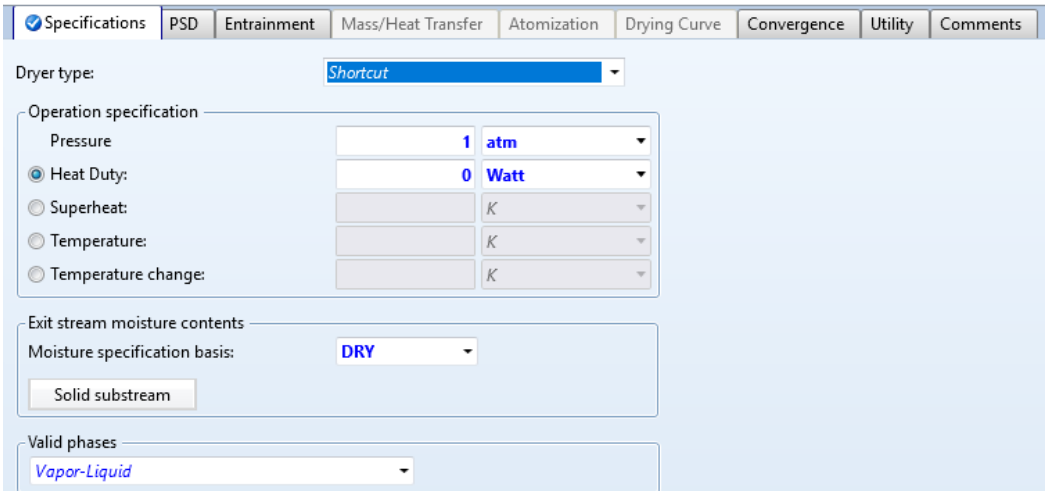


Figure 26. Parameters for dryer´s design.

For the azeotropic distillation system, the amount of MTBE fed into the extraction column was the suitable one in order to keep the proportions from the simulation reference scheme [33].

Table 7 shows the approximated values of the Heat Transfer Coefficient (k) used for each heat exchanger, with the assumption that all of the heat exchangers are tubular [38]:

Table 7. Heat exchanger coefficients [38].

Number of stream	Respective heat exchanger on simulation	Application	Value (kW/m^2K)
1	W-102	Liquids inside and outside tubes	0.525
2	W-103	Liquids inside and outside tubes	0.525
3	W-104	Condensation of organic vapors (phase change)	0.45
4	W-105	Gas at high pressure inside and liquid outside	0.3
5	W-106	Gas at high pressure inside and liquid outside	0.3
6	W-202	Gas at high pressure inside and liquid outside	0.3
7	W-203	Gas at high pressure inside and liquid outside	0.3
8	W-204	Liquids inside and outside tubes	0.525
9	H-301	Liquids inside and outside tubes	0.525

In Chapter 4.2 a cost estimation is presented. It should be noticed that HINT software assumes by default shell and tube heat exchangers. It also assumes that the material of construction is carbon steel and that the operating pressure is 150 psi. All of those parameters can be changed to other type of heat exchangers, different materials and other values of pressure. They can only provide an estimation of the order of magnitude of capital costs.

4 Results and comparisons

From the simulation of the process created in Aspen Plus®, the variable costs of the new improvements of the plant can be estimated based on the quantities of chemicals fed into the process, as well as the costs due to utilities for the energy integration of the plant. plant. The simulation can also be used to create a preliminary list of equipment, which allows estimating the cost of capital. Next, the results that can be obtained from the simulation of the process are presented. The focus is on results, which can be identified as the biggest drivers of costs.

A list of all material flows with the mass flows for all components (mass flows in kg/h), mass fractions, temperature and pressure data of the flows as well as the volume flows (l/s) is attached in the Appendix (Chapter 9). In addition, the complete flow chart of the simulation is shown.

4.1 Streams and utilities

The initial variable costs were analyzed in the previous project of a simulation in Aspen Plus® mentioned in Chapter 3.1 [21]. However, the conclusions will just focus on the improvements of new simulation.

The changed variable costs of the improved adipic acid production plant consist mainly in the energy requirements for the operation of the heat exchange network, but it also consist in the feeding of methyl *tert*-butyl ether, which corresponds to stream 01-MTBE.

As it has been mentioned in Chapter 3.3.2, the amount of MTBE that is fed to the water removal sub-process ($3.08 \cdot 10^5$ kg/s) is not real. The amount of MTBE present in that stream is 24.7 kg/s, which is exactly the same amount that is fed in 01-MTBE stream. That means that there are no loses, which is not realistic. Taking in consideration that the streams 04-P and 01-MTBE are conceived as a pseudo-recycle, it should be necessary to add an additional small amount of MTBE in 01-MTBE stream. Table 8 shows the feeding amount of MTBE necessary to separate successfully the required amounts of this process plant, according to *Kung-Li et. al (2014*) [33].

Table 8. Necessary mass and volume flows for the new part of the process plant.

Stream	Type of stream	Mass flow	Volume flow
01-MTBE	Entrainer	$3.6 \cdot 10^{-5}$ kg/s	$4.1 \cdot 10^{-12}$ cm^3/s

The mass flow can be used for calculating the raw material costs.

In the previous project work, it was also estimated the yield of the process using the Equation 1:

(1) $$Overall\ process\ yield: Y_{k,i} = 1 - \frac{\dot{n}_{i,t} - n_{k,O}}{\dot{n}_{i,t}} \cdot \frac{v_i}{v_k}$$

With a molar flow of adipic acid (k) of 253.44 kmol/h, a molar mass flow of glucose (i) of 258.4 kmol/h and with the stoichiometric coefficients of 1 and -1 respectively, the total yield of the process is 98,1%. The resulting yield is a little bit lower comparing to the overall yield from the previous project work (99.4 %), but more realistic [21].

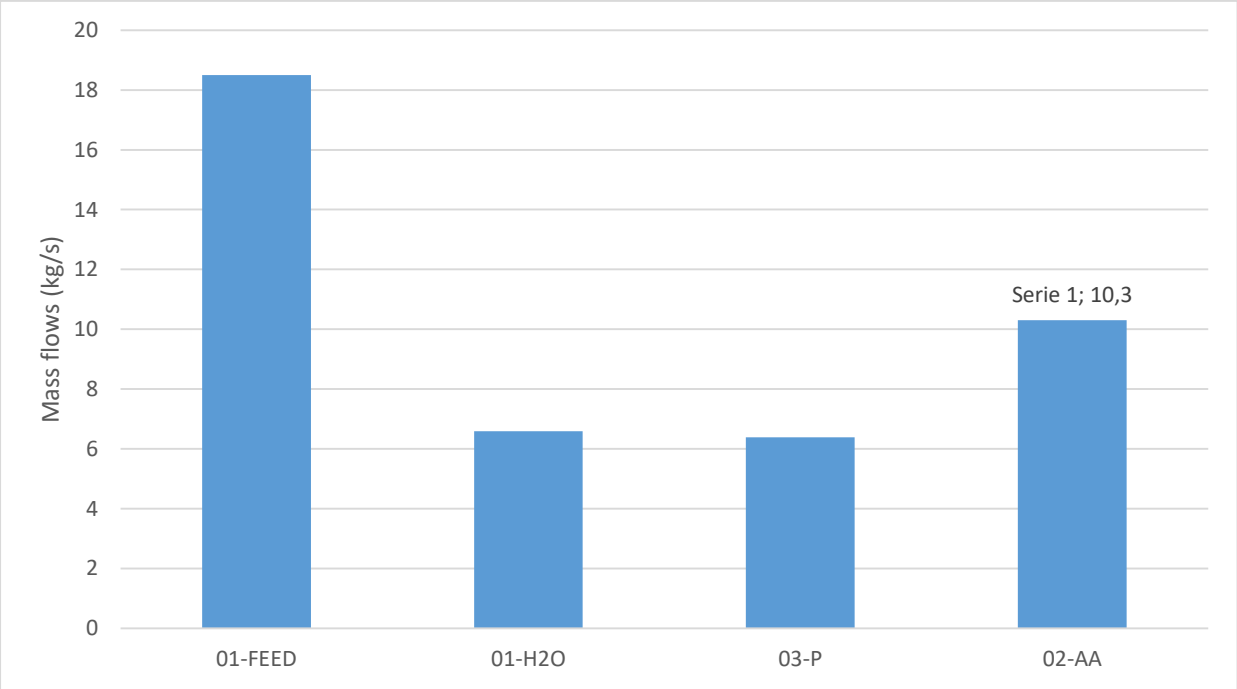


Figure 27. Comparison of the component mass flows of glucose in the input stream 01-FEED and output stream 01-H2O and the glucaric acid in the purge stream 03-P compared with the product mass flow of adipic acid in 02-AA.

In the Figure 27 above, the leakage currents of glucose and glucaric acid are compared with the mass flow of adipic acid and glucose.

		Absolute	Relative consumption per product quantity	
Adipic acid production	324	kt/a		
Feedstocks				
Glucose/dextrose	407	kt/a	1.26	t/t adipic acid
Utilities				
Minimum heating duty	12 418	kW	335 622	kWh/t adipic acid
Minimum cooling duty	852	kW	23 027	kWh/t adipic acid
Electrical power	376.58	MW	10 177.84	MWh/t adipic acid

Figure 28. Absolute and relative to adipic acid consumption of feedstocks and utilities.

Figure 28 shows the absolute consumption of feedstocks and utilities, as well as relative consumption per product quantity of adipic acid. The electrical power has been calculated considering only the power necessary for the columns. The electrical power necessary for the pumps and other units operations such as the crystallizer has a negligible value in comparison with the one mentioned.

Regarding the changed heat exchange integration, some new costs in heating and cooling utilities are necessary. Heating and cooling duties are calculated by HINT software, as it is shown in Figure 28, which would be enough information for a cost estimation. It should be noted that the acquisition costs of the heat exchangers should be taken into account in the next chapter. As it can be noticed, the cooling water and the associate costs (public services) necessary for the production plant are very low.

