



# **Treball Final de Grau**

**Etherification of furfuryl alcohol to butyl levulinate using ion-exchange resins**

**Eterificació de l'alcohol furfurílic a levulinat de butil utilitzant resines d'intercanvi iònic**

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*Si tú no trabajas por tus sueños, alguien te contratará para que trabajes por los suyos.*

Steve Jobs

M'agradaria agrair al meu tutor Roger Bringué, pel seu suport total en el treball, sobretot en el procés experimental, demostrant una elevada paciència en els problemes que han anat sorgint.

A més, altres persones m'han donat consells i ajuda quan les necessitava. Per aquesta raó i l'amabilitat que han provat tenir, són dignes de menció els companys de laboratori Rodrigo, Jordi and Ravi.

Finalment, apreciar els ànims que els meus pares m'han donat durant tot el projecte i la carrera, així com a cada pas que he decidit donar a la meva vida.



**REPORT**





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## 1. SUMMARY

The objective of this research is the study of the synthesis reaction of butyl levulinate (BL) from furfuryl alcohol (FA) and 1-butanol (BUT) by using commercial ion-exchange resins as catalysts. There's two stages in the reaction: a conversion of FA to 2-(butoxymethyl)furan (Bmf) and the production of BL from the intermediate mentioned. The main drawback of this reaction is the polymerization of FA, producing some insoluble substances as oligomeric products, for example, 5-5-dibutoxy-2-pentanone (DBPent), resulting in a drop of selectivity.

During the last years, the production of BL is being investigated, since interest in the use of lignocellulosic biomass for the production of chemicals, fuel or energy increases at the same time that global awareness do about fuels resource depletion and the environmental impact causes to carry out some industrial processes. So the search for an effective and economical process for obtaining this product without bringing about severe changes in the environment is imperative.

The project will work at a temperature of 100°C using different types of ion-exchange resins (macroreticulars and gel-type resins) to carry out a comparison of the selectivity, conversion and yield obtained with the use of each of them and give possible explanations of observed facts through their individual characteristics (degree of crosslinking, acid capacity and DVB percentage). To see the reaction rates varying the catalysts, representations of the evolution of Bmf and BL moles produced will be realized.

The effect of the temperature in the reaction is studied too, carrying out the reaction at temperatures among 80 °C and 110 °C. Finally, two different initial molar ratio are used to see the effect of this parameter along the reaction course.

**Keywords:** butyl levulinate, furfuryl alcohol, ion-exchange resins, etherification.



## 2. RESUM

L'objectiu d'aquesta investigació és l'estudi de la reacció de síntesi de levulinat de butil (BL) a partir d'alcohol furfúric (FA) i 1-butanol (BUT) mitjançant l'ús de resines d'intercanvi iònic comercials com a catalitzadors. Hi ha dues etapes en la reacció: una conversió de FA de 2-(butoximetil)furan (BMF) i la producció de BL a partir de l'intermedi esmentat. El principal inconvenient d'aquesta reacció és la polimerització de FA, produint algunes substàncies insolubles com productes oligomèrics com, per exemple, 5-5-dibutoxi-2-pentanona (DBPent), resultant en un descens de la selectivitat.

Durant els últims anys, s'està investigant la producció de BL, ja que actualment l'interès en la utilització de biomassa lignocel·lulòsica per a la producció de químics, gasolina o energia augmenta al mateix temps que la conscienciació global tant en l'esgotament de recursos en combustibles fòssils com en l'impacte ambiental que es provoca al portar a terme segons quins processos industrials. Llavors, la recerca d'un procés econòmic i efectiu per a la obtenció d'aquest producte sense provocar greus canvis en el medi ambient és imperatiu.

El projecte treballarà a una temperatura de 100 °C per mitjà de diferents tipus de resines d'intercanvi iònic (macroreticulars i resines de tipus gel) per dur a terme una comparació de la selectivitat, conversió i el rendiment obtingut amb l'ús de cada un d'ells i donar possibles explicacions dels fets observats a través de les seves característiques individuals (grau de reticulació, capacitat d'àcid i el percentatge de DVB). Per veure les diferents velocitats de reacció que varien amb cada catalitzador, es realitzaran representacions de l'evolució dels mols de Bmf i BL produïts.

L'efecte de la temperatura en la reacció es va estudiar també, duent a terme la reacció a temperatures entre 80 °C i 110 °C. Finalment, dos relacions molars inicials diferents s'han utilitzat per veure l'efecte d'aquest paràmetre al llarg del curs de la reacció.

**Paraules clau:** levulinat de butil, alcohol furfúric, resina d'intercanvi iònic, eterificació.



## 3. INTRODUCTION

### 3.1. USING BIOMASS TO PRODUCE CHEMICALS

Declining reserves of fossil resources and increasing environmental damage caused by their use (such as the increase of global warming) has encouraged investigating new energy sources. Ago, fossil energy sources were used because of its abundance and low cost, but the environmental concerns and population increase make that source unsustainable, rising prices and forcing to find a renewable source. Biomass-derived carbohydrates are abundant (nature produces over 150 billion tonnes of biomass per year by photosynthesis, with only 3-4% used by humans for food and non-food purposes) and of a reasonable price. Therefore, this type of renewable energy source is earning importance, making investigators research for such converting this type of material in chemicals used to produce gasoline or other products on an industrial scale.

Biomass allows the production of different platform chemicals, which are capable of reacting to become other compounds of interest for use in many applications. Furthermore, in contrast to other renewable energy resources, biomass is the only renewable resource of fixed coal, which is essential for the production of liquid hydrocarbon fuels and chemicals.

On the available biomass sources, the most important is lignocellulose, which is mainly composed of lignin, cellulose and hemicellulose. Lignin is a three-dimensional polymer formed of methoxylated phenylpropane structures (because of that fact is why lignin is regarded as source of aromatic molecules). Cellulose and hemicellulose are polymers composed of glucose or different carbohydrate units, respectively, and a depolymeration process of them gives sugars (xylose, mannose, glucose) from non-edible and widely available renewable sources. Sugars and derivatives are of wide applicability due to their variety of use and transformation to important commodity or platform chemicals, just like furans or sorbitol, used nowadays to produce alkyl levulinates.

Nowadays, research is focused on trying to find the most suitable path reaction to produce alkyl levulinates on an industrial scale. That is, the starting compounds to be used must be available on an industrial scale at an economical price and the reaction route must be as short as

possible. There are two approaches in the conversion of biomass, the thermochemical and the biochemical processes, being the first normally chosen. In the context of this study levulinic acid is produced from biomass, to be used, then, to produce levulinic esters and use them as gasoline and diesel additives.

These levulinic esters are suitable candidates as additives to biodiesel transportation fuels. Moreover, those bio-based chemicals are not toxic, of a high lubricity, with a stable point of flammability and with good conditions of low temperature flow, enabling the replacement of current chemicals produced from petro-chemical routes for these alkyl levulinates.

Another important aspect about this type of organic compounds is their versatility, because of the different possible uses that can be given, for example, as a condiment, plastic agent, fragrance or substrate for different types of reaction (such as condensation or addition to an ester or keto group).

For all these reasons mentioned above, biodiesel fuel is a good candidate as blender for petroleum diesel fuel, as well as having other properties such as biodegradability, miscibility with petroleum diesel, increased lubricity, high flash point and it reduces emissions of particulate matter, unburned hydrocarbons and CO-upconditions during fully warmed.

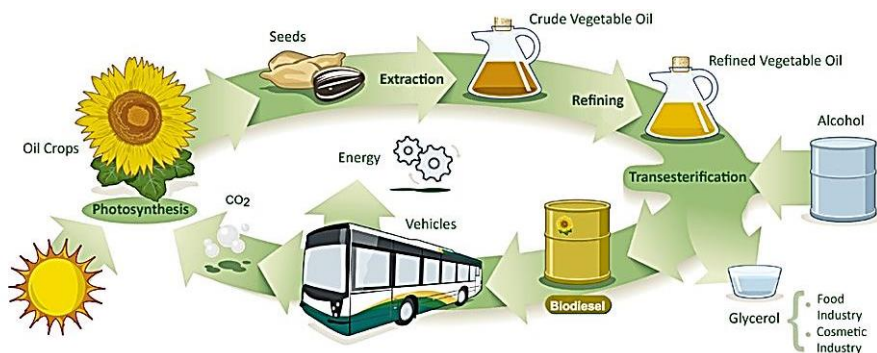


Figure 1. Biodiesel cycle.



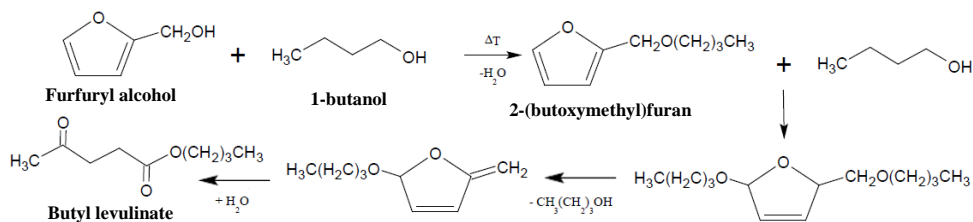
### 3.2. SOME REACTION ROUTES AND ALTERNATIVES TO BUTYL LEVULINATE

This work deals with the synthesis reaction of BL from butanol and furfuryl alcohol. However, there are other routes to reach the same target compound, using the same chemical procedure (acid catalysis and previous dehydration process) but starting from other reactants.

Alkyl levulinates have some functional groups (a ketone group and an ester group). For this reason, it is why are worldwide utilized as building blocks for the synthesis of various chemicals and drugs. Those levulinates may be obtained by alcoholysis in the presence of acid catalysts as well as by direct esterification of levulinic acid or from sugars.

In the first option, furfuryl alcohol is obtained by hydrogenation of furfural (an important biomass feedstock obtained from dehydration of xylan hemicellulose, component of lignocellulosic biomass), where the former, reacts with 1-butanol to produce an intermediate, Bmf, which in contact with water originates butyl levulinate. Additionally, some byproducts can be formed, such as DBPent and humins, which are oligomeric products resulting from the polymerization of furfuryl alcohol. To reduce the synthesis of these compounds, an excess of butanol is added and ion-exchange resins are used, since the use of mineral acids causes the apparition of these humins.

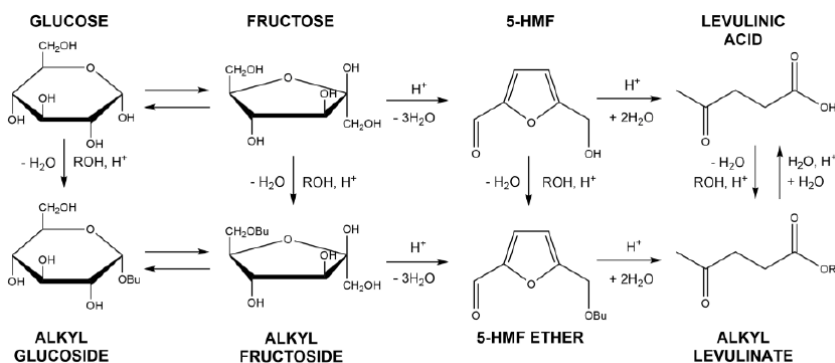
The solvents formed from furfural have various applications, such as the production of dark thermostatic resins resistant to bases, acids and other solvents, for phenolic resins or pigments at low solubility or others like those mentioned in the previous sections on the uses of butyl levulinate.



Scheme 1. Butyl levulinate production using furfuryl alcohol.

There is a second path to produce alkyl levulinates. An acid hydrolysis of cellulose and sugars results in levulinic acid, a compound that has been highlighted by the United States Department of Energy in 2004 and again in 2010 as a promising building block for chemistry, produced by the Biofine process nowadays. This is the main industrial process to obtain levulinic esters, that is, by means of the esterification of levulinic acid with alkyl alcohols in the presence of sulfuric acid, obtaining a high yield of products. However, acid hydrolysis results in a mixture of compounds in solution of very difficult separation, such as levulinic acid, water, formic acid, furans (5-hydroxymethylfurfural and furfural) or polymers. Moreover, levulinic acid is of high cost and that is why, at present, full of researchers are investigating how to produce alkyl levulinates economically.