4.2 Appliances

In the following chapter the costs corresponding to the changed appliances will be analyzed (in the case of heat exchange network) and qualitatively estimated for the new parts of the simulation. As the heat exchange network is totally different from the previous simulation, they will be included as well.

The transferred heat in each heat exchanger and the initial and final temperatures of each

heat exchanger are shown in Figure 29:

H.E.	Heat (kW)	Hot Str.	T1 (K)	T2 (K)	Cold Str.	T1 (K)	T2 (K)	Area (m2)	Cost ($)
1	10150.85	7	433.15	382.15	2	372.15	372.15	1485.4	1.574e+005
2	1724.997	4	382.15	324.013	10	303.15	372.15	611.69	8.67e+004
3	1725.004	6	382.15	316.9609	13	303.15	372.15	765.54	1.007e+005
4	11743.15	7	382.15	323.15	14	311.8884	372.15	4213.1	3.216e+005
5	16721.	1	362.1	303.15	Ut.	-	-	189.15	4.07e+004
6	5010.1	Ut.	-	-	2	372.15	372.15	53.59	1.953e+004
7	14216.	3	362.991	313.15	Ut.	-	-	158.14	3.645e+004
8	2106.	4	432.265	361.2871	Ut.	-	-	20.021	1.21e+004
9	243.	5	324.371	303.15	Ut.	-	-	2.9052	6541
10	1715.	6	433.15	368.339	Ut.	-	-	16.136	1.105e+004
11	852.	8	288.189	285.15	Ut.	-	-	11.128	9569
12	1702.9	Ut.	-	-	15	372.15	372.15	18.215	1.162e+004

Figure 29. Results from the heat exchangers.

As it was mentioned in Chapter 3.3.3, HINT software offers the possibility of checking a cost estimation of the heat exchange network. Those costs have been calculated taking into account the assumptions mentioned in Chapter 3.4.2. It can be easily noticed in Figure 29 that the biggest heat exchangers are the numbers 1, 2, 3 and 4, which means higher amount of heat transferred. Thus, they lead to the higher costs. Those results make sense since they are the only heat exchangers that allows the heat transference between two streams from the plant. Their associate costs of the acquisition are also the biggest, as expected.

In addition to the heat exchangers, the capital costs of the new parts of simulation will be mainly influenced by the price of the columns, the crystallizers, the centrifuge and the rotary dryer. Tables 9 and 10 list the parameters that would be necessary for a cost estimation.

Table 9. Crystallizers parameters.

Designation	Usage	Residence time
Z-301	Adipic acid crystallization	1 h
Z-302	Adipic acid crystallization	1 h

According to the example of adipic acid crystallization given on the Patent US 5,471,001, a normal value for the residence time of the particles could be approximately 1 hour [39]. This value is not totally reliable because there are a lot of factors that affect crystallization, such us supersaturation or mechanical agitation. However, this value can be useful for a cost estimation or the crystallizers that are needed for the plant.

Table 10 shows the necessary parameters for the columns involved in the water removal (acetic acid recovery) section for a cost estimation.

Table 10. Columns parameters.

Designation	Usage	Height	Diameter
C-401 (Distill)		10 m	2.03 m
C-402 (RadFrac)		15 m	13.8 m
C-403 (Distill)		4 m	0.43 m
C-404 (Distill)		20 m	0.58 m
E-401 (Extract)		4 m	0.96 m

The height has been calculated assuming that the distance between stages is 0.5 m. The procedure of the calculation of the columns diameters involves Formulas 2, 3, 4 and 5, and it is shown in the Appendix (Chapter 8).

(2) $$A = \pi r^2$$

(3) $$Pv = nRT$$

(4) $$[f.Factor] = u \cdot \sqrt{\rho}$$

(5) $$Reduced\ [f.Factor] = [f.Factor] \cdot A$$

When the diameter of the column is too high (more than 7-8 m approximately), the equipment in the reality would be substituted for more than one column located in parallel, in order to achieve the required output and simplifying the construction. However, the calculations of the new equipment are not the aim of this project, but only a qualitatively estimation of the costs.

Regarding the centrifuge and the rotary dryer, the necessary parameters would be the dimensions (diameter and height) and the area, respectively. Despite Rennovia patents [23] and other scientific articles [29] mention the centrifuge and dryer, they do not make public the quantitative size data. Although the characteristics of these unit operations suppose a very well-kept secret, those equipments will not be very responsible of the capital costs compering to the columns.

5. Discussion

It was shown the Rennovia process can be carried out on industrial scale with available state-of-the art plant equipment.. An exact evaluation of the economic competitiveness compared to conventional oil-based adipic acid production will require additional work, elucidating the following unknowns:

5.1 Limitations

The side reactions that take place in the reactors R-101 and R-201 could not be taken into account due to the lack of information. Laboratory test and experiments in the pilot plan would be necessary in order to get accurate data about the exact course of the reaction with all side reaction. The effect of those side reactions would be a decrease on the selectivity, but the decrease is not expected to be very remarkable thanks to the recycles on both reactors.

The black box mentioned in Chapter 3.2 refers to T-101 device. It separates the glucaric acid from water and glucose. T-101 is considered a black box because the exact separation is not listed in the patent followed for previous simulation [22]. This has a huge impact on the production simulation plant's cost because it is impossible to estimate energy and capital costs without knowing which unit operations are involved. The other two black boxes (T-201 and T-202) have been replaced for the crystallization section and the acetic acid recovery section, respectively. However, there was not possible to simulate a substitutive section for the first black box (T-101) because the program Aspen Adsorption was necessary, which is a variant of Aspen Plus®. However, that is not the aim of this project. Rennovia Inc. presented a patent in 2013 where it is described an accepted and proved process for the separation at least one mono- or di-carboxylic compound by selective elution from an ion exchange chromatography medium [40].

5 Summary

This project work contains an extensive literature research to get introduced into the context, where bio-based adipic acid production from glucose via Rennovia process has been compared with the conventional processes. From a technical point of view, the installation gains in security. It presents less possibilities of contact with hazardous chemical substances (such us nitric acid). From an environmental point of view, CO_2 emissions are reduced. From an economical point of view, there is an advantage to avoid the exhaustible feedstocks.

The aim of this project work was to complement the previous one, particularly regarding to separation and purification of adipic acid, acetic acid recovery and heat exchange integration network.

For this purpose, some new assumptions were made regarding the crystallization principles (such us solubility data, particle size distribution…), specific parameters or efficiencies of different apparatus, input flows and heat transfer coefficient values for the different heat exchanges (see Chapter 3.4.2).

It is important to remember that in Chapter 3.3.2 (which corresponds to acetic acid recovery section), a pseudo-recycle was used due to numerical convergence problems. However, in the real production plan this would not be necessary.

Chapter 4 shows a qualitatively estimation about the highest cost about the new improvements of the simulation.

Finally, it was concluded that the overall process yield of adipic acid from dextrose (component of glucose used in Aspen Plus® simulation) input is 98.1%, as mentioned in Chapter 4.1.

The simulation shows that the largest single column in terms of diameter is C-402 with approximately 13.8 m, and C-404 the highest column with 20 meters long.

The biggest heat exchanger is expected to be the heat exchanger number 4 (see Table 29 from Chapter 4.2), with a heat exchange area of 4213.1 m^2. The overall heat exchange area is 745.02 m^2.

According to pinch method, the minimum heating duty is 12418 kW and the minimum cooling duty is 852 kW.

6 Perspective

After running the simulation, a well-functioning adipic acid from glucose production plant was proven. However, there was no enough time at the end of the project to make a detailed cost estimation based on the power and equipment used. However, the required parameters can be found in Aspen Plus® simulation.

Industries such as automotive, electronics and footwear are a key driving factor of adipic acid consumption in China and India. Asia has recently been the biggest consumer of adipic acid with more than 35 % of the market in 2013. Moreover, it is expected an increase of 5.3 % between 2014 and 2020. In Europe it is also expected a growth in consumption of about 4.2 % in that period [41].

Nowadays, the main manufacturers of adipic acid are BASF, Rhodia, and INVISTA and Ascend Performance Materials. All of them together accounted 60 % of the manufacture. Rennovia Inc., was the first company using this innovative chemo-catalytic process [40].

Rennovia's bio-based adipic acid process has proven to be a potentially competitive alternative to the conventional process. In a future, there should be taken in consideration new patent publications of Rennovia.

7 References

[1] Ed de Jong, Adrian Higson, Patrick Walsch & Maria Wellisch (2012): *"Product developments in the bio-based quemicals arena".*

[2] Harold A. Wittcoff, Bryan G. Reuben & Jeffery S. Plotkin (2013): *"Industrial organic chemicals"*.

[3] Education.afpm.org: *"What is a cracker and why should I care?"*. [http://education.afpm.org/petrochemicals/what-is-a-cracker-and-why-should-i-care/].

[4] Judith Becker, Anna Lange, Jonathan Fabarius & ChristophWittmann (2015): *"Top value platform chemicals: bio-based production of organic acids"*.

[5] ICIS Chemical Business (2011): *"European chemical profile: Adipic acid"*. [https://www.icis.com/resources/news/2011/02/28/9439026/european-chemical-profile-adipic-acid/].

[6] Adipic Acid – The Chemical Company. [https://thechemco.com/chemical/adipic-acid/].

[7] Tino Polen, Markus Spelberg & Michael Bott (2013): *"Toward biotechnological production of adipic acid and precursors from biorenewables"*.

[8] National Institute of Environmental Health Sciences (1994): *"Environmental Health Perspectives"*. [https://ehp.niehs.nih.gov/wp-content/uploads/103/6/ehp.95103564.pdf].