Levulinic acid ester is produced from glucose or fructose by acid catalyzed dehydration esterification via 5-(hydroxymethyl)furfural and levulinic acid in alcoholic medium. Levulinic acid/based solvents may have application for the realization of synthetic fibers, pesticides, textiles and coatings, among others. These solvents do not show a high risk of ecotoxicity, for which it is used both in food industry and pharmaceutical and also treated as biodegradable compounds, so that means a great incentive for use as substitutes for traditional chemicals due to the environmental concern at present.



Scheme 2. Different routes to produce butyl levulinate.

As before mentioned, other possible compounds for the synthesis of alkyl levulinates, used in other studies, are sugars, just like mono or disaccharides (glucose or fructose, for example), obtained through acid hydrolysis of polysaccharides. Due to this chemical process, an intermediate is obtained, the 5-(hydroxymethyl)furfural, that reacts with water to form levulinic acid and, through the previous route, form an alkyl levulinate. An advantage of these routes is the low production of byproducts, as well as milder conditions.

### 3.3. ION-EXCHANGE RESINS

Ion-exchange resins are polymers capable of exchanging specific ions within the polymer with ions in a solution that is passed through them. That ability is also seen in natural systems such as soils and living cells. Synthetic resins are primarily used for purifying water, but also have some various applications as separating out some inorganics and organics elements.

Those catalyst materials are insoluble substances (acid or bases which have insoluble salts) containing loosely held ions which are able to be exchanged with other ions in solutions which come in contact with them. That process takes place without any physical alteration to the catalyst. The presence of salts in the resin enables them to exchange either positively or negatively charged ions. So many natural substances such as proteins, cellulose, living cells or soil particles, exhibit ion-exchange properties, making an important function in nature.

Synthetic ion-exchange materials based on coal and phenolic resins were first introduced for industrial use during the year 1930. Years later, some catalysts were developed consisting of polystyrene (PS) and divinylbenzene (DVB) with sulfonic groups to form cation exchangers or amine groups to form anion exchangers. These two kinds of resin are still the most commonly used resins today.

The resins are prepared as spherical beads of 0.5 to 1.0 mm in diameter. These appear solid even under the microscope, but on a molecular scale the structure is quite open. That fact makes the possibility of making an intimate contact with the exchange sites of the crosslinked polymer and a chemical solution.

Some of the studies that have made a comparison between the results of this etherification reaction and publications that have emerged over the years on this subject, have concluded that the use of homogeneous catalysis provides greater conversions than the use of an heterogeneous

catalyst. Even so, it is not used due to some drawbacks, such as the danger in handling these substances, the corrosion which causes to the equipment, pollution (because of the solid waste that is created from the subsequent neutralization acid used) and problems in their separation, disposal and regeneration because of its corrosive and toxic nature.

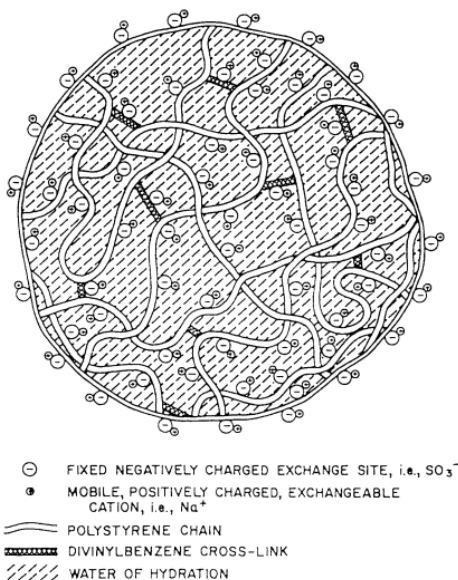


Figure 2. Polystyrene-divinylbenzene resin expanded view.

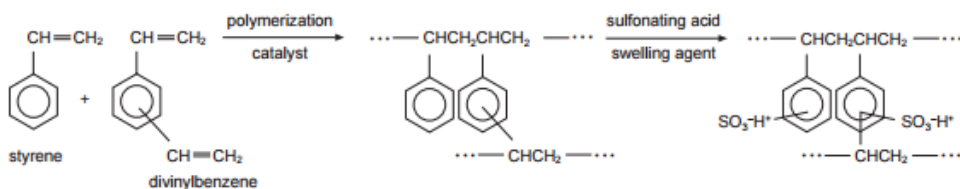
Furthermore, the use of mineral acids favors the reaction pathway that results in the humins. For the reasons mentioned above, the use of acid catalysts as substitutes for mineral acids has been growing over the recent years, due to the existence of the globally environmental concern. All this makes the heterogeneous catalysis interesting, in which acidic or basic groups are attached to insoluble solid structures in the reaction medium, enabling they simple separation by mechanical methods. However, it has to be considered that the presence of the resins in the mixture may influence the catalytic effect of them due to the constraint of accessibility of the reactants to the active centers and to the interaction of the polymer chains with reagents, solvent and catalytic groups, affecting the kinetics of the reaction that takes place.

Ion-exchange resins in its acid form, contains  $-SO_3H$  groups, anchored in a polymeric structure of polystyrene (PS) with a certain percentage of divinylbenzene (DVB) (which varies depending on the type of resin), the last acting as crosslinking agent, benefiting the link between the polymer chains. They are able to present a quasi-homogeneous behavior in an aqueous medium or quasi-heterogeneous in a nonpolar gaseous or liquid medium. When the medium is aqueous or of a high polarity, the polymer chains are separated, the catalyst spheres swell, thus facilitating access of the reactants to the  $-SO_3H$  groups. But, when the medium is apolar, a significant separation does not occur in the polymer chains, thus limiting the catalytic capacity of the resin in a few superficially acid groups.

Resins are classified, according to its acid activity, as non-sulfonated and over-sulfonated resins, by its pore size in macroporous/macroporous and microporous/gel-type and, finally, by the percentage of divinylbenzene, which is closely related to the degree of crosslinking, in high, medium and low.

The degree of crosslinking affects various parameters of the resins, such as flexibility, the melting point, the viscosity or the ion-exchange capacity. For example, low cross-link densities decrease the viscosities, whereas high cross-link densities can cause materials to become very rigid. Furthermore, the effect of crosslinking makes ion-exchange capacity decrease, prolonging the time needed to accomplish the process but, indeed, improves the robustness of the resin.

Generally, porosity is inversely related to the DVB cross-linking. For example, a high percentage of DVB would mean a high degree of crosslinking of the polymer, therefore, the resin, in contact with a polar medium, will not swell that much than another with a smaller percentage, and then, pores would not suffer a big change in size neither.



Scheme 3. Polymerization and swelling of a polystyrene-divinylbenzene resin.

According to the pore size, the two possible kinds of catalyst have a few differences between them:

**Macroporous or macroreticular resin:** Those catalysts are made from a rigid and tough material, with a lower capacity than microporous resins. A positive point face to the other type of resin is the longer operating life they have and the fact that they are be able to effect separations that gel-type catalyst couldn't perform. In the catalyst regeneration process, high-molecular-weight ions can be more completely removed from solution and more completely eluted from the resin. In addition, the open structure allows application with tough copolymers which would be too dense for use microporous resins.

A macroporous resin is a macroreticular resin with more than 20% crosslinkage, with pore diameters up to several hundred Angstroms, with a surface area about 500 m<sup>2</sup>/g or higher, generally higher crosslinking than gel-type resins and, therefore, exhibit little volume change. Therefore, the oxidation stability improves.

Some of the drawbacks we can consider are the poorer regeneration efficiencies, lower capacities, higher regeneration costs and that at similar crosslinkages, macroporous resins have greater exposure to potential oxidants than gel resins due to their greater porosity and surface area.

The sponge-like structure of macroreticular resins offers superior physical and chemical properties to those available with conventional gel-type resins.

**Microporous or gel-type resin:** With pores diameters typically up to 10 or 15 Ångstroms, in a non-swelling medium, that is, where environmental conditions do not allow the polymer chains to separate easily, not exposing the inner of the catalyst, such kind of resins of flexible polymeric chains can become ineffective. That's because of the small pore size because, if swelling does not occur, the pores are too small for the reactants to access their active centers. Particularly, in nonpolar media, where gel-type resins do not perform satisfactorily because of their inaccessibility to the reactants, it does not cause swelling of the pores and therefore, being too small to allow access to the active sites of reactants, macroporous resins could be used as a better option than microporous, because of the sponge-like structure that offers superior physical and chemical properties to those available with conventional gel-type resins.

The studied reaction can be carried out catalyzed or without catalyst, but the absence in the use of an acid catalyst causes a reaction rate too slow. Some papers showed that the most important feature of the catalyst for a better development of the reaction is the accessibility of furfuryl alcohol to the acid sites whereas the acid strength seems not to play an important role<sup>[8]</sup>.

Depending on the size of the pores, between the two types of existing resins, the gel-type present more accessibility to their active centers to 1-butanol than to furfuryl alcohol, a less polar compound, fact that encourages alternative reaction pathways producing the undesired oligomeric products<sup>[15]</sup>.

However, disordered mesoporous catalysts have a wide distribution of pore sizes and a low surface area while ordered mesoporous catalysts are more beneficial, due to a better distribution of pore size, greater surface area and a high pore volume, causing a greater number of active sites and increasing the rate of mass transfer of reactants and products within the pores. In this study, some reactions have been developed with specific resin sizes and, because of the similar data obtained and the results of some other authors, it is considered that the rate of mass transfer is not important versus the reaction rate, being the last as the controlling stage of the system.

#### **3.4. STATE OF ART OF THE FURFURYL ALCOHOL ETHERIFICATION REACTION**

The reaction of alcoholysis of furfuryl alcohol, occurs in two steps: the conversion of reactant occurs, reacting with the alcohol, to produce an intermediate (typically 2-(alkoxymethyl)furan)<sup>[8]</sup>, which undergoes a transformation by the addition of alkyl groups, generating other alcohol, which then reacts with water to produce the levulinate alkyl.

This reaction produces the polymerization<sup>[33]</sup> of the furfuryl alcohol giving, as a result, high molecular mass compounds, such as oligomeric products, called humins (insoluble organic products in water at all pH's, that comprise about 50% of the organic matter in soils), causing a decrease in reaction selectivity and yield. In addition, various byproducts were formed by non-sequential reactions, probably produced from furfuryl alcohol and its intermediate. One of the most widespread hypothesis about the alcoholysis reaction that occurs is the succession of furfuryl alcohol dehydration to  $\alpha$ -angelica lactone, subsequently attacked by alcohols to form alkyl levulinates.

The field of study where it is found more information on the production of these compounds is in the reaction carried out from levulinic acid by homogeneous catalysis<sup>[13]</sup>, that is, using mineral acids as catalyst (just like sulfuric acid), delivering a high product performance to be obtained. Because of the various drawbacks pertaining to use of these acids mentioned in previous sections, they have now being replaced by solid catalysts. Most papers that have used resins, they were synthesized themselves, with few recreations of the process of obtaining alkyl levulinates from mostly commercial catalysts as used in this study: the Amberlyst and DOWEX.

These investigations are currently published (due to the emergence of a consciousness for environmental issues) and show very good results, with a selectivity and conversion almost 100 %, at temperatures above 100 °C temperatures. For this investigation, it is trying to find a process the more economical as it could, so lower temperatures and low cost catalysts available on the market were applied. That objective fixed will affect the parameters mentioned, the selectivity and the conversion, decreasing considerably in comparison from other publications on which they have used synthesized catalyst or higher temperatures.

## 4. OBJECTIVES

The main objective of this work is to study the influence of some operation conditions on the synthesis reaction of butyl levulinate from furfuryl alcohol and 1-butanol using ion-exchange resins as catalyst. Reactant conversion, selectivity of the reaction and yield to BL will be followed. Mainly, this study is focused on the points listed below:

- **Type of catalyst:** Watching the influence of the percentage of divinylbenzene (factor that modifies the degree of crosslinking), sulfonation and pores sizes of the commercial ion-exchange resins used.

- **Initial molar ratio:** Varying the initial molar ratio in the reaction to see its effects. Two FA-BUT ratios were chosen: 1:4 and 1:8, with mass values of 15,19 g FA and 45,91 g BUT for the first ratio mentioned and 8,39 g FA and 50,68 g BUT for the second one.

- **Temperature:** Consider the differences obtained in the same procedure to conduct different temperatures: 110°C, 100°C, 90°C and 80°C.



## 5. EXPERIMENTAL

### 5.1. REAGENTS AND CATALYSTS USED

Some chemicals, as resins, compounds and other substances, were necessary to carry out the experiments seen in the present work. Those materials are presented below:

**Water:** provided by the faculty of physics and chemistry of UB, Milli-Q type.

**Butyl levulinate and furfuryl alcohol:** provided by Sigma Aldrich, 98 % purity each.

**1-butanol:** provided by Across Organics, 99.5 % purity.

Whereas the 1-butanol and furfuryl alcohol were involved as reactants in the reaction process, these, along with water and butyl levulinate, were used to perform the calibration of the gas chromatograph.

Various gases were useful for the realization of the investigation:

**Nitrogen:** Inert gas used to pressurize the reactor or return the sample to it. Its purity is 99.9995 %, supplied by the company Abello Linde.

**Helium gas:** used as mobile phase in gas chromatography. Its purity is 99.998 %, supplied by the company Abello Linde.

**Compressed air:** auxiliary gas applied to set on some valves inside the chromatograph.

In the presented work, various acidic ion-exchange resins of different types and characteristics were used.

The following tables showed each resin types used, classified according to the previously mentioned properties:

Table 1. Catalysts characteristics.

Catalyst	Structure	%DVB	Sulfonation	H <sup>+</sup> (eq/g)	T <sub>max</sub> (°C)
A15	Macroreticular	20	Monosulfonated	4,81	120
A16	Macroreticular	12	Monosulfonated	4,8	130
A31	Gel-type	4	Monosulfonated	4,84	130
A35	Macroreticular	20	Oversulfonated	5,32	150
A36	Macroreticular	12	Oversulfonated	5,4	150
A39	Macroreticular	8	Monosulfonated	4,81	130
A70	Macroreticular	8	Monosulfonated	2,65	190
A121	Gel-type	2	Monosulfonated	4,8	130
DOWEX 50x2	Gel-type	2	Monosulfonated	5,06	150
DOWEX 50x4	Gel-type	4	Monosulfonated	4,95	150
DOWEX 50x8	Gel-type	8	Monosulfonated	4,83	150

Table 2. BET and ISEC measures.

Catalyst	BET mesures				ISEC mesures		dp (nm)
	d <sub>p</sub> (nm)	V <sub>g</sub> (cm <sup>3</sup> /g)	V <sub>sp</sub> (cm <sup>3</sup> /g)	S <sub>g</sub> (m <sup>2</sup> /g)	V <sub>g</sub> (cm <sup>3</sup> /g)	S <sub>g</sub> (m <sup>2</sup> /g)	
A15	31,8	0,328	0,765	42,01	0,616	192	16,1
A16	29,7	0,013	1,129	1,69	0,188	46	10,3
A31	15,3	0,00033	1,904	0,1	0	0	0
A35	23,6	0,21	0,504	28,9	0,72	199	15,0
A36	27	0,143	0,61	21	0,259	68	9,1
A39	17,6	0,00029	1,624	0,09	0,155	56	7,9
A70	22	0	1,257	0,02	0,22	66	8,1
A121	32,9	0,00035	3,236	0,02	0	0	0
DOWEX 50x2	0	0	2,657	1,32	0	0	0
DOWEX 50x4	0	0	1,84	0,0296	0	0	0
DOWEX 50x8	0	0	1,25	0,23	0	0	0

## 5.2. EXPERIMENTAL DEVICE

The equipment used can be divided into two parts: the reactor with the process controller and the gas chromatograph (GC).

The reactor used (from Autoclave Engineers, mini-reactor series) is of stainless steel, of a nominal volume of 100 mL with operating conditions limit of 2900 psi pressure and a temperature of 600 F. The reactor is composed of various supplements: a filter for sampling, a stirrer, a thermocouple to measure the temperature inside the reactor, a rupture disk if an unexpected pressure increase takes place, a pressure relief valve to release pressure and return part of the sample into the reactor, a catalyst injector and a purge stream system.

The figure below shows a diagram of the whole experimental system:

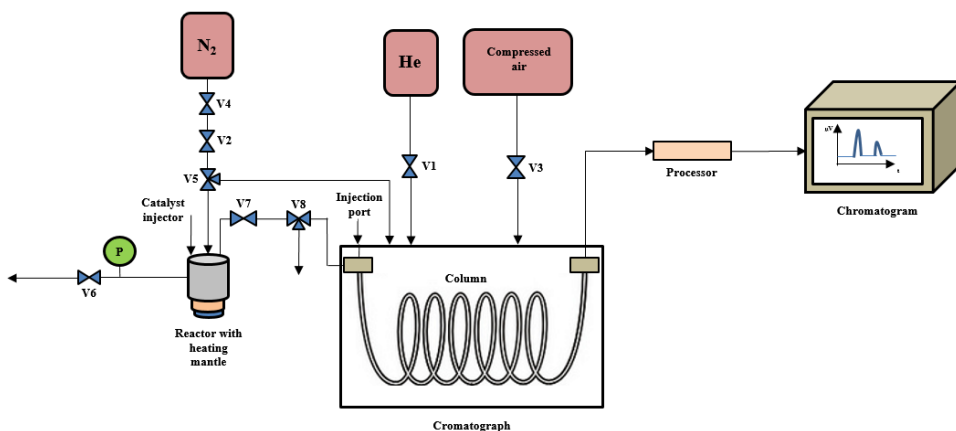


Figure 3. Experimental device scheme.

In the next figure all the elements mentioned can be appreciated:

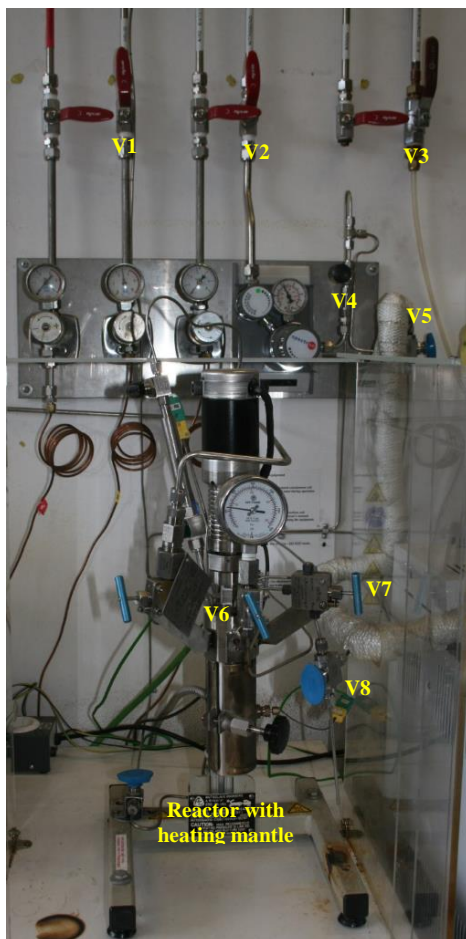


Figure 4. Reactor and valves system.

The gas chromatograph performs the separation and detection of the compounds present in the sample obtained from the mixture in the reactor. Samples can be taken semi-automatically through a filter, which is in contact with the mixture, or by manual injection with a needle.

After taking the sample, it travels through the chromatograph column, which will carry out the separation of compounds. The separation is done by passing the mobile phase (helium in this case) through the column, which contains the stationary phase. The mobile phase only aims to

elute the sample and transport it to the detector whereas the stationary phase (in this case, an inert solid) has the function of adsorbing analytes, retaining them to his subsequent separation and reaching the detector at different times. The times are characteristic for each compound although, at similar interactions to the stationary phase, it can produce the arrival of them at the same time, overlapping the peaks. The use of a solid as stationary phase has limited application because of semipermanent retention of polar molecules and obtaining queues peaks due to non-linear adsorption. However, it may be used for the separation of gaseous molecules of low molecular weight. This column, which is located inside a temperature-controlled oven, is connected to an injector and a detector from different ends.

The detector is the responsible to identify the presence of these compounds when they leave the column, relating the amount of compound detected with an electrical signal and displaying it on a chromatogram. By calibration, it is possible to relate the percentage of the area appeared in the peaks in the chromatogram with the mass fraction of the compound in solution. There are several types of detectors (FID, TCD, NPD, FPD ...). In this case, it is working with TCD (thermal conductivity detector), which is a technique used to analyze inorganic gases and small hydrocarbon molecules based on the comparison of thermal conductivities between two gas streams and the reference shows where, in this case, the first will be helium. TCD detector was chosen because it permits the detection and quantification of water.

## 5.3. EXPERIMENTAL PROCEDURE

### 5.3.1. CATALYST PRETREATMENT

At the beginning, the catalyst contains a percentage of water of about 60 %. This amount of water is problematic because it decreases the catalytic activity of the resin due to the hindrance of other substances to get into their pores. In addition, if after pretreatment is not dry enough, it is possible to originate errors in the measurement of water production in the reaction studied.

Therefore, to prevent all the mentioned problems, the water content of the resins has to be eliminated. The drying procedure is as follows: first, most of the free water contained in the catalyst is removed at room temperature for a day and then, the resin is placed for two hours in an atmospheric oven at 110 °C. Finally, the catalyst is located into a vacuum oven at 100°C for

at least 14h. Final content in the resin beads after vacuum-drying was 3-5%wt. (analyzed by Karl-Fischer titration in our laboratory).



Figure 5. Example of a dried ion-exchange resin.

### 5.3.2. STARTUP AND PROCESS

To carry out the experiment, the GC must be at BUL\_VALV\_PONA.M operating method to reach the appropriate temperatures and pressures for each of its components. The way to start each experiment, after having introduced the mixture of reactants necessary to the reactor and the reactor placed in the autoclave position, is as follows, according to the figure showed:

1. Direction valve V5 to make nitrogen circulates within the reactor and open valve V4 to a pressure of 40 bar inside the reactor (corresponding to the work pressure).
2. Once this value is reached, close the valve V4 and wait a few seconds to see if pressure inside the reactor gets lower, which would mean that there is a leakage and system must be dismantled.
3. If there is not any leakage, the valve V6 is opened to eject the nitrogen introduced before. Then, the heating procedure of reactor starts with the aid of a heating mantle and connecting the stirring at 500 rpm. The heating time is about 25 minutes, with a setpoint of 150 °C, in order to prevent an out of control of the temperature rising.
4. Reached the desired temperature, open valve V4 to reach the desired pressure and keep it open throughout the experiment.

5. Subsequently, the valve V7 is opened to take a sample of the reactor content and wait about 7 minutes to ensure the filling of the chromatograph loop.
6. After that, the method starts and must wait 30 seconds for the sample to circulate into the chromatograph and, in order to return the sample that has not been introduced into the chromatograph, change the direction of the valve V5, open the valve V6 over 20 bar, close that valve and the valve V7 and proceed to purge the system by changing the direction of the valve V8 repeatedly until the content of output is as clean as possible. Once this is done, put valves V8 and V5 to the starting position at the beginning of the experiment.
7. Points 5 and 6 are repeated periodically until the end of the experiment (6 hours).
8. Once the experiment ends, the reactor is depressurized as mentioned in point 3, the position of the set point temperature gets the value of 0 °C to reduce the temperature of the heating mantle gradually and displaces the reactor of its working position.