[9] Online Trade Magazine: *"Crude oil's impact on renewable energy: energy alternative or energy staple?"*. [https://www.altenergymag.com/article/2015/06/crude-oil%E2%80%99s-impact-on-renewable-energy-energy-alternative-or-energy-staple/20384/].

[10] Rennovia Inc. [http://www.rennovia.com/].

[11] Rolf Beerthuis , Gadi Rothenberg & N. Raveendran Shiju (2014): *"Catalytic routes towards acrylic acid, adipic acid and ε-caprolactam starting from biorenewables".*

[12] Gary M. Diamond, Vince Murphy & Thomas R. Boussie (2014): "*Modern Applications of High Throug hput R&D in Heterogeneous Catalysis".* Chapter 8: "*Application of High Throughput Experimentation to the Production of Commodity Chemicals from Renewable Feedstocks".*

[13] Fabrizio Cavani et al: "*Chemicals and fuels from bio-based building blocks".* Chapter 6 (Thomas R. Boussie, Gary M. Diamond, Eric Dias & Vince Murphy: "*Synthesis of adipic acid*

starting from renewable raw materials".

[14] Robin Jastrzebski, Emily J. van den Berg, Bert M. Weckhuysen & Pieter C. A. Bruijnincx (2015): "*Sustainable production of d dimethyl adipate by non-heme iron(III) catalysed oxidative cleavage of catechol*".

[15] Easy Biology Class: *"Indrustrial fermentation process: batch, fed-batch and continuous fermentation".* [http://www.easybiologyclass.com/industrial-fermentation-process-batch-fed-batch-and-continuous-fermentation/]

[16] Niu W1, Draths KM & Frost JW (2002): *"Benzene-free synthesis of adipic acid".*

[17] Stijn Van de Vyver & Yuriy Román-Leshkov (2013): *"Emerging catalytic processes for the production of adipic acid".*

[18] Johnson Matthey & Rennovia (2015): *"Johnson Matthey process technologies and Rennovia announce on time start-up of mini-plant for bio-based glucaric acid production using jointly developed technology".*

[19] Doris de Guzman (2013): *"Rennovia produces 100% bio-based nylon".* Green chemicals blog. [/]

[20] Intratec Solutions (2017): "*Technology Profile: Bio-based Adipic Acid Production from Glucose"*. [http://www.chemengonline.com/bio-based-adipic-acid-production-from-glucose/].

[21] Martina Amend & Jonathan Pamer (2017): *"Fakultät Angewandte Chemie Prozess Design: Adipinsäure aus Glucose nach Rennovia-Verfahren".*

[22] T.Boussie, E.Dias, Z.Fresco, V.Murphy, J.Shoemaker, R.Archer & H. Jiang (2015): *"Production of adipic acid and derivates from carbohydrate-containing materials".* Rennovia Inc., Santa Clara, CA (US) 2015 (US 9,434,709 B2).

[23] Johannes C. fioeterhroelr, Geleeu & Renter J. L. Graif (1963): *"Three step crystallization of adipic acid".* Stamicarbon N.V., Heerlen, Netherlands 1957 (US3,096,369).

[24] Cristalización: introducción. [http://www.uap.edu.pe/intranet/fac/material/24/20102BT240224218240104021/20102BT240224218240104021215 91.pdf].

[25] William B. Clark & Robert E. Gee (1953): *"Adipic acid crystallization".* Willmington, Del., US 2,813,122.

[26] Melt crystallization & hydraulic wash column: *"Crystallization"*. [http://www.soliqz.com/crystallization/]

[27] Slide player: *"What is a solution?"* [http://slideplayer.com/slide/8659041/].

[28] Nucleación. [https://cv3.sim.ucm.es/wiki/site/curriculo-3313-1/Nucleaci%C3%B3n@2.html].

[29] Michael Tuttle Musser (2005): *"Adipic acid"*. E.I. DuPont de Nemours & Co., Sabine River Laboratory, Orange, Texas 77631, United States.

[30] Chemindustrial Systems, Inc.: *"Hydrocyclone frequently asked questions"*. [https://hydrocyclone.com/faq.htm].

[31] Hafiz Muhammad Irfan Anwar (2011): *"Simulation of solid processes by Aspen Plus"*. Master thesis in chemical and process engineering.

[32] Lloyd Berg (1992): *"Dehydration of acetic acid by azeotropic distillation"*. Lloyd Berg, Bozeman, Mont., US 5,160,412.

[33] Kung-Ling Li, I-Lung Chien & Cheng-Liang Chen (2014): *"Design and optimization of acetic acid dehydration processes"*.

[34] Ángel Martín & Fidel A. Mato (2007): *"Hint: an educational software for heat exchanger network design with the pinch mehtod"*. Elsevier.

[35] Pinch technology: basics for the beginners. The chemical engineers' resource page. [*http://pages.mtu.edu/~jwsuther/erdm/pinchtech.pdf*].

[36] Binwei Shen et al. (2013): *"Solubilities of adipic acid in acetic acid + water mixtures and acetic acid + cyclohexane mixtures"*. Journal of chemical & engineering data.

[37] Ralf Beck & Jens-Petter Andreassen (2011): *"Influence of crystallization conditions on crystal morphology and size of $CaCO_3$ and their effect on pressure filtration"*.

[38] Overall heat transfer coefficient table charts and equation [*https://www.engineersedge.com/thermodynamics/overall_heat_transfer-table.htm*].

[39] Howard W. Anderson et at (1995): *"Crystallization of adipic acid"*. E. I. Du Pont de Nemours and Company. US 5,471,001.

[40] Raymon Archer et. al (2013): *"Process for the separation of mono- and di-carboxylic acid*

compounds". Rennovia Inc., Menlo Park, CA (US). US 2013/0345473.

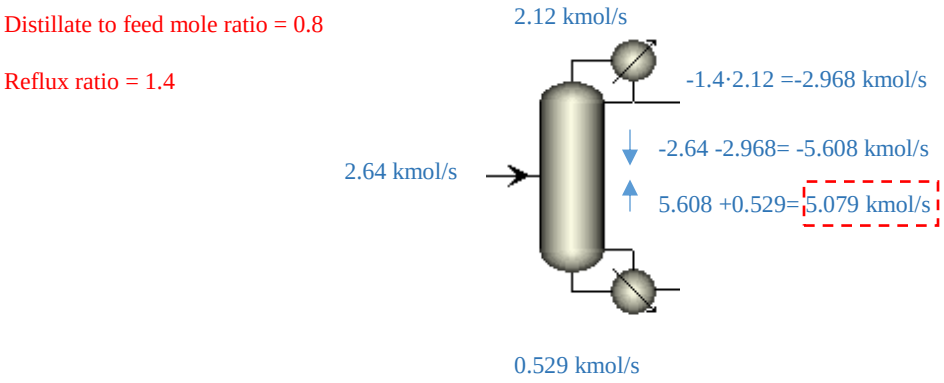
[41] Grand view research (2013): *"Adipic acid market analysis by application (nylon 6,6 fiber, nylon 6,6 resin, polyurethane, adipate ester) and segment forecasts to 2020"*. [https://www.grandviewresearch.com/industry-analysis/adipic-acid-market].

[42] Johannes Rauber: *"Design practice for packed liquid-liquid extraction column".* [http://folk.ntnu.no/skoge/prost/proceedings/aiche-2006/data/papers/P73337.pdf].

8 Appendix

For the calculation of the columns diameters it has been assumed that the $[f.Factor]$ is equal to 1:

- **C-401 (Distill)**



According to the hydraulics profile of C-402 (RadFrac) column in Aspen Plus®, the molecular weight can be assumed to be constant along the column. The gas flow going through column C-401 is 5.079 kmol/s, and it will have approximately the same molecular weight than at the bottom of the column:

$$M = \frac{Mass\ flow}{Mole\ flow} = \frac{150\ kg/s}{0.529\ kmol/s} = 283.55\ g/mol$$

For the density calculation, the temperature will be taken from the bottom of the column because the mole flow of gas is bigger at the bottom:

$$Pv = nRT \rightarrow Pv = \frac{m}{M}RT \rightarrow \rho = \frac{PM}{RT} = \frac{1 \cdot 283.55}{0.082 \cdot 392.952} = 8.8\frac{g}{L} = 8800\ g/m^3$$

According to formula 4 (see Chapter 4.2) and to the assumption mentioned before:

$$[f.Factor] = 1 = u \cdot \sqrt{\rho} \rightarrow u = \frac{1}{\sqrt{8800}} = 0.011\ m/s$$

Considering the volume flow at the bottom of the column:

$$\dot{v} = u \cdot A \rightarrow A = \frac{0.035}{0.011} = 3.182\ m^2$$

$$A = \pi r^2 \rightarrow r = \sqrt{\frac{3.182}{\pi}} = 1.013\ m \rightarrow D = 2.03\ m$$

- **C-402 (RadFrac)**

The maximum reduced f-Factor's value has been taken from the hydraulics profile of C-402 in Aspen Plus®.

$$Reduced\ [f.Factor] = [f.Factor] \cdot A$$

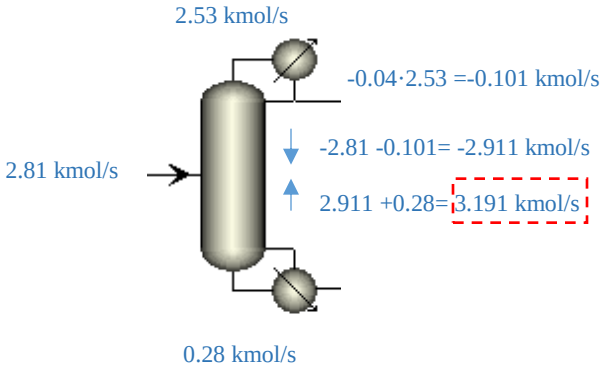
$$A = \frac{149.778 \frac{\sqrt{kgm^3}}{s}}{1\sqrt{\frac{kg}{m}}\frac{1}{s}} = 149.778\ m^2$$

$$A = \pi r^2 \rightarrow r = \sqrt{\frac{149.778}{\pi}} = 6.9\ m \rightarrow D = 13.8\ m$$

- **C-403 (Distill)**

Distillate to feed mole ratio = 0.9

Reflux ratio = 0.04



Following the same procedure as in C-401:

$$M = \frac{Mass\ flow}{Mole\ flow} = \frac{5.267\ kg/s}{0.281\ kmol/s} = 18.74\ g/mol$$

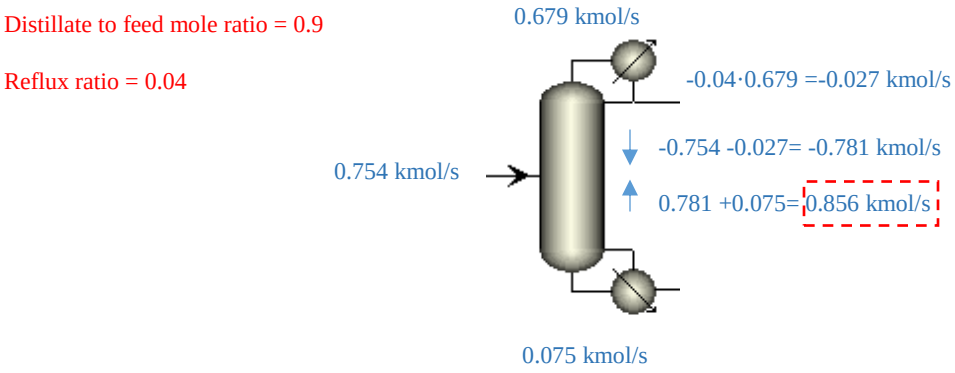
$$Pv = nRT \rightarrow Pv = \frac{m}{M}RT \rightarrow \rho = \frac{PM}{RT} = \frac{1 \cdot 18.74}{0.082 \cdot 375.551} = 0{,}609\frac{g}{L} = 609\ g/m^3$$

$$[f.Factor] = 1 = u \cdot \sqrt{\rho} \rightarrow u = \frac{1}{\sqrt{609}} = 0.041\ m/s$$

$$\dot{v} = u \cdot A \rightarrow A = \frac{0.006}{0.041} = 0.146\ m^2$$

$$A = \pi r^2 \rightarrow r = \sqrt{\frac{0.146}{\pi}} = 0.216\ m \rightarrow D = 0{,}43\ m$$

- **C-404 (Distill)**



Following the same procedure as in C-401:

$$M = \frac{Mass\ flow}{Mole\ flow} = \frac{4.528\ kg/s}{0.075\ kmol/s} = 60.37\ g/mol$$

$$Pv = nRT \rightarrow Pv = \frac{m}{M}RT \rightarrow \rho = \frac{PM}{RT} = \frac{1 \cdot 60.37}{0.082 \cdot 395.899} = 1.860\frac{g}{L} = 1860\ g/m^3$$

$$[f.Factor] = 1 = u \cdot \sqrt{\rho} \rightarrow u = \frac{1}{\sqrt{1860}} = 0.023\ m/s$$

$$\dot{v} = u \cdot A \rightarrow A = \frac{0.005}{0.023} = 0.217\ m^2$$

$$A = \pi r^2 \rightarrow r = \sqrt{\frac{0.217}{\pi}} = 0.263\ m \rightarrow D = 0{,}58\ m$$

- **E-401 (Extract)**

The extraction column separates mainly MTBE from water. The density different is big: 740 kg/m^3 and 997 kg/m^3, respectively. For liquid-liquid extraction columns with high density difference, it can be assumed a capacity of flooding of 70 m^3/m^2/h [42].

$$A = \frac{Liquid\ flow\ input}{Flooding\ capacity} = \frac{50}{70} = 0.714\ m^2$$

$$A = \pi r^2 \rightarrow r = \sqrt{\frac{0.714}{\pi}} = 0.48\ m \rightarrow D = 0{,}96\ m$$

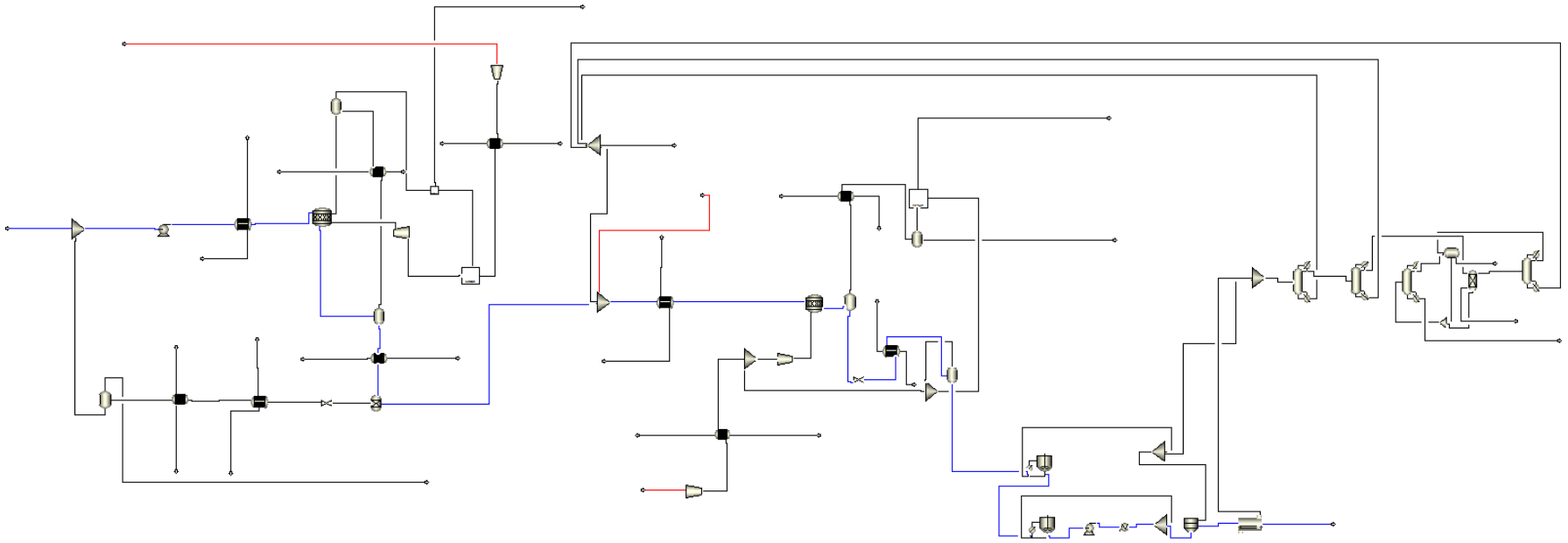


Figure 30. Representation of the complete process plant including the main stream in blue and the input streams of air acetic acid and air in red.

Table 11. List of all material flows – part 1.