## 6. RESULTS AND DISCUSSION

### 6.1. DESCRIPTION OF AN EXPERIMENT

Several experiments have been planned to check the influence of the initial molar ratio, temperature and the characteristics of the catalyst on the reaction. With this objective, the Gas Chromatograph was calibrated to relate compounds mass fractions with the percentage of the areas of each compound in the sample taken. Thanks to that information, the conversion of the data obtained into mass fractions and those, in moles of each compound in the mixture of the reactor, could take place. That allows the possibility to calculate the necessary data of conversion of furfuryl alcohol, selectivity and yield to the desired product.

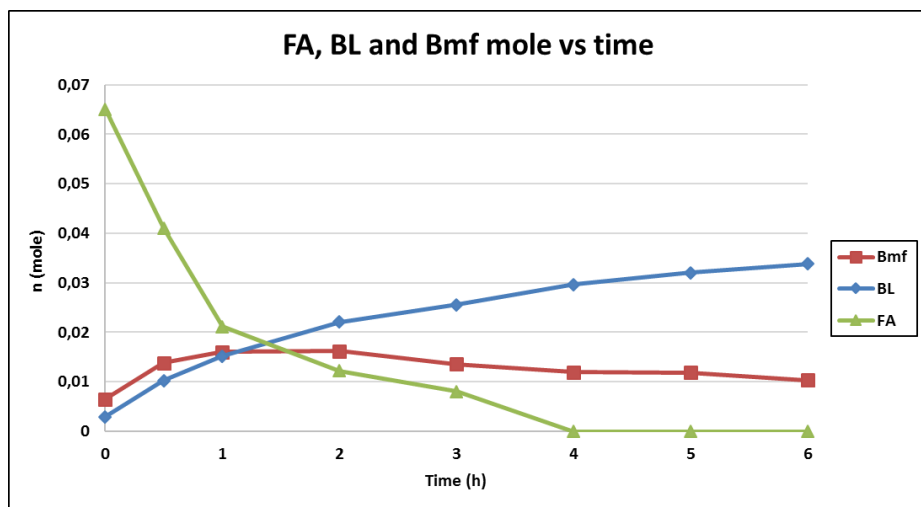


Figure 6. Example of the evolution of FA, BL and BL mole.

Figure 6 shows the evolution of the mole profiles of a model experiment: A39,  $T = 80\text{ }^{\circ}\text{C}$  and ratio 1:8. What is shown is the decreasing of FA due to various reactions happening simultaneously (both oligomeric and the main reaction) while the BL moles are taking place. As



an intermediate, Bmf moles were initially formed and, the less FA moles are about to react, the less quantity of intermediate is produced during the reaction.



Figure 7. FA, BUT, BL and products obtained in the reaction respectively.

Once the reaction finished, the mass balance was accomplished within 10%. As shown in figure 7, products obtained are darker than the BL colour. The reason of that difference is the oligomeric products formed in the mixture apart from the BL.

Other assays were performed with the aim to see how reaction varies changing some experimental conditions. In all experiments, the stirring speed was set to 500 rpm and the pressure to 40 bars to maintain the compounds in liquid state inside the reactor.

In previous experiments the effect of the initial amount of catalyst was checked. Initially, two grams of resin was used, but the reaction was almost complete during the initial heating period of the reactor. Using 2 grams of the catalyst A39 at a temperature of 100 °C with an initial molar ratio of 1:8, the full conversion is achieved in about 1 hour, whereas using 1 gram, the complete conversion is reached in 3 hours. Thus, for all experiments, 1 gram of resin was used to assess the evolution of reactants into products along 6 hours.

Finally, some experiments were conducted with the aim to compare the performance of a resin with the commercial distribution of particle diameters, and some sieved fractions of it. The catalysts used are commercial and were not sieved in most cases owing to, carrying out a comparison between the process with sieved resins (diameter comprised between 0.63 and 0.4) and not sieved, a significant change was not seen in the final results. That comparison was made using A39 at a temperature of 100 °C and an initial molar ratio of 1:8, obtaining results inside the replications made for the A39 resin.

In addition, according to some papers, the variation in the size of commercial resins used seems not to influence the reaction rate. Therefore, at the fixed stirring and using the resins mentioned, internal mass transfer resistance can be negligible.

In addition, due to lack of Bmf, its calibration has been realised with BL, using Bmf common area percentages during the reaction.

Here are the formulas used to calculate the necessary data:

To calculate the conversions:

$$X_j(t) = \frac{n_j^0 - n_j(t)}{n_j^0} \quad (1)$$

With furfuryl alcohol as a reactant:

$$X_{FA}(t) = \frac{n_{FA}^0 - n_{FA}(t)}{n_{FA}^0} \quad (2)$$

The selectivity could be found as:

$$S_j^k(t) = \frac{\text{Mole of reactant converted into } k}{\text{Mole of } j \text{ reacted}} = \frac{n_k(t)}{n_j^0 - n_j(t)} \quad (3)$$

Knowing that the reactions have a stoichiometry of 1:1 in both productions of Bmf and BL,  $n_k = n_{BL} = n_{Bmf}$ , thus:

$$S_{FA}^{BL}(t) = \frac{n_{BL}(t)}{n_{FA}^0 - n_{FA}(t)} \quad (4)$$

$$S_{FA}^{Bmf}(t) = \frac{n_{Bmf}(t)}{n_{FA}^0 - n_{FA}(t)} \quad (5)$$

Where total selectivity is calculated as the sum of the two selectivity because, once FA is turned into Bmf, will be a matter of time for it to react producing BL:

$$S^{BL}(t) = S_{FA}^{Bmf}(t) + S_{FA}^{BL}(t) \quad (6)$$

Yield is calculated taking into account the BL selectivity:

$$Y_j^k(t) = Y_{FA}^{BL}(t) = X_{FA}(t) \cdot S^{BL}(t) \quad (7)$$

## 6.2. CATALYST SCREENING

Different catalysts were used at the same conditions of temperature (100 °C) and initial molar ratio (1:8) to see the differences in the results due to the characteristics of each of them.

As shown in table 3, the catalyst which best performs in selectivity is A16 along with A70, although neither of these comes to a complete conversion. The one which gets the best results reaching a total conversion is A39. That's why it has been used to study the effects of other variables such as temperature or initial molar ratio.

Gel-type resins are those that provide a lower yield and selectivity in the reaction, although in all cases, except of DOWEX 50x8 and A31, full conversion is reached, which in many macroreticular catalysts does not happen. A possible explanation for this could be that, this kind of resin, may enhance reactions that produce humins apart from the main reaction. Otherwise, the sum of selectivity calculated in the table presented should be unity. As it is not, the existence of these unwanted products, not detected by GC, is confirmed. To determine the experimental error, several replications were done for A39 and A35. In table 3, the error for each parameter is shown, considering similar values for the rest of the ion-exchange resins.

Table 3. Experiments results for each catalyst at t = 6 h.

Catalyst	$X_{FA}$	$Y_{FA}^{BL}$	$S_{FA}^{Bmf}$	$S_{FA}^{BL}$	$S^{BL}$
A15	1,00	0,51	0,09	0,51	0,60
A16	0,70	0,39	0,15	0,56	0,71
A31	0,26	0,03	0,34	0,12	0,45
A35	1,00±0,00	0,40±0,02	0,14±0,01	0,40±0,02	0,54±0,02
A36	0,27	0,09	0,28	0,35	0,63
A39	1,00±0,00	0,57±0,03	0,04±0,04	0,57±0,04	0,61±0,03
A70	0,93	0,48	0,13	0,51	0,65
A121	1,00	0,50	0,03	0,50	0,53
DOWEX 50x2	1,00	0,47	0,05	0,47	0,52
DOWEX 50x4	1,00	0,20	0,25	0,20	0,44
DOWEX 50x8	0,00	0,00	0,00	0,00	0,00

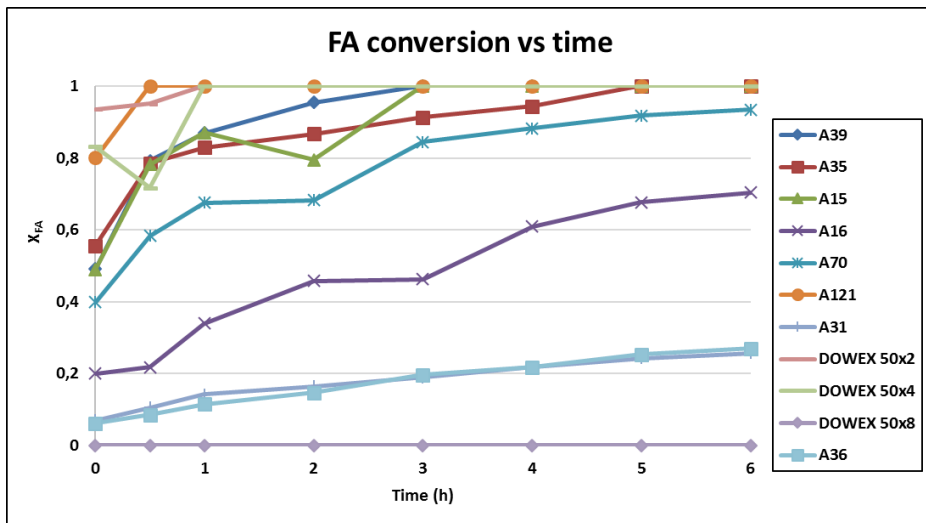


Figure 8. Evolution of FA conversion.

Figure 8 shows that most resins reach a complete or almost complete conversion in a time less than 3 hours. Some exceptions are DOWEX 50x8, A16, A70, A39, A36 and A31 (the last two nearly overlapping), where no reaction occurs in the first catalyst mentioned. A39 reach full conversion in a time of 5 hours, while A70 doesn't reach that maximum value at any time, but the conversion is almost complete at 6 hours.

Furthermore, the catalyst which faster gets full conversion is A121, followed by DOWEX 50x2, DOWEX 50x4 and the two that come to similar time, A39 and A15.

The catalyst A121 is the gel-type resin of lower %DVB and  $H^+/V_{sp}$  ratio, characteristics that beneficiates the reactant conversion. It has very similar properties than DOWEX 50x2, followed by DOWEX 50x4 which duplicates the parameters values of both catalysts. The last DOWEX mentioned has practically the same properties as A31. Nevertheless, very different results in this section (although selectivity are almost the same) are obtained for each resin. The only variation between them is in pore diameter, where A31 has a value of 15 nm while the other is almost 0. The effect of the last parameter seems to be more important, as there is not too much variation in the ratio shown between DOWEX 50x2 and A121 (with 2 %DVB) or between DOWEX 50x4 and A31 (4 %DVB), where DOWEX have an almost unappreciable diameter.

In macroreticulars type, the results are less obvious: at similar pore size or %DVB, in some cases give better results the ones whose have a higher  $H^+/V_{sp}$  ratio, other cases are the ones whose has a smaller ratio, and the other way around. Generally, it seems that at quite high values of %DVB, the faster to get a complete conversion. Although other parameters are affecting it, it appears to be an optimal in their values because of the large variation of the data obtained.

Although A31 and A36 give very similar conversions, their characteristics are so different in  $H^+/V_{sp}$  ratio and %DVB, surpassing to A31 in both aspects.

The conversion would also be explained with the same argument for A15 and A16: the two of the same resin type, similar acid capacity but of varied %DVB. For the same reason, DOWEX 50x8 does not react because of its high %DVB. However, A39 and A15, whose give very similar results, have a very different %DVB, being higher for the last mentioned. Nevertheless, the  $H^+/V_{sp}$  ratio and the pore diameter is favourable for A39, possibly offsetting the difference in %DVB.

Finally, A35 and A70 differ in all parameters. As A35 has higher features values, gives better conversion results.

To appreciate the reaction rate for each kind of catalyst, is important to see how Bmf moles changes along the time of the reaction:

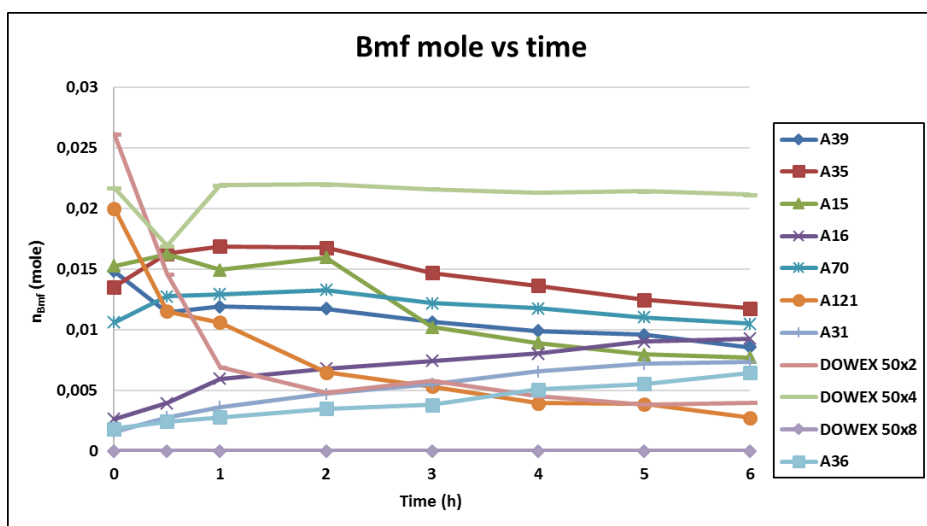


Figure 9. Evolution of Bmf mole.

In the graphic above, different behaviour in the evolution of Bmf moles are represented. All of them have the same similitude, despite of that the reaction rate varies for each catalyst, showing different forms. For example, in DOWEX 50x2 or A121, the curve only decrease, whereas in A31 or A36 is only increasing. Initially, the amount of Bmf increases as it is produced, until FA has completely reacted and, therefore, the intermediate compound is not produced anymore, decreasing his mole quantity, reacting with water to produce BL.

Because of the difference in reaction rate in the use of certain catalysts, this trend is not appreciated significantly, since in some cases, at the reactor preheating stage, almost all FA has undergone a complete conversion.

In gel-type resins, a similar behaviour than in the previous section is appreciated. High %DVB and low pore size are the better characteristics to achieve a high rate of intermediate production. In this kind of catalyst, the reaction rate for the formation of Bmf is so low, seeing in most cases only an increase in the number of moles, except of A121 and DOWEX 50x2, of similar properties but of very different pore diameters (with a very low value for the DOWEX). In addition, even though the trend is a decrease of these moles, in DOWEX 50x4 these moles remain constant. One cause could be the deactivation of the catalyst due to the adsorption of humins, thus keeping off the access to the catalytic centers.

For macroreticular resins, the rate is higher, although some are not that much, as in the case of A36 or A16. It is appreciated again the possibility of the presence of some optimal parameters values due to so different results. For example, in the ones of a high reaction rate, the first has a rather high %DVB and  $H^+/V_{sp}$  ratio and, between the second one (A39) and the third one (A70), all of them with the same %DVB, gives better results a higher ratio. Furthermore, comparing the third one with A35, although the above mentioned parameters are much more favourable for the last mentioned, A70 gives better results. A similar case occurs between A35 and A15 that, although having the same %DVB, the last, which has less  $H^+/V_{sp}$  value, gets better data.

Even if the reaction rate to produce this intermediate is so important to the global reaction, the main objective in this study is to get the most BL mole as it could.

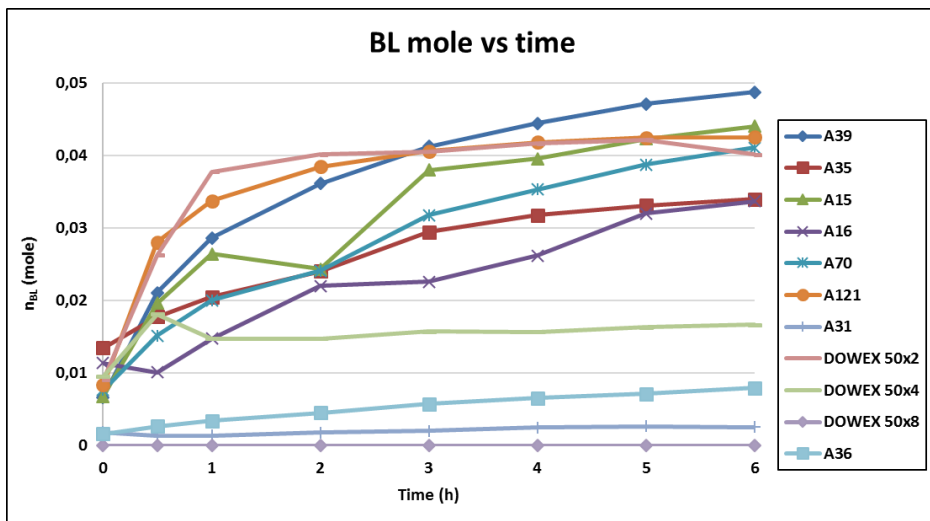


Figure 10. Evolution of BL mole.

In figure 10 it is shown that BL moles produced are quite similar in some resins, but also there are different cases. The catalysts that produced a higher BL mole are A39, A15 and A121 whereas A36, A31 and DOWEX 50x8 are the least (the last gives no amount of BL).

The parameters seem to influence in the same way as they do in previous sections. In gel-type, a low %DVB benefits BL production, while the pore diameter and the  $H^+/V_{sp}$  ratio decrease it.

The conclusion for macroreticulars catalyst results it is similar too, suggesting the presence of an optimal in %DVB,  $H^+/V_{sp}$  and pore diameter.

At similar and equal %DVB and pore diameter, for example, between A70 and A39, a high  $H^+/V_{sp}$  ratio give plenty of BL mole, whilst between A16 and A36 it is found the opposite.

Although A35 or A16 initially produces a higher amount of BL, reaction rate decreases during the course of the process. Even though at similar diameters and higher %DVB, that which has a lower  $H^+/V_{sp}$  ratio is benefited (both A70 and A35).

The resins curve of DOWEX 50x2 and A121 are very similar because of their characteristics, which A121 has a much larger pore diameter, which seems to have no importance in front of %DVB. It is appreciate comparing A31 and DOWEX 50x4, ion-exchange resins of similar

characteristics but of a higher pore diameter in the DOWEX. This fact implies that, as long as %DVB increases, other factors take more at considering.

DOWEX 50x4 curve increases at the beginning of the reaction but remains almost constant for the rest of time, both in production of BL and Bmf, possibly because a deactivation of the catalyst due to the adsorption of humins. The same happens with A31 and A36, but in these cases BL is been producing over the time. One possible explanation could be a very low reaction rate in the use of these catalysts.

The figures that follows exhibit some variables that could influence the selectivity of each ion-exchange resin used. Nevertheless, selectivity is not the most important parameter to take into account, because some of the catalyst shown have a high selectivity but, during a 6 hours, are only capable to produce a very low BL mole.

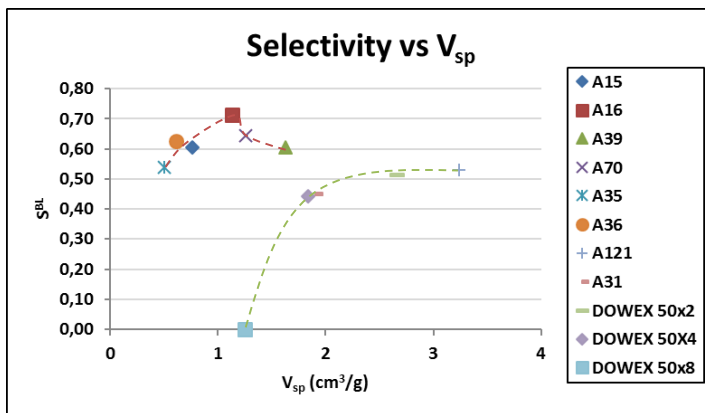


Figure 11. Variation of catalyst selectivity with volume of the swollen phase.

The representation above shows that, for macroreticulars catalyst, there seems to be an optimal about 1 cm<sup>3</sup>/g, which is where the catalyst with higher selectivity is found, the A16, whilst others increase their selectivity as long as they approach to this value.

For gel-type resins, it appears that selectivity is proportional to the  $V_{sp}$ , increasing as it does, does not reacting to values close to 1 cm<sup>3</sup>/g.



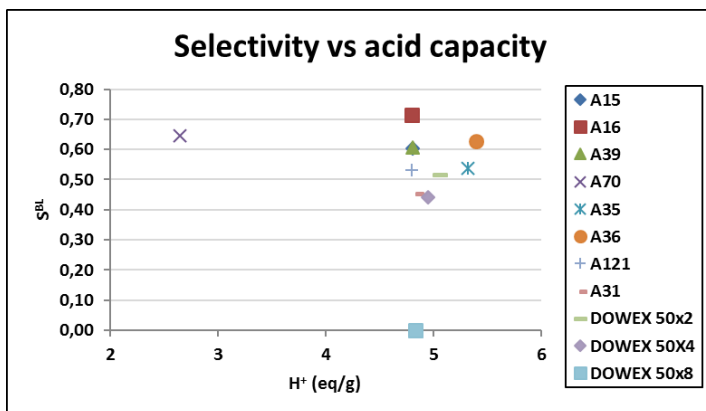


Figure 12. Variation of catalyst selectivity with acid capacity.

At high and similar acid capacity, very different results for all resins, ranging from a value of selectivity of 0,7 to 0,45 or even 0. In addition, for very low acid capacity as A70, the selectivity is one of the highest. This parameter seems to have no significant importance in the reaction and does not seem to be many differences between macroreticulars and gel-type resins.

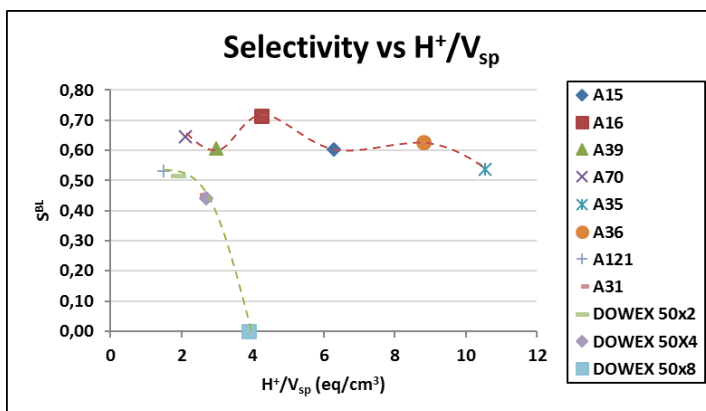


Figure 13. Variation of catalyst selectivity with number of sulfonic groups per volume of swollen gel-phase.

As the number of sulfonic groups per volume of swollen gel-phase are reduced, the selectivity of the gel-type resins increases. That is, for this kind of catalyst, the effect of this parameter is

inversely proportional to the selectivity. When this ratio is lower, the greater the selectivity of the reaction is due to a more appropriate sulfonic groups concentration.

In macroreticulars catalyst does not seem to have any significant effect. All of their selectivity remain quite similar for very different values. However, at high values seem to suffer a decrease in selectivity.

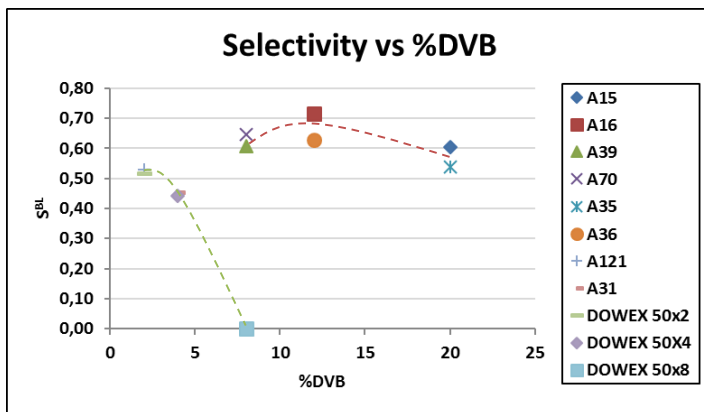


Figure 14. Variation of catalyst selectivity with divinylbenzene percentage.