Stream Name	Units	01-AA	01-AIR	01-FEED	01-GAS	01-H2	01-H2O	01-HD	01-KD	01-MTBE	01-P	01-R	01-S	02-AA
From		F-301			G-101		G-103		W-101		G-203	TRENN01	M-101	T-301
To		T-301	K-102	M-101	W-105	K-201		W-101		E-401		V-101	P-101	
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	2,85E+02	2,93E+02	2,93E+02	3,63E+02	2,93E+02	3,73E+02	4,25E+02	4,25E+02	3,13E+02	3,03E+02	3,03E+02	3,56E+02	2,85E+02
Pressure	N/sqm	1,01E+05	1,00E+05	1,00E+05	4,90E+05	3,00E+06	1,00E+05	5,00E+05	5,00E+05	1,01E+05	4,00E+06	4,90E+05	1,00E+05	1,01E+05
Molar Vapor Fraction		0,00E+00	1,00E+00	0,00E+00	1,00E+00	1,00E+00	1,00E+00	1,00E+00	9,83E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Enthalpy	J/kg	-8,22E+06	-5,11E+03	-9,73E+06	-1,15E+06	-7,26E+04	-1,33E+07	-1,32E+07	-1,32E+07	-4,48E+06	-8,57E+06	-1,48E+07	-1,32E+07	-6,83E+06
Mass Entropy	J/kg-K	-4,33E+03	1,31E+02	-7,19E+03	-2,80E+02	-1,42E+04	-2,03E+03	-2,52E+03	-2,61E+03	-6,62E+03	-4,27E+03	-8,67E+03	-7,52E+03	-6,07E+03
Mass Density	kg/cum	1,10E+03	1,18E+00	1,14E+03	4,38E+00	2,48E+00	5,81E-01	2,55E+00	2,59E+00	8,08E+02	1,04E+03	1,01E+03	1,00E+03	1,36E+03
Enthalpy Flow	Watt	-1,32E+09	-1,47E+05	-1,80E+08	-6,45E+07	-5,73E+04	-8,75E+07	-3,66E+04	-3,67E+04	-1,38E+08	-1,75E+07	-8,71E+08	-9,32E+08	-7,03E+07
Average MW		5,90E+01	2,88E+01	4,87E+01	2,70E+01	2,02E+00	1,80E+01	1,80E+01	1,80E+01	7,88E+01	5,21E+01	2,01E+01	2,40E+01	1,46E+02
Mole Flows	kmol/sec	2,71E+00	1,00E+00	3,79E-01	2,07E+00	3,92E-01	3,66E-01	1,54E-04	1,54E-04	3,91E-01	3,93E-02	2,92E+00	2,94E+00	7,04E-02
Mass Flows	kg/sec	1,60E+02	2,88E+01	1,85E+01	5,58E+01	7,90E-01	6,59E+00	2,78E-03	2,78E-03	3,08E+01	2,04E+00	5,87E+01	7,06E+01	1,03E+01
OXYGE-01	kg/sec	0,00E+00	6,40E+00	0,00E+00	5,91E+00	0,00E+00	2,74E-04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,74E-04	8,49E-09	0,00E+00
WATER	kg/sec	5,16E+00	0,00E+00	5,54E+00	5,10E+00	0,00E+00	6,59E+00	2,78E-03	2,78E-03	2,34E-01	1,35E-01	5,20E+01	5,10E+01	0,00E+00
HYDRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	7,90E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,10E-17	0,00E+00	0,00E+00	0,00E+00
GLUCARAC	kg/sec	1,85E+00	0,00E+00	0,00E+00	1,63E-09	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,91E-08	0,00E+00	0,00E+00	0,00E+00
DEXTR-01	kg/sec	0,00E+00	0,00E+00	1,29E+01	4,38E-09	0,00E+00	1,79E-08	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,66E+00	1,96E+01	0,00E+00
NITRO-01	kg/sec	0,00E+00	2,24E+01	0,00E+00	4,48E+01	0,00E+00	1,14E-04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,14E-04	1,76E-10	0,00E+00
ADIPI-01	kg/sec	3,24E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,48E-03	0,00E+00	0,00E+00	0,00E+00
ACETI-01	kg/sec	1,40E+02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	5,85E+00	1,91E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-02	kg/sec	1,03E+01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,03E+01
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,47E+01	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Fractions														
OXYGE-01		0,00E+00	2,22E-01	0,00E+00	1,06E-01	0,00E+00	4,17E-05	0,00E+00	0,00E+00	0,00E+00	0,00E+00	4,68E-06	1,20E-10	0,00E+00
WATER		3,22E-02	0,00E+00	3,00E-01	9,14E-02	0,00E+00	1,00E+00	1,00E+00	1,00E+00	7,60E-03	6,60E-02	8,86E-01	7,22E-01	0,00E+00
HYDRO-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	5,40E-18	0,00E+00	0,00E+00	0,00E+00
GLUCARAC		1,16E-02	0,00E+00	0,00E+00	2,93E-11	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,42E-08	0,00E+00	0,00E+00	0,00E+00
DEXTR-01		0,00E+00	0,00E+00	7,00E-01	7,85E-11	0,00E+00	2,72E-09	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,14E-01	2,78E-01	0,00E+00
NITRO-01		0,00E+00	7,78E-01	0,00E+00	8,03E-01	0,00E+00	1,73E-05	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,94E-06	2,49E-12	0,00E+00
ADIPI-01		2,02E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	7,25E-04	0,00E+00	0,00E+00	0,00E+00
ACETI-01		8,72E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,90E-01	9,33E-01	0,00E+00	0,00E+00	0,00E+00
ADIPI-02		6,42E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E+00
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	8,02E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Volume Flow	cum/sec	1,46E-01	2,44E+01	1,62E-02	1,27E+01	3,18E-01	1,13E+01	1,09E-03	1,07E-03	3,81E-02	1,97E-03	5,79E-02	7,03E-02	7,54E-03

Table 12. List of all material flows – part 2.

Stream Name	Units	02-AIR	02-FEED	02-GAS	02-H2	02-H2O	02-HD	02-KD	02-P	02-R	02-S	03-AIR	03-GAS	03-H2
From		K-102		W-105	K-201	C-403		W-102	S-202	V-101	P-101	W-106	G-102	W-202
To		W-106	M-201	G-102	W-202		W-102			W-103	W-101	M-102	ROX	M-202
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	4,32E+02	2,93E+02	3,13E+02	3,24E+02	3,76E+02	2,93E+02	3,11E+02	3,03E+02	3,03E+02	3,56E+02	3,03E+02	3,13E+02	3,03E+02
Pressure	N/sqm	3,15E+05	1,00E+05	4,90E+05	4,00E+06	1,09E+05	1,00E+05	1,00E+05	4,00E+06	1,00E+05	5,10E+05	3,15E+05	4,80E+05	4,00E+06
Molar Vapor Fraction		1,00E+00	0,00E+00	8,76E-01	1,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E+00	0,00E+00	0,00E+00	1,00E+00	0,00E+00	1,00E+00
Mass Enthalpy	J/kg	1,38E+05	-8,06E+06	-1,41E+06	3,80E+05	-1,51E+07	-1,59E+07	-1,58E+07	-7,77E+04	-1,48E+07	-1,32E+07	5,11E+03	-1,58E+07	7,26E+04
Mass Entropy	J/kg-K	1,99E+02	-4,02E+03	-1,02E+03	-1,39E+04	-7,81E+03	-9,14E+03	-8,89E+03	-1,47E+04	-8,67E+03	-7,52E+03	-1,66E+02	-8,86E+03	-1,49E+04
Mass Density	kg/cum	2,53E+00	1,08E+03	5,80E+00	2,99E+00	9,12E+02	9,99E+02	9,82E+02	3,26E+00	1,01E+03	1,00E+03	3,60E+00	9,80E+02	3,20E+00
Enthalpy Flow	Watt	3,98E+06	-8,96E+07	-7,87E+07	3,00E+05	-7,95E+07	-3,53E+09	-3,51E+09	-1,69E+04	-8,71E+08	-9,31E+08	1,47E+05	-7,28E+07	5,73E+04
Average MW		2,88E+01	6,01E+01	2,70E+01	2,02E+00	1,88E+01	1,80E+01	1,80E+01	2,05E+00	2,01E+01	2,40E+01	2,88E+01	1,80E+01	2,02E+00
Mole Flows	kmol/sec	1,00E+00	1,85E-01	2,07E+00	3,92E-01	2,81E-01	1,23E+01	1,23E+01	1,06E-01	2,92E+00	2,94E+00	1,00E+00	2,56E-01	3,92E-01
Mass Flows	kg/sec	2,88E+01	1,11E+01	5,58E+01	7,90E-01	5,27E+00	2,22E+02	2,22E+02	2,18E-01	5,87E+01	7,06E+01	2,88E+01	4,61E+00	7,90E-01
OXYGE-01	kg/sec	6,40E+00	0,00E+00	5,91E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,74E-04	8,49E-09	6,40E+00	1,79E-04	0,00E+00
WATER	kg/sec	0,00E+00	0,00E+00	5,10E+00	0,00E+00	4,97E+00	2,22E+02	2,22E+02	3,85E-04	5,20E+01	5,10E+01	0,00E+00	4,61E+00	0,00E+00
HYDRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	7,90E-01	0,00E+00	0,00E+00	0,00E+00	2,14E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	7,90E-01
GLUCARAC	kg/sec	0,00E+00	0,00E+00	1,63E-09	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,75E-23	0,00E+00	0,00E+00	0,00E+00	1,63E-09	0,00E+00
DEXTR-01	kg/sec	0,00E+00	0,00E+00	4,38E-09	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,66E+00	1,96E+01	0,00E+00	4,38E-09	0,00E+00
NITRO-01	kg/sec	2,24E+01	0,00E+00	4,48E+01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,14E-04	1,76E-10	2,24E+01	1,19E-04	0,00E+00
ADIPI-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	7,44E-09	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ACETI-01	kg/sec	0,00E+00	1,11E+01	0,00E+00	0,00E+00	2,98E-01	0,00E+00	0,00E+00	3,52E-03	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-02	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Fractions														
OXYGE-01		2,22E-01	0,00E+00	1,06E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	4,68E-06	1,20E-10	2,22E-01	3,90E-05	0,00E+00
WATER		0,00E+00	0,00E+00	9,14E-02	0,00E+00	9,43E-01	1,00E+00	1,00E+00	1,77E-03	8,86E-01	7,22E-01	0,00E+00	1,00E+00	0,00E+00
HYDRO-01		0,00E+00	0,00E+00	0,00E+00	1,00E+00	0,00E+00	0,00E+00	0,00E+00	9,82E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E+00
GLUCARAC		0,00E+00	0,00E+00	2,93E-11	0,00E+00	0,00E+00	0,00E+00	0,00E+00	8,02E-23	0,00E+00	0,00E+00	0,00E+00	3,55E-10	0,00E+00
DEXTR-01		0,00E+00	0,00E+00	7,85E-11	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,14E-01	2,78E-01	0,00E+00	9,51E-10	0,00E+00
NITRO-01		7,78E-01	0,00E+00	8,03E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,94E-06	2,49E-12	7,78E-01	2,58E-05	0,00E+00
ADIPI-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	3,41E-08	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ACETI-01		0,00E+00	1,00E+00	0,00E+00	0,00E+00	5,66E-02	0,00E+00	0,00E+00	1,61E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-02		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Volume Flow	cum/sec	1,14E+01	1,03E-02	9,63E+00	2,64E-01	5,77E-03	2,22E-01	2,26E-01	6,70E-02	5,79E-02	7,03E-02	8,00E+00	4,70E-03	2,47E-01

Table 13. List of all material flows – part 3.

Stream Name	Units	03-HD	03-KD	03-P	03-R	03-S	04-AIR	04-GAS	04-H2	04-HD	04-KD	04-P	04-R	04-S
From		H-101	W-103	S-201	W-103	S-101	S-101	G-102	M-202		W-104	D-401	W-104	ROX
To		W-103			W-104			S-101	K-202	W-104			G-103	G-101
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	3,83E+02	3,73E+02	3,91E+02	3,72E+02	3,56E+02	3,13E+02	3,13E+02	3,03E+02	5,23E+02	5,23E+02	3,13E+02	3,73E+02	3,63E+02
Pressure	N/sqm	1,00E+05	1,00E+05	1,01E+05	1,00E+05	5,05E+05	4,75E+05	4,80E+05	4,00E+06	4,00E+06	4,00E+06	1,01E+05	1,00E+05	4,95E+05
Molar Vapor Fraction		1,00E+00	1,11E-01	7,05E-04	1,20E-04	0,00E+00	1,00E+00	1,00E+00	1,00E+00	1,00E+00	1,08E-01	0,00E+00	1,25E-01	4,08E-01
Mass Enthalpy	J/kg	-1,33E+07	-1,53E+07	-7,93E+06	-1,46E+07	-1,32E+07	-1,15E+05	-1,15E+05	-6,29E+03	-1,30E+07	-1,45E+07	-4,78E+06	-1,43E+07	-8,03E+06
Mass Entropy	J/kg-K	-1,98E+03	-7,44E+03	-3,98E+03	-7,79E+03	-7,52E+03	-3,08E+02	-3,11E+02	-1,48E+04	-3,07E+03	-6,04E+03	-6,39E+03	-7,10E+03	-4,28E+03
Mass Density	kg/cum	5,66E-01	5,22E+00	7,07E+02	8,04E+02	1,00E+03	5,16E+00	5,21E+00	3,23E+00	1,66E+01	1,29E+02	8,28E+02	5,15E+00	1,02E+01
Enthalpy Flow	Watt	-1,10E+08	-1,27E+08	-5,06E+07	-8,54E+08	-9,31E+08	-2,94E+06	-5,88E+06	-1,05E+04	-1,27E+08	-1,42E+08	-1,60E+08	-8,39E+08	-1,04E+09
Average MW		1,80E+01	1,80E+01	6,13E+01	2,01E+01	2,40E+01	2,83E+01	2,83E+01	2,03E+00	1,80E+01	1,80E+01	7,66E+01	2,01E+01	2,56E+01
Mole Flows	kmol/sec	4,61E-01	4,61E-01	1,04E-01	2,92E+00	2,94E+00	9,06E-01	1,81E+00	8,17E-01	5,41E-01	5,41E-01	4,38E-01	2,92E+00	5,06E+00
Mass Flows	kg/sec	8,31E+00	8,31E+00	6,39E+00	5,87E+01	7,06E+01	2,56E+01	5,12E+01	1,66E+00	9,75E+00	9,75E+00	3,36E+01	5,87E+01	1,30E+02
OXYGE-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	2,74E-04	8,49E-09	2,95E+00	5,91E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,74E-04	5,91E+00
WATER	kg/sec	8,31E+00	8,31E+00	6,95E-03	5,20E+01	5,10E+01	2,49E-01	4,97E-01	1,54E-03	9,75E+00	9,75E+00	2,64E-01	5,20E+01	5,71E+01
HYDRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,65E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC	kg/sec	0,00E+00	0,00E+00	8,34E-02	0,00E+00	0,00E+00	1,02E-22	2,04E-22	6,99E-23	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,51E+01
DEXTR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	6,66E+00	1,96E+01	4,36E-21	8,72E-21	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,66E+00	6,66E+00
NITRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	1,14E-04	1,76E-10	2,24E+01	4,48E+01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,14E-04	4,48E+01
ADIPI-01	kg/sec	0,00E+00	0,00E+00	1,46E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,98E-08	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ACETI-01	kg/sec	0,00E+00	0,00E+00	6,15E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,41E-02	0,00E+00	0,00E+00	8,59E+00	0,00E+00	0,00E+00
ADIPI-02	kg/sec	0,00E+00	0,00E+00	9,35E-04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,47E+01	0,00E+00	0,00E+00
Mass Fractions														
OXYGE-01		0,00E+00	0,00E+00	0,00E+00	4,68E-06	1,20E-10	1,15E-01	1,15E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	4,68E-06	4,56E-02
WATER		1,00E+00	1,00E+00	1,09E-03	8,86E-01	7,22E-01	9,71E-03	9,71E-03	9,27E-04	1,00E+00	1,00E+00	7,86E-03	8,86E-01	4,41E-01
HYDRO-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	9,91E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC		0,00E+00	0,00E+00	1,31E-02	0,00E+00	0,00E+00	3,99E-24	3,99E-24	4,21E-23	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,16E-01
DEXTR-01		0,00E+00	0,00E+00	0,00E+00	1,14E-01	2,78E-01	1,70E-22	1,70E-22	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,14E-01	5,14E-02
NITRO-01		0,00E+00	0,00E+00	0,00E+00	1,94E-06	2,49E-12	8,75E-01	8,75E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,94E-06	3,46E-01
ADIPI-01		0,00E+00	0,00E+00	2,28E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,79E-08	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ACETI-01		0,00E+00	0,00E+00	9,63E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	8,47E-03	0,00E+00	0,00E+00	2,56E-01	0,00E+00	0,00E+00
ADIPI-02		0,00E+00	0,00E+00	1,46E-04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	7,36E-01	0,00E+00	0,00E+00
Volume Flow	cum/sec	1,47E+01	1,59E+00	9,03E-03	7,30E-02	7,03E-02	4,96E+00	9,82E+00	5,15E-01	5,89E-01	7,54E-02	4,05E-02	1,14E+01	1,27E+01

Table 14. List of all material flows – part 4.

Stream Name	Units	05-GAS	05-H2	05-HD	05-KD	05-R	05-S	06-GAS	06-HD	06-KD	06-R	06-S	07-GAS	07-HD
From		S-101	K-202		W-105	G-103	G-101	M-102		W-106	S-301	W-102	K-101	
To		M-102	RHYD	W-105		M-101	W-102	K-101	W-106		Z-302	TRENN01	ROX	W-201
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	3,13E+02	3,26E+02	2,93E+02	3,13E+02	3,73E+02	3,63E+02	3,08E+02	2,93E+02	3,13E+02	2,85E+02	3,03E+02	3,63E+02	4,25E+02
Pressure	N/sqm	4,75E+05	4,90E+06	1,00E+05	1,00E+05	1,00E+05	4,90E+05	3,10E+05	1,00E+05	1,00E+05	1,01E+05	4,90E+05	5,00E+05	5,00E+05
Molar Vapor Fraction		1,00E+00	1,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,00E+00	1,00E+00
Mass Enthalpy	J/kg	-1,15E+05	3,17E+05	-1,59E+07	-1,58E+07	-1,44E+07	-1,32E+07	-5,13E+04	-1,59E+07	-1,58E+07	-8,22E+06	-1,35E+07	5,99E+03	-1,32E+07
Mass Entropy	J/kg-K	-3,08E+02	-1,46E+04	-9,14E+03	-8,86E+03	-7,74E+03	-7,30E+03	-1,67E+02	-9,14E+03	-8,85E+03	-4,33E+03	-8,00E+03	-1,35E+02	-2,52E+03
Mass Density	kg/cum	5,16E+00	3,68E+00	9,99E+02	9,80E+02	9,48E+02	1,00E+03	3,46E+00	9,99E+02	9,79E+02	1,10E+03	1,06E+03	4,73E+00	2,55E+00
Enthalpy Flow	Watt	-2,94E+06	5,27E+05	-2,65E+09	-2,63E+09	-7,52E+08	-9,77E+08	-2,79E+06	-7,06E+08	-7,02E+08	-3,30E+08	-9,94E+08	3,26E+05	-3,66E+04
Average MW		2,83E+01	2,03E+00	1,80E+01	1,80E+01	2,04E+01	2,46E+01	2,86E+01	1,80E+01	1,80E+01	5,91E+01	2,46E+01	2,86E+01	1,80E+01
Mole Flows	kmol/sec	9,06E-01	8,17E-01	9,25E+00	9,25E+00	2,56E+00	3,00E+00	1,91E+00	2,47E+00	2,47E+00	6,79E-01	3,00E+00	1,91E+00	1,54E-04
Mass Flows	kg/sec	2,56E+01	1,66E+00	1,67E+02	1,67E+02	5,21E+01	7,38E+01	5,44E+01	4,44E+01	4,44E+01	4,01E+01	7,38E+01	5,44E+01	2,78E-03
OXYGE-01	kg/sec	2,95E+00	0,00E+00	0,00E+00	0,00E+00	8,49E-09	2,74E-04	9,35E+00	0,00E+00	0,00E+00	0,00E+00	2,74E-04	9,35E+00	0,00E+00
WATER	kg/sec	2,49E-01	1,54E-03	1,67E+02	1,67E+02	4,54E+01	5,20E+01	2,49E-01	4,44E+01	4,44E+01	1,29E+00	5,20E+01	2,49E-01	2,78E-03
HYDRO-01	kg/sec	0,00E+00	1,65E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC	kg/sec	1,02E-22	6,99E-23	0,00E+00	0,00E+00	0,00E+00	1,51E+01	1,02E-22	0,00E+00	0,00E+00	4,64E-01	1,51E+01	1,02E-22	0,00E+00
DEXTR-01	kg/sec	4,36E-21	0,00E+00	0,00E+00	0,00E+00	6,66E+00	6,66E+00	4,36E-21	0,00E+00	0,00E+00	0,00E+00	6,66E+00	4,36E-21	0,00E+00
NITRO-01	kg/sec	2,24E+01	0,00E+00	0,00E+00	0,00E+00	1,76E-10	1,14E-04	4,48E+01	0,00E+00	0,00E+00	0,00E+00	1,14E-04	4,48E+01	0,00E+00
ADIPI-01	kg/sec	0,00E+00	2,98E-08	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	8,09E-01	0,00E+00	0,00E+00	0,00E+00
ACETI-01	kg/sec	0,00E+00	1,41E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	3,49E+01	0,00E+00	0,00E+00	0,00E+00
ADIPI-02	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,60E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Fractions														
OXYGE-01		1,15E-01	0,00E+00	0,00E+00	0,00E+00	1,63E-10	3,72E-06	1,72E-01	0,00E+00	0,00E+00	0,00E+00	3,72E-06	1,72E-01	0,00E+00
WATER		9,71E-03	9,27E-04	1,00E+00	1,00E+00	8,72E-01	7,05E-01	4,57E-03	1,00E+00	1,00E+00	3,22E-02	7,05E-01	4,57E-03	1,00E+00
HYDRO-01		0,00E+00	9,91E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC		3,99E-24	4,21E-23	0,00E+00	0,00E+00	0,00E+00	2,04E-01	1,88E-24	0,00E+00	0,00E+00	1,16E-02	2,04E-01	1,88E-24	0,00E+00
DEXTR-01		1,70E-22	0,00E+00	0,00E+00	0,00E+00	1,28E-01	9,03E-02	8,01E-23	0,00E+00	0,00E+00	0,00E+00	9,03E-02	8,01E-23	0,00E+00
NITRO-01		8,75E-01	0,00E+00	0,00E+00	0,00E+00	3,38E-12	1,55E-06	8,24E-01	0,00E+00	0,00E+00	0,00E+00	1,55E-06	8,24E-01	0,00E+00
ADIPI-01		0,00E+00	1,79E-08	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,02E-02	0,00E+00	0,00E+00	0,00E+00
ACETI-01		0,00E+00	8,47E-03	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	8,71E-01	0,00E+00	0,00E+00	0,00E+00
ADIPI-02		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,47E-02	0,00E+00	0,00E+00	0,00E+00
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Volume Flow	cum/sec	4,96E+00	4,51E-01	1,67E-01	1,70E-01	5,50E-02	7,36E-02	1,57E+01	4,45E-02	4,54E-02	3,66E-02	6,93E-02	1,15E+01	1,09E-03