As crosslinkage agent, DVB influence in the swelling of the pores of the catalyst. If the percentage in the resin is so high, there will be more cross-linking among polymer chains, making it more rigid. When it happens, it will be more difficult to the catalyst to swell. Therefore, pores get smaller, keeping away the reactants of the internal sulfonic groups, interacting only with those located over the surface.

In gel-type resins, the less the crosslinking they have, the better the selectivity results are. In macroreticular resins, it appears to be an optimal around A16 and A36 %DVB values. Comparing the resins that have the same %DVB, it could be seen that, all of which give a better selectivity have a lower acid capacity or  $H^+/V_{sp}$  ratio than his pertinent partner, except for DOWEX 50x8.

As %DVB is related to the accessibility of reactants to active sites, it makes sense to think that these results could be produced because too much swelling can cause a greater reaction rate in the production of BL and others byproducts.

At both kind of catalysts, an increasing in the pores could mean a large increase in the access of unwanted reactants to produce humins, which are larger molecules.

In macroreticular resins, the optimal means the border between this change in the access of reactants of higher volume values whereas in the microporous only means a drop in accessibility.

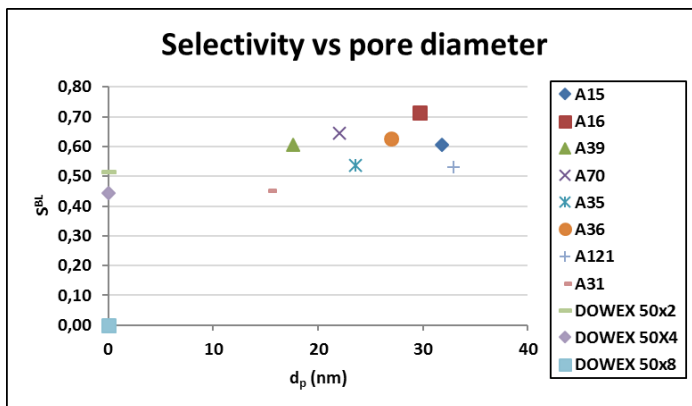


Figure 15. Variation of catalyst selectivity with pore diameter.

A large pore diameter allows the introduction of reactants inside the catalyst, facilitating their interaction with sulfonic groups. According to figure 15, for most ion-exchange resins, an increase of this parameter benefits selectivity, with the exception of DOWEX 50x2, with a much lower diameter than the rest, but giving a similar selectivity as A31 and A35. One explanation could be that, being microporous, the lower %DVB than A31 causes the effects mentioned in figure 14, which also explain why A121 is the gel-type resin which gives more selectivity with a much large diameter. The difference between the resins A16 and A15 are due to the existence of an optimal in %DVB, while the contrast in acid capacity between A16 and A36 is what makes the difference between their selectivity. These two factors also influence the results among A35 and A70.

### 6.3. TEMPERATURE INFLUENCE

As mentioned, the effect of temperature on the reaction is also studied. A39 has been used for this purpose as it has achieved the higher values of selectivity of all who have reached full conversion of FA. The studied temperatures were 110 °C, 100 °C, 90 °C and 80 °C, with an initial molar ratio of 1:8.

The figures show the collected data:

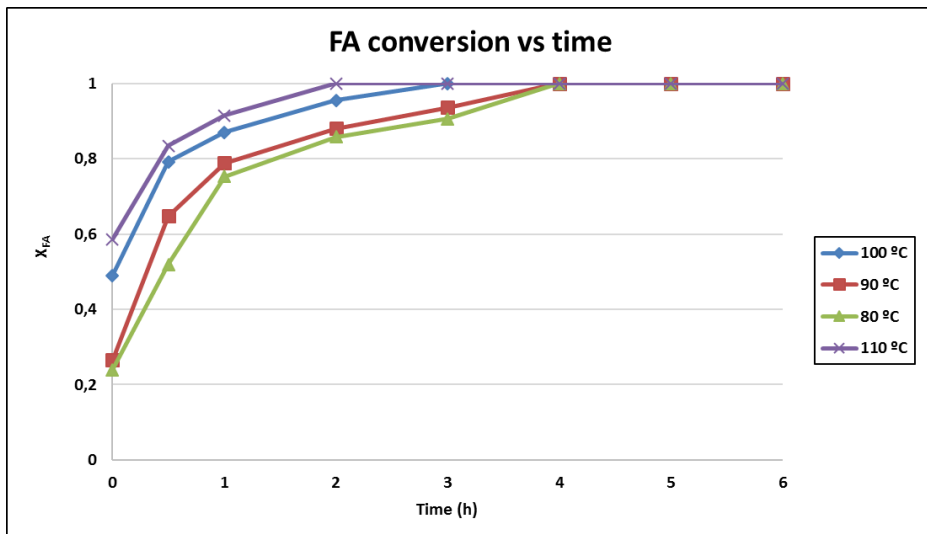


Figure 16. Evolution of FA conversion changing temperatures.

The conversion curves at a temperature of 80 °C and 90 °C are so similar, but when the reaction works at 90 °C, the difference between them are significant. Full conversion is more rapidly achieved with an increasing of temperature, probably due to better reaction rate to produce BL than oligomeric products.

In figure 17, at higher temperatures, all the Bmf mole curve it's not seen, due to a higher reaction rate, whereas at 80 °C or even at 90 °C, a great quantity of Bmf moles produced can be appreciated. As far as the temperature is increased during the preheating, the stage where Bmf moles only fall to produce BL, is already reached.

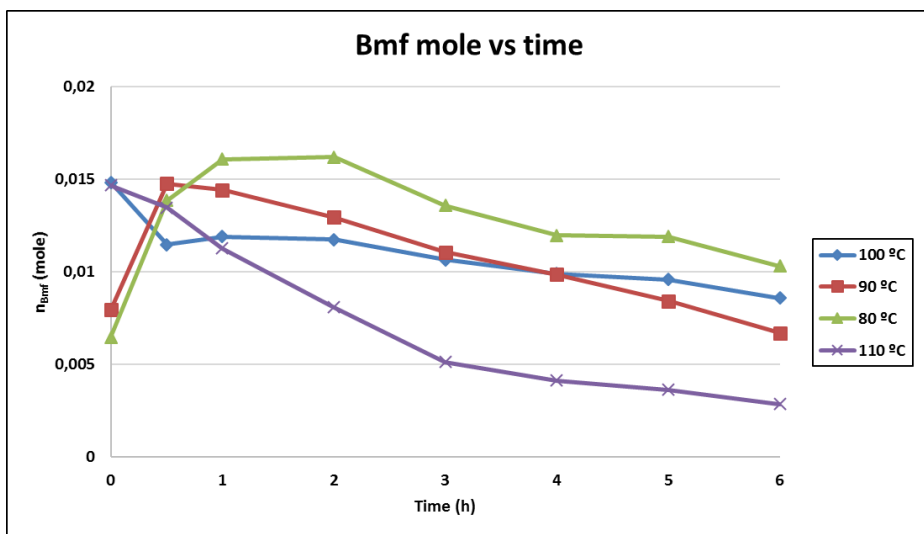


Figure 17. Evolution of Bmf mole changing temperatures.

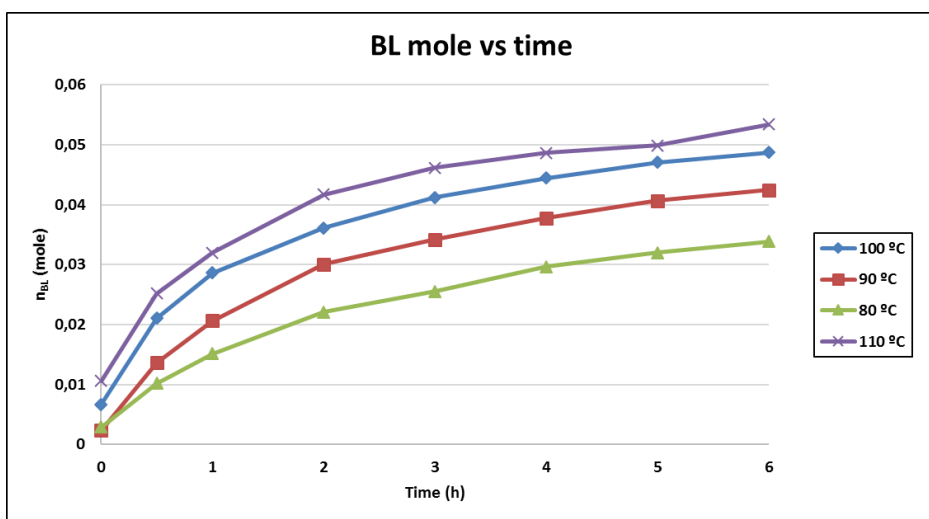


Figure 18. Evolution of BL mole changing temperatures.

As temperature decreases, so does the selectivity (fewer BL moles are obtained), producing a larger amount of unwanted products. Therefore, BL moles obtained drop along the temperature reduction.

### 6.3. INITIAL MOLAR RATIO INFLUENCE

In addition, the effect of the initial ratio of the reactants it is also taken into account. Experiments were accomplished with a FA-BUT ratio of 1:4 and 1:8, for a time reaction of 6 hours at a temperature of 100 °C.

The following figures show the differences between the two ratios, using A39:

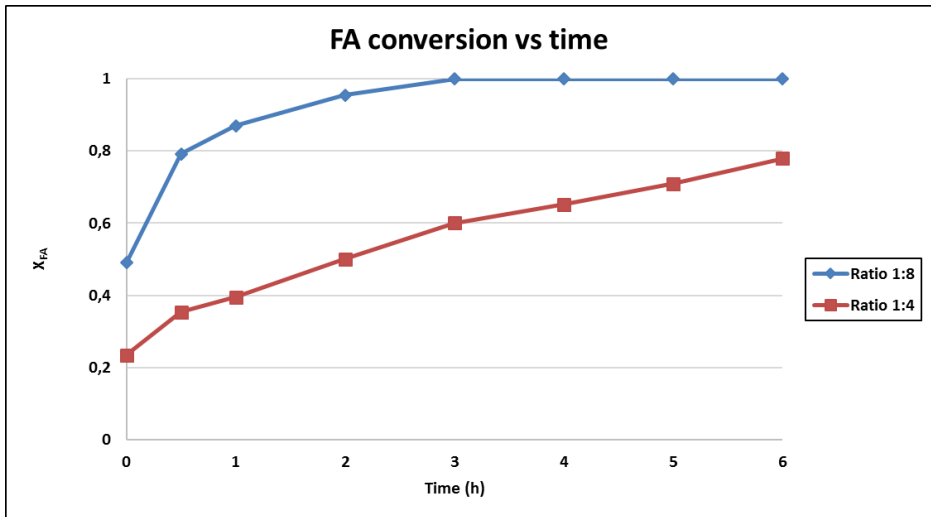


Figure 19. Evolution of FA conversion changing initial molar ratio.

Working in a 1:4 ratio, the initial FA moles are higher than in 1:8 ratio. At  $t = 0h$ , the conversion of FA in the lower ratio is almost half of the value obtained in 1:8 ratio. That's means the initial molar ratio definitely influence the reaction, accelerating the production of the intermediate and so does with BL.