Table 15. List of all material flows – part 5.

Stream Name	Units	07-KD	07-R	07-S	08-GAS	08-HD	08-KD	08-R	08-S	09-GAS	09-HD	09-KD	09-R	09-S
From		W-201	S-302	TRENN01	G-201		W-202	S-201	M-201	W-203		W-203	C-401	W-201
To			Z-301	M-201	W-203	W-202		M-201	W-201	G-203	W-203		S-201	RHYD
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	4,25E+02	2,85E+02	3,03E+02	4,33E+02	2,93E+02	3,14E+02	3,91E+02	3,68E+02	3,03E+02	2,93E+02	3,01E+02	3,93E+02	3,68E+02
Pressure	N/sqm	5,00E+05	1,01E+05	4,90E+05	4,90E+06	1,00E+05	1,00E+05	1,01E+05	1,00E+05	4,90E+06	1,00E+05	1,00E+05	1,01E+05	1,00E+05
Molar Vapor Fraction		9,83E-01	0,00E+00	0,00E+00	1,00E+00	0,00E+00	0,00E+00	7,05E-04	0,00E+00	9,31E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Enthalpy	J/kg	-1,32E+07	-7,57E+06	-8,10E+06	-4,52E+06	-1,59E+07	-1,58E+07	-7,93E+06	-7,95E+06	-5,61E+06	-1,59E+07	-1,59E+07	-7,81E+06	-7,95E+06
Mass Entropy	J/kg-K	-2,61E+03	-5,14E+03	-5,58E+03	-5,38E+03	-9,14E+03	-8,85E+03	-3,98E+03	-4,09E+03	-8,18E+03	-9,14E+03	-9,03E+03	-4,09E+03	-4,09E+03
Mass Density	kg/cum	2,59E+00	1,21E+03	3,71E+03	7,47E+00	9,99E+02	9,79E+02	7,07E+02	1,04E+03	1,14E+01	9,99E+02	9,92E+02	9,96E+02	1,04E+03
Enthalpy Flow	Watt	-3,67E+04	-1,26E+06	-1,22E+08	-1,42E+07	-4,41E+07	-4,39E+07	-1,07E+09	-1,29E+09	-1,76E+07	-1,68E+09	-1,67E+09	-2,73E+08	-1,29E+09
Average MW		1,80E+01	8,17E+01	2,10E+02	5,49E+00	1,80E+01	1,80E+01	6,13E+01	6,55E+01	5,49E+00	1,80E+01	1,80E+01	6,62E+01	6,55E+01
Mole Flows	kmol/sec	1,54E-04	2,03E-03	7,18E-02	5,71E-01	1,54E-01	1,54E-01	2,21E+00	2,47E+00	5,71E-01	5,86E+00	5,86E+00	5,29E-01	2,47E+00
Mass Flows	kg/sec	2,78E-03	1,66E-01	1,51E+01	3,13E+00	2,78E+00	2,78E+00	1,36E+02	1,62E+02	3,13E+00	1,06E+02	1,06E+02	3,50E+01	1,62E+02
OXYGE-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
WATER	kg/sec	2,78E-03	2,86E-03	0,00E+00	1,37E-01	2,78E+00	2,78E+00	1,48E-01	1,48E-01	1,37E-01	1,06E+02	1,06E+02	1,38E-03	1,48E-01
HYDRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	1,07E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,07E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC	kg/sec	0,00E+00	1,03E-03	1,51E+01	2,91E-08	0,00E+00	0,00E+00	1,77E+00	1,69E+01	2,91E-08	0,00E+00	0,00E+00	1,85E+00	1,69E+01
DEXTR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
NITRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-01	kg/sec	0,00E+00	1,79E-03	0,00E+00	1,48E-03	0,00E+00	0,00E+00	3,09E+00	3,09E+00	1,48E-03	0,00E+00	0,00E+00	3,24E+00	3,09E+00
ACETI-01	kg/sec	0,00E+00	7,74E-02	0,00E+00	1,93E+00	0,00E+00	0,00E+00	1,31E+02	1,42E+02	1,93E+00	0,00E+00	0,00E+00	2,99E+01	1,42E+02
ADIPI-02	kg/sec	0,00E+00	8,31E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,98E-02	1,98E-02	0,00E+00	0,00E+00	0,00E+00	2,08E-02	1,98E-02
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Fractions														
OXYGE-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
WATER		1,00E+00	1,72E-02	0,00E+00	4,37E-02	1,00E+00	1,00E+00	1,09E-03	9,12E-04	4,37E-02	1,00E+00	1,00E+00	3,94E-05	9,12E-04
HYDRO-01		0,00E+00	0,00E+00	0,00E+00	3,42E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	3,42E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC		0,00E+00	6,18E-03	1,00E+00	9,27E-09	0,00E+00	0,00E+00	1,31E-02	1,04E-01	9,27E-09	0,00E+00	0,00E+00	5,30E-02	1,04E-01
DEXTR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
NITRO-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-01		0,00E+00	1,08E-02	0,00E+00	4,73E-04	0,00E+00	0,00E+00	2,28E-02	1,91E-02	4,73E-04	0,00E+00	0,00E+00	9,25E-02	1,91E-02
ACETI-01		0,00E+00	4,66E-01	0,00E+00	6,14E-01	0,00E+00	0,00E+00	9,63E-01	8,76E-01	6,14E-01	0,00E+00	0,00E+00	8,54E-01	8,76E-01
ADIPI-02		0,00E+00	5,00E-01	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,46E-04	1,23E-04	0,00E+00	0,00E+00	0,00E+00	5,94E-04	1,23E-04
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Volume Flow	cum/sec	1,07E-03	1,38E-04	4,06E-03	4,20E-01	2,78E-03	2,84E-03	1,92E-01	1,56E-01	2,75E-01	1,06E-01	1,06E-01	3,51E-02	1,56E-01

Table 16. List of all material flows – part 6.

Stream Name	Units	10-GAS	10-HD	10-KD	10-R	10-S	11-R	11-S	12-GAS	12-R	12-S	13-GAS	13-R	13-S	14-S
From		S-202		W-204	C-402	RHYD	C-404	G-201	M-203	C-403	V-201	T-301	C-404	W-204	G-202
To		M-203	W-204		S-201	G-201	D-401	V-201	M-202	D-401	W-204	M-401	S-201	G-202	Z-301
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	3,03E+02	2,93E+02	3,09E+02	3,91E+02	4,33E+02	3,33E+02	4,33E+02	3,03E+02	3,31E+02	4,33E+02	2,85E+02	3,96E+02	3,23E+02	3,23E+02
Pressure	N/sqm	4,00E+06	1,00E+05	1,00E+05	1,01E+05	4,90E+06	1,01E+05	4,90E+06	4,00E+06	1,01E+05	5,00E+05	1,01E+05	1,18E+05	5,00E+05	1,00E+05
Molar Vapor Fraction		1,00E+00	0,00E+00	0,00E+00	0,00E+00	1,74E-01	0,00E+00	0,00E+00	1,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Enthalpy	J/kg	-7,77E+04	-1,59E+07	-1,58E+07	-7,97E+06	-7,95E+06	-6,32E+06	-8,02E+06	-7,77E+04	-1,50E+07	-8,02E+06	-8,31E+06	-7,95E+06	-8,16E+06	-8,16E+06
Mass Entropy	J/kg-K	-1,47E+04	-9,14E+03	-8,92E+03	-3,95E+03	-4,08E+03	-6,52E+03	-4,06E+03	-1,47E+04	-8,49E+03	-4,06E+03	-4,21E+03	-3,94E+03	-4,25E+03	-4,25E+03
Mass Density	kg/cum	3,26E+00	9,99E+02	9,84E+02	9,44E+02	2,73E+02	8,29E+02	8,99E+02	3,26E+00	9,49E+02	8,99E+02	1,08E+03	9,38E+02	1,05E+03	1,05E+03
Enthalpy Flow	Watt	-6,78E+04	-5,30E+09	-5,27E+09	-8,16E+08	-1,30E+09	-2,25E+08	-1,29E+09	-6,78E+04	-7,17E+08	-1,29E+09	-1,25E+09	-3,60E+07	-1,31E+09	-1,31E+09
Average MW		2,05E+00	1,80E+01	1,80E+01	5,98E+01	4,97E+01	5,25E+01	5,90E+01	2,05E+00	1,89E+01	5,90E+01	5,67E+01	6,01E+01	5,90E+01	5,90E+01
Mole Flows	kmol/sec	4,25E-01	1,85E+01	1,85E+01	1,71E+00	3,29E+00	6,79E-01	2,71E+00	4,25E-01	2,53E+00	2,71E+00	2,64E+00	7,54E-02	2,71E+00	2,71E+00
Mass Flows	kg/sec	8,72E-01	3,33E+02	3,33E+02	1,02E+02	1,63E+02	3,56E+01	1,60E+02	8,72E-01	4,78E+01	1,60E+02	1,50E+02	4,53E+00	1,60E+02	1,60E+02
OXYGE-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
WATER	kg/sec	1,54E-03	3,33E+02	3,33E+02	1,53E-01	5,29E+00	5,21E+00	5,16E+00	1,54E-03	4,49E+01	5,16E+00	5,16E+00	1,13E-06	5,16E+00	5,16E+00
HYDRO-01	kg/sec	8,57E-01	0,00E+00	0,00E+00	0,00E+00	1,07E+00	0,00E+00	5,09E-20	8,57E-01	0,00E+00	5,09E-20	0,00E+00	0,00E+00	5,09E-20	0,00E+00
GLUCARAC	kg/sec	6,99E-23	0,00E+00	0,00E+00	0,00E+00	1,85E+00	0,00E+00	1,85E+00	6,99E-23	0,00E+00	1,85E+00	1,85E+00	0,00E+00	1,85E+00	1,85E+00
DEXTR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
NITRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-01	kg/sec	2,98E-08	0,00E+00	0,00E+00	0,00E+00	1,35E+01	0,00E+00	1,35E+01	2,98E-08	0,00E+00	1,35E+01	3,24E+00	0,00E+00	1,35E+01	1,35E+01
ACETI-01	kg/sec	1,41E-02	0,00E+00	0,00E+00	1,02E+02	1,42E+02	8,28E+00	1,40E+02	1,41E-02	3,06E-01	1,40E+02	1,40E+02	4,53E+00	1,40E+02	1,40E+02
ADIPI-02	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,98E-02	0,00E+00	1,98E-02	0,00E+00	0,00E+00	1,98E-02	0,00E+00	0,00E+00	1,98E-02	1,98E-02
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,22E+01	0,00E+00	0,00E+00	2,55E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Fractions															
OXYGE-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
WATER		1,77E-03	1,00E+00	1,00E+00	1,50E-03	3,24E-02	1,46E-01	3,22E-02	1,77E-03	9,40E-01	3,22E-02	3,44E-02	2,49E-07	3,22E-02	3,22E-02
HYDRO-01		9,82E-01	0,00E+00	0,00E+00	0,00E+00	6,55E-03	0,00E+00	3,18E-22	9,82E-01	0,00E+00	3,18E-22	0,00E+00	0,00E+00	3,18E-22	0,00E+00
GLUCARAC		8,02E-23	0,00E+00	0,00E+00	0,00E+00	1,13E-02	0,00E+00	1,16E-02	8,02E-23	0,00E+00	1,16E-02	1,24E-02	0,00E+00	1,16E-02	1,16E-02
DEXTR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
NITRO-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-01		3,41E-08	0,00E+00	0,00E+00	0,00E+00	8,27E-02	0,00E+00	8,44E-02	3,41E-08	0,00E+00	8,44E-02	2,16E-02	0,00E+00	8,44E-02	8,44E-02
ACETI-01		1,61E-02	0,00E+00	0,00E+00	9,99E-01	8,67E-01	2,32E-01	8,72E-01	1,61E-02	6,41E-03	8,72E-01	9,32E-01	1,00E+00	8,72E-01	8,72E-01
ADIPI-02		0,00E+00	0,00E+00	0,00E+00	0,00E+00	1,21E-04	0,00E+00	1,24E-04	0,00E+00	0,00E+00	1,24E-04	0,00E+00	0,00E+00	1,24E-04	1,24E-04
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	6,21E-01	0,00E+00	0,00E+00	5,34E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Volume Flow	cum/sec	2,68E-01	3,34E-01	3,39E-01	1,08E-01	5,98E-01	4,30E-02	1,78E-01	2,68E-01	5,03E-02	1,78E-01	1,39E-01	4,83E-03	1,53E-01	1,53E-01

Table 17. List of all material flows – part 7.

Stream Name	Units	15-S	16-S	17-S	18-S	19-S	20-S	21-S	22-S	23-S	24-S	25-S	26-S	27-S	28-S
From		Z-301	Z-302	P-301	H-301	S-301	F-301	S-302	M-401	C-401	C-402	E-401	E-401	D-401	M-402
To		Z-302	P-301	H-301	S-301	F-301	S-302	M-401	C-401	C-402	E-401	C-404	M-402	M-402	C-403
Stream Class		MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD	MIXCIPSD
Temperature	K	2,95E+02	2,88E+02	2,88E+02	2,85E+02	2,85E+02	2,85E+02	2,85E+02	2,85E+02	3,88E+02	3,77E+02	3,34E+02	3,13E+02	3,13E+02	3,12E+02
Pressure	N/sqm	1,01E+05	1,01E+05	1,51E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05	1,01E+05
Molar Vapor Fraction		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
Mass Enthalpy	J/kg	-8,20E+06	-8,21E+06	-8,21E+06	-8,22E+06	-8,22E+06	-7,57E+06	-7,57E+06	-8,31E+06	-8,30E+06	-1,10E+07	-6,51E+06	-4,48E+06	-1,58E+07	-1,51E+07
Mass Entropy	J/kg-K	-4,32E+03	-4,33E+03	-4,33E+03	-4,33E+03	-4,33E+03	-5,14E+03	-5,14E+03	-4,21E+03	-4,07E+03	-5,42E+03	-6,20E+03	-6,62E+03	-8,86E+03	-8,71E+03
Mass Density	kg/cum	1,08E+03	1,09E+03	1,09E+03	1,10E+03	1,10E+03	1,21E+03	1,21E+03	1,08E+03	9,33E+02	8,95E+02	8,44E+02	8,08E+02	9,92E+02	9,69E+02
Enthalpy Flow	Watt	-1,32E+09	-1,65E+09	-1,65E+09	-1,65E+09	-1,32E+09	-1,57E+06	-3,15E+05	-1,25E+09	-9,54E+08	-1,38E+08	-2,61E+08	-1,42E+07	-7,88E+08	-8,02E+08
Average MW		5,91E+01	5,91E+01	5,91E+01	5,91E+01	5,91E+01	8,17E+01	8,17E+01	5,67E+01	5,44E+01	3,11E+01	5,33E+01	7,88E+01	1,80E+01	1,89E+01
Mole Flows	kmol/sec	2,72E+00	3,40E+00	3,40E+00	3,40E+00	2,72E+00	2,54E-03	5,08E-04	2,64E+00	2,12E+00	4,04E-01	7,54E-01	4,04E-02	2,77E+00	2,81E+00
Mass Flows	kg/sec	1,60E+02	2,01E+02	2,01E+02	2,01E+02	1,60E+02	2,08E-01	4,15E-02	1,50E+02	1,15E+02	1,26E+01	4,02E+01	3,18E+00	4,99E+01	5,30E+01
OXYGE-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
WATER	kg/sec	5,16E+00	6,45E+00	6,45E+00	6,45E+00	5,16E+00	3,57E-03	7,14E-04	5,16E+00	5,15E+00	5,00E+00	5,21E+00	2,42E-02	4,99E+01	4,99E+01
HYDRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC	kg/sec	1,85E+00	2,32E+00	2,32E+00	2,32E+00	1,85E+00	1,28E-03	2,57E-04	1,85E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
DEXTR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
NITRO-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-01	kg/sec	6,36E+00	4,05E+00	4,05E+00	4,05E+00	3,24E+00	2,24E-03	4,48E-04	3,24E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ACETI-01	kg/sec	1,40E+02	1,75E+02	1,75E+02	1,75E+02	1,40E+02	9,68E-02	1,94E-02	1,40E+02	1,10E+02	7,56E+00	1,28E+01	6,04E-01	0,00E+00	6,04E-01
ADIPI-02	kg/sec	7,27E+00	1,30E+01	1,30E+01	1,30E+01	1,04E+01	1,04E-01	2,08E-02	2,08E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01	kg/sec	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	2,22E+01	2,55E+00	0,00E+00	2,55E+00
Mass Fractions															
OXYGE-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
WATER		3,22E-02	3,22E-02	3,22E-02	3,22E-02	3,22E-02	1,72E-02	1,72E-02	3,44E-02	4,48E-02	3,98E-01	1,30E-01	7,60E-03	1,00E+00	9,40E-01
HYDRO-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
GLUCARAC		1,16E-02	1,16E-02	1,16E-02	1,16E-02	1,16E-02	6,18E-03	6,18E-03	1,24E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
DEXTR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
NITRO-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ADIPI-01		3,96E-02	2,02E-02	2,02E-02	2,02E-02	2,02E-02	1,08E-02	1,08E-02	2,16E-02	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ACETI-01		8,71E-01	8,71E-01	8,71E-01	8,71E-01	8,71E-01	4,66E-01	4,66E-01	9,32E-01	9,55E-01	6,02E-01	3,19E-01	1,90E-01	0,00E+00	1,14E-02
ADIPI-02		4,53E-02	6,47E-02	6,47E-02	6,47E-02	6,47E-02	5,00E-01	5,00E-01	1,39E-04	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
ISOPR-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00
METHY-01		0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	0,00E+00	5,51E-01	8,02E-01	0,00E+00	4,81E-02
Volume Flow	cum/sec	1,48E-01	1,84E-01	1,84E-01	1,83E-01	1,46E-01	1,72E-04	3,44E-05	1,39E-01	1,23E-01	1,40E-02	4,76E-02	3,93E-03	5,02E-02	5,47E-02