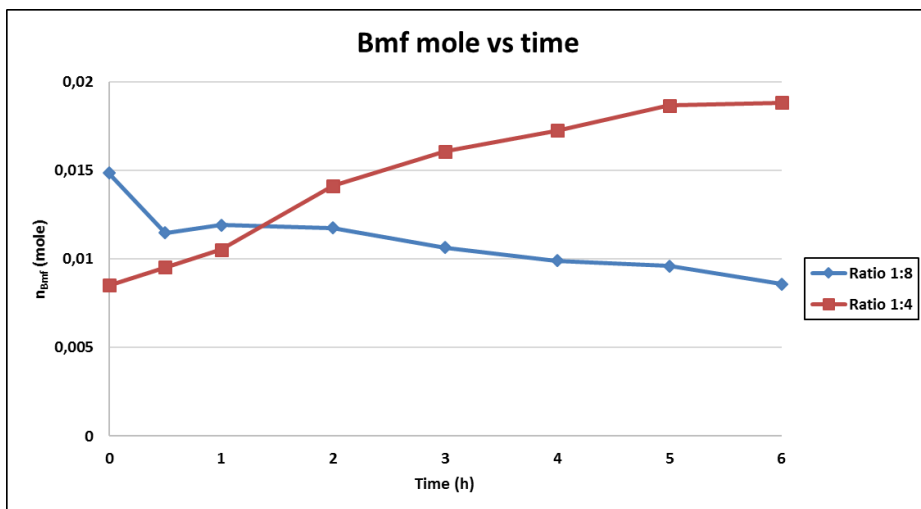


Figure 20. Evolution of Bmf mole changing initial molar ratio.

When the ratio is higher, there's a small quantity of FA about to react. Therefore, because of the depletion of the limiting reactant, the production of Bmf decrease while the BL moles continue increasing, showing a decline in Bmf moles.

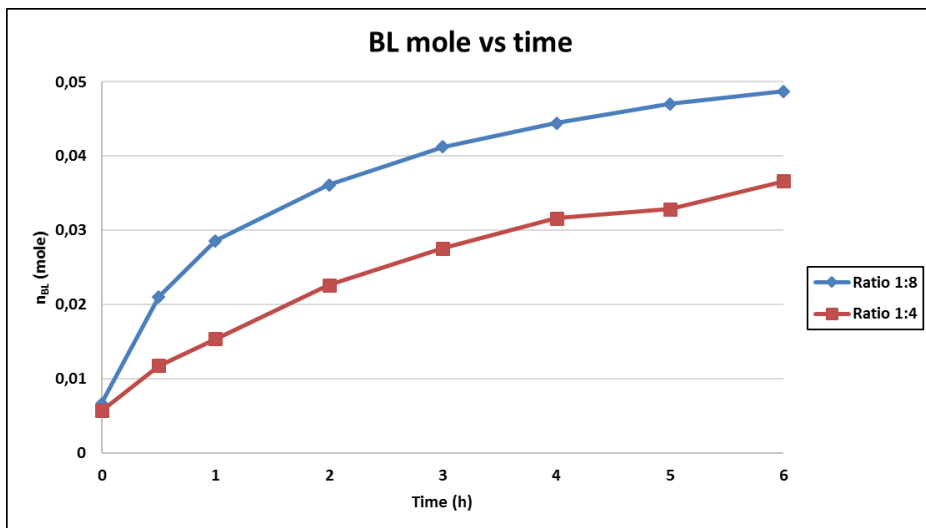


Figure 21. Evolution of BL mole changing initial molar ratio.

Results indicate an improvement in selectivity (0,46 and 0,61 for ratios of 1:4 and 1:8, respectively), as well as they do in conversion and yield, using the higher ratio. That is because excess of BUT limits the polymerization reaction of FA, decreasing the concentration of the limiting reactant, preventing excessive formation of oligomeric products.

Also, as it can be seen, the production of BL moles is higher in 1:8 ratio, the opposite in the case of Bmf. According to better reaction rate producing BL, the moles of the intermediate decrease at the beginning of the representation for the upper ratio. That is because of the depletion of the reactant. The response to 1:4 ratio is quite different: the reaction rate to produce BL moles is lower and full conversion is not reached, remaining FA moles to react. That increase these moles, keeping almost constant due to the low rate.



## 7. CONCLUSIONS

The present work shows the results of all the experiments performed to appreciate how some variables influence in various aspects of the reaction studied.

The use of acidic ion-exchange resins improves the reaction rate to produce BL, although other byproducts were formed, such as oligomeric products because of FA polymerization.

The conversion of FA to Bmf is produced in half of the cases in a time less than 3 hours. In the rest of the catalysts used, full conversion does not take place. The ion-exchange resin which gives a better BL moles production is the macroporous type A39, with a complete conversion at a time of 5 hours. Despite of this result, it is not the one with a high selectivity. A16 confers the best selectivity with a value of 0,71 (in spite of not to reach a complete conversion) in front of 0,61 of A39.

Nevertheless, gel-type resins give the worst results, with a very low selectivity, being the DOWEX 50x8 useless in this reaction.

In addition, acid capacity and pore diameter seems not to influence significantly in the reaction course, whereas %DVB, the volume of the swollen phase of the catalyst and the number of sulfonic groups per volume of swollen gel-phase makes some difference between each catalyst.

For macroporous resins, in all cases an optimal value can be appreciated. In gel-type resins, it is found an increase in selectivity and reaction rate for high values of  $V_{sp}$  but the opposite happens for high values of %DVB and  $H^+/V_{sp}$  ratio.

As expected, an increasing in temperature assure better selectivity, conversions and yield results, with a rather difference between the higher temperature and the lower used. Changing the initial molar ratio, upper ratios improved all the aspects studied.



## 8. REFERENCES AND NOTES

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## 9. ACRONYMS

FA: furfuryl alcohol.

BUT: 1-butanol.

Bmf: 2-(butoxymethyl)furan.

BL: butyl levulinate.

DBPent: 5-5-dibutoxy-2-pentanone.

Hmf: 5-(hydroxymethyl)furfural.

dp: pore diameter (nm).

%DVB: divinylbenzene percentage.

H<sup>+</sup>: acid capacity (eq/g).

ISEC: Inverse Steric Exclusion Chromatography.

BET: Brunauer, Emmett and Teller.

PS: polystyrene.

GC: Gas Chromatograph.

TCD: Thermal Conductivity Detector.

T<sub>max</sub>: maximum temperature (°C).

S<sub>g</sub>: mesoporous surface area (m<sup>2</sup>/g).

V<sub>g</sub>: pore volume (cm<sup>3</sup>/g).

V<sub>sp</sub>: volume of the swollen phase (cm<sup>3</sup>/g).

j: reactant.

k: product.

X<sub>j</sub>: conversion of reactant j.

Y<sub>j</sub><sup>k</sup>: yield of reactant j to product k.

S<sub>j</sub><sup>k</sup>: selectivity of reactant j to product k.

$S^k$ : total selectivity to product k.

$n_i$ : moles of the compound i.



# APPENDICES



## APPENDIX 1: CHROMATOGRAPHIC ANALYSIS

Table 4. Retention time of the substances detected by GC.

Compound	Retention time (min)
BUT	8,432
FA	10,363
H <sub>2</sub> O	4,616
Bmf	11,693
BL	12,236
N <sub>2</sub>	4,408
DBPent	14,069

The calibration of the intermediate Bmf and BL are the same because of the lack of the intermediate compound. In the BL calibration, current % area of Bmf are been used.

Table 5. Vials used for the calibration.

Vials	%Mass	BL		BUT		FA		H <sub>2</sub> O	
		%Area	%Mass	%Area	%Mass	%Area	%Mass	%Area	%Mass
1	11,120	8,614	88,880	91,386	0,000	0,000	0,000	0,000	0,000
	11,120	8,371	88,880	91,629	0,000	0,000	0,000	0,000	0,000
	11,120	8,466	88,880	91,534	0,000	0,000	0,000	0,000	0,000
2	1,364	3,707	93,288	95,353	5,111	0,940	0,000	0,000	0,000
	1,364	3,905	93,288	95,165	5,111	0,930	0,000	0,000	0,000
	1,364	3,824	93,288	95,204	5,111	0,973	0,000	0,000	0,000
3	0,000	0,000	71,590	79,644	15,926	20,360	0,000	0,000	0,000
	0,000	0,000	71,590	79,576	15,926	20,424	0,000	0,000	0,000
	0,000	0,000	71,590	79,324	15,926	20,676	0,000	0,000	0,000
4	44,000	38,263	56,000	61,737	0,000	0,000	0,000	0,000	0,000
	44,000	38,574	56,000	61,426	0,000	0,000	0,000	0,000	0,000
	44,000	38,881	56,000	61,119	0,000	0,000	0,000	0,000	0,000

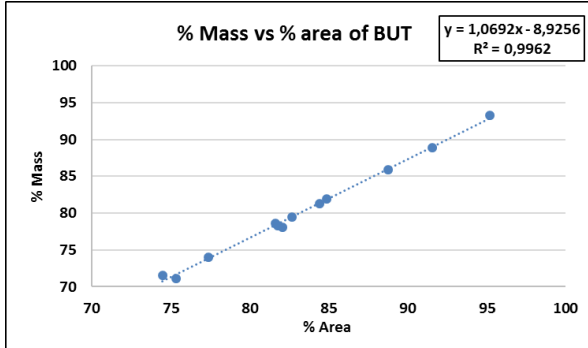
5	1,582	1,249	78,095	82,228	20,323	16,556	0,000	0,000
	1,582	1,270	78,095	81,900	20,323	16,831	0,000	0,000
	1,582	1,216	78,095	82,072	20,323	16,679	0,000	0,000
6	8,663	6,921	81,879	84,854	8,154	6,511	1,305	1,714
	8,663	6,910	81,879	84,892	8,154	6,509	1,305	1,689
	8,663	6,918	81,879	84,856	8,154	6,504	1,305	1,721
7	12,915	10,413	81,296	84,444	4,595	3,673	1,194	1,471
	12,915	10,605	81,296	84,261	4,595	3,653	1,194	1,481
	12,915	10,431	81,296	84,467	4,595	3,650	1,194	1,452
8	16,213	13,050	79,461	82,671	3,068	2,456	1,258	1,542
	16,213	13,334	79,461	82,944	3,068	2,465	1,258	1,539
	16,213	13,328	79,461	82,661	3,068	2,453	1,258	1,558
9	19,045	15,625	78,261	81,664	1,633	1,303	1,061	1,324
	19,045	15,525	78,261	81,861	1,633	1,302	1,061	1,312
	19,045	15,716	78,261	81,758	1,633	1,293	1,061	1,316
10	21,050	17,523	71,141	75,245	7,041	6,108	0,767	0,484
	21,050	17,463	71,141	75,348	7,041	6,103	0,767	0,472
	21,050	17,398	71,141	75,416	7,041	6,147	0,767	0,464
11	21,050	17,528	73,993	77,404	3,567	3,162	1,389	1,856
	21,050	17,477	73,993	77,490	3,567	3,172	1,389	1,861
	21,050	17,615	73,993	77,366	3,567	3,182	1,389	1,887
12	13,715	10,977	78,577	81,613	5,518	4,626	2,190	2,736
	13,715	11,080	78,577	81,562	5,518	4,609	2,190	2,748
	13,715	11,025	78,577	81,643	5,518	4,625	2,190	2,755
13	10,825	8,753	71,590	74,492	15,926	13,397	1,660	3,287
	10,825	8,955	71,590	74,282	15,926	13,487	1,660	3,275
	10,825	8,826	71,590	74,550	15,926	13,410	1,660	3,285
14	3,680	2,613	0,000	0,000	95,587	97,748	0,733	0,725
	3,680	2,708	0,000	0,000	95,587	97,651	0,733	0,720
	3,680	2,655	0,000	0,000	95,587	97,643	0,733	0,723
15	0,000	0,000	85,841	88,772	14,159	11,283	0,000	0,000
	0,000	0,000	85,841	88,758	14,159	11,242	0,000	0,000
	0,000	0,000	85,841	88,717	14,159	11,228	0,000	0,000
16	4,725	4,120	0,000	0,000	94,468	96,702	0,832	1,023
	4,725	4,003	0,000	0,000	94,468	96,700	0,832	1,005
	4,725	4,005	0,000	0,000	94,468	96,613	0,832	1,013
17	4,503	3,504	0,000	0,000	94,974	97,175	0,526	0,541
	4,503	3,487	0,000	0,000	94,974	97,150	0,526	0,532
	4,503	3,503	0,000	0,000	94,974	97,165	0,526	0,532

Table 6. %Average area of BL obtained after making replicas of the vials.

Vials	%Mass	%Area 1	%Area 2	%Area 3	%Average area		
1	11,12	8,614	8,371	8,466	8,484	±	0,139
2	1,364	3,707	3,905	3,824	3,812	±	0,113
3	0,000	0,000	0,000	0,000	0,000	±	0,000
4	44,000	38,263	38,574	38,881	38,573	±	0,350
5	1,582	1,249	1,270	1,216	1,245	±	0,031
6	8,663	6,921	6,910	6,918	6,916	±	0,006
7	12,915	10,413	10,605	10,431	10,483	±	0,120
8	16,213	13,050	13,334	13,328	13,237	±	0,184
9	19,045	15,625	15,525	15,716	15,622	±	0,108
10	21,050	17,523	17,463	17,398	17,461	±	0,071
11	21,050	17,528	17,477	17,615	17,540	±	0,079
12	13,715	10,977	11,080	11,025	11,027	±	0,058
13	10,825	8,753	8,955	8,826	8,845	±	0,116
14	3,680	2,613	2,708	2,655	2,659	±	0,054
15	0,000	0,000	0,000	0,000	0,000	±	0,000
16	4,725	4,120	4,003	4,005	4,043	±	0,076
17	4,503	3,504	3,487	3,503	3,498	±	0,011

Table 7. Equation of the calibration of each compound, where y is %mass and x is %area.

Compound	Equation	R <sup>2</sup>
BUT	$y = (1,0692 \pm 0,001)x - (8,9256 \pm 0,0098)$	0,9982
FA	$y = (1,2156 \pm 0,0015)x$	0,9980
H <sub>2</sub> O	$y = (0,7967 \pm 0,0081)x$	0,9743
Bmf	$y = (1,2276 \pm 0,0019)x$	0,9973
BL	$y = (1,2276 \pm 0,0019)x$	0,9973



22. Calibration of BUT.

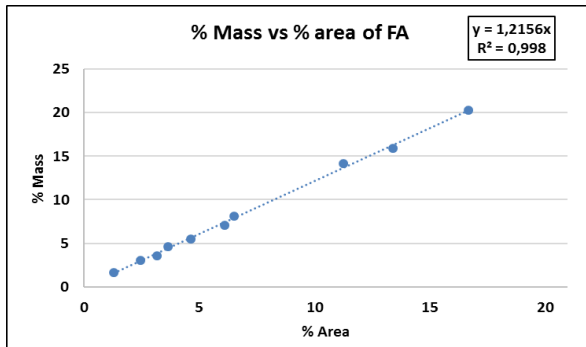


Figure 23. Calibration of FA

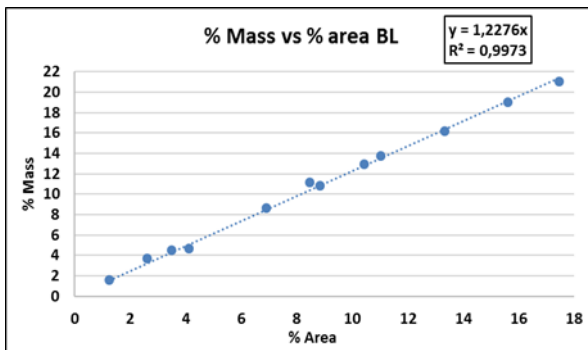


Figure 24. Calibration of BL

## APPENDIX 2: SAFETY DATA SHEETS

Now, some information about the dangerous substances used in the present work are shown:

- Furfuryl alcohol information:

### SIGMA-ALDRICH

[sigma-aldrich.com](http://sigma-aldrich.com)

#### SAFETY DATA SHEET

according to Regulation (EC) No. 453/2010

Version 6.0 Revision Date 08.09.2015


Print Date 09.02.2016

GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

#### SECTION 1: Identification of the substance/mixture and of the company/undertaking

<b>1.1 Product identifiers</b>	
Product name	: Furfuryl alcohol
Product Number	: 185930
Brand	: Aldrich
Index-No.	: 603-018-00-2
REACH No.	: A registration number is not available for this substance as the substance or its uses are exempted from registration, the annual tonnage does not require a registration or the registration is envisaged for a later registration deadline.
CAS-No.	: 98-00-0
<b>1.2 Relevant identified uses of the substance or mixture and uses advised against</b>	
Identified uses	: Laboratory chemicals, Manufacture of substances
<b>1.3 Details of the supplier of the safety data sheet</b>	
Company	: Sigma-Aldrich Quimica, S.L. Ronda de Poniente, 3 Aptdo. Correos 278 E-28760 TRES CANTOS -MADRID
Telephone	: +34 91 6619977
Fax	: +34 91 6619642
E-mail address	: eurtechserv@sial.com
<b>1.4 Emergency telephone number</b>	
Emergency Phone #	: 704100087

#### SECTION 2: Hazards identification

<b>2.1 Classification of the substance or mixture</b>	
Classification according to Regulation (EC) No 1272/2008	
Acute toxicity, Oral (Category 3), H301	
Acute toxicity, Inhalation (Category 2), H330	
Acute toxicity, Dermal (Category 3), H311	
Skin irritation (Category 2), H315	
Eye irritation (Category 2), H319	
Carcinogenicity (Category 2), H351	
Specific target organ toxicity - single exposure (Category 3), Respiratory system, H335	
Specific target organ toxicity - repeated exposure, Inhalation (Category 2), Nose, H373	
For the full text of the H-Statements mentioned in this Section, see Section 16.	
<b>2.2 Label elements</b>	
Labelling according Regulation (EC) No 1272/2008	
Pictogram	

Signal word	Danger
Hazard statement(s)	
H301 + H311	Toxic if swallowed or in contact with skin
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.
H373	May cause damage to organs (Nose) through prolonged or repeated exposure if inhaled.
Precautionary statement(s)	
P260	Do not breathe dust/ fume/ gas/ mist/ vapours/ spray.
P280	Wear protective gloves/ protective clothing/ eye protection/ face protection.
P284	Wear respiratory protection.
P301 + P310 + P330	IF SWALLOWED: Immediately call a POISON CENTER or doctor/ physician. Rinse mouth.
P304 + P340 + P310	IF INHALED: Remove person to fresh air and keep comfortable for breathing. Immediately call a POISON CENTER or doctor/ physician.
P403 + P233	Store in a well-ventilated place. Keep container tightly closed.
Supplemental Hazard Statements	none

### 2.3 Other hazards

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

## SECTION 3: Composition/information on ingredients

### 3.1 Substances

Synonyms	: 2-(Hydroxymethyl)furan
Formula	: $C_5H_6O_2$
Molecular weight	: 98,10 g/mol
CAS-No.	: 98-00-0
EC-No.	: 202-626-1
Index-No.	: 603-018-00-2

#### Hazardous ingredients according to Regulation (EC) No 1272/2008

Component	Classification	Concentration
<b>Furfuryl alcohol</b>		
CAS-No.	98-00-0	Acute Tox. 3; Acute Tox. 2; Acute Tox. 3; Skin Irrit. 2; Eye Irrit. 2; Carc. 2; STOT SE 3; STOT RE 2; H301, H330, H311, H315, H319, H351, H335, H373
EC-No.	202-626-1	
Index-No.	603-018-00-2	
		<= 100 %

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first aid measures

#### General advice

Consult a physician. Show this safety data sheet to the doctor in attendance.



**If inhaled**

If breathed in, move person into fresh air. If not breathing, give artificial respiration. Consult a physician.

**In case of skin contact**

Wash off with soap and plenty of water. Take victim immediately to hospital. Consult a physician.

**In case of eye contact**

Rinse thoroughly with plenty of water for at least 15 minutes and consult a physician.

**If swallowed**

Do NOT induce vomiting. Never give anything by mouth to an unconscious person. Rinse mouth with water. Consult a physician.

**4.2 Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

**4.3 Indication of any immediate medical attention and special treatment needed**

No data available

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**SECTION 5: Firefighting measures****5.1 Extinguishing media****Suitable extinguishing media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide.

**5.2 Special hazards arising from the substance or mixture**

Carbon oxides

**5.3 Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

**5.4 Further information**

Use water spray to cool unopened containers.

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**SECTION 6: Accidental release measures****6.1 Personal precautions, protective equipment and emergency procedures**

Wear respiratory protection. Avoid breathing vapours, mist or gas. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Beware of vapours accumulating to form explosive concentrations. Vapours can accumulate in low areas.

For personal protection see section 8.

**6.2 Environmental precautions**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

**6.3 Methods and materials for containment and cleaning up**

Contain spillage, and then collect with an electrically protected vacuum cleaner or by wet-brushing and place in container for disposal according to local regulations (see section 13). Keep in suitable, closed containers for disposal.

**6.4 Reference to other sections**

For disposal see section 13.

---

**SECTION 7: Handling and storage****7.1 Precautions for safe handling**

Avoid contact with skin and eyes. Avoid inhalation of vapour or mist.

Keep away from sources of ignition - No smoking. Take measures to prevent the build up of electrostatic charge.

For precautions see section 2.2.

**7.2 Conditions for safe storage, including any incompatibilities**

Store in cool place. Keep container tightly closed in a dry and well-ventilated place. Containers which are opened must be carefully resealed and kept upright to prevent leakage.

Air sensitive.

Aldrich - 185930

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Storage class (TRGS 510): Non-combustible, acute toxic Cat. 1 and 2 / very toxic hazardous materials

**7.3 Specific end use(s)**

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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**SECTION 8: Exposure controls/personal protection**

**8.1 Control parameters**

**Components with workplace control parameters**

**8.2 Exposure controls**

**Appropriate engineering controls**

Avoid contact with skin, eyes and clothing. Wash hands before breaks and immediately after handling the product.

**Personal protective equipment**

**Eye/face protection**

Face shield and safety glasses Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU).

**Skin protection**

Handle with gloves. Gloves must be inspected prior to use. Use proper glove removal technique (without touching glove's outer surface) to avoid skin contact with this product. Dispose of contaminated gloves after use in accordance with applicable laws and good laboratory practices. Wash and dry hands.

The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

**Full contact**

Material: butyl-rubber

Minimum layer thickness: 0,3 mm

Break through time: 480 min

Material tested:Butoject® (KCL 897 / Aldrich Z677647, Size M)

**Splash contact**

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm

Break through time: 30 min

Material tested:Camatr® (KCL 730 / Aldrich Z677442, Size M)

data source: KCL GmbH, D-36124 Eichenzell, phone +49 (0)6659 87300, e-mail sales@kcl.de, test method: EN374

If used in solution, or mixed with other substances, and under conditions which differ from EN 374, contact the supplier of the CE approved gloves. This recommendation is advisory only and must be evaluated by an industrial hygienist and safety officer familiar with the specific situation of anticipated use by our customers. It should not be construed as offering an approval for any specific use scenario.

**Body Protection**

Complete suit protecting against chemicals. The type of protective equipment must be selected according to the concentration and amount of the dangerous substance at the specific workplace.

**Respiratory protection**

Where risk assessment shows air-purifying respirators are appropriate use a full-face respirator with multi-purpose combination (US) or type ABEK (EN 14387) respirator cartridges as a backup to engineering controls. If the respirator is the sole means of protection, use a full-face supplied air respirator. Use respirators and components tested and approved under appropriate government standards such as NIOSH (US) or CEN (EU).

**Control of environmental exposure**

Prevent further leakage or spillage if safe to do so. Do not let product enter drains.

**SECTION 9: Physical and chemical properties****9.1 Information on basic physical and chemical properties**

a) Appearance	Form: clear, liquid Colour: colourless
b) Odour	No data available
c) Odour Threshold	No data available
d) pH	No data available
e) Melting point/freezing point	Melting point/range: -29 °C - lit.
f) Initial boiling point and boiling range	170 °C - lit.
g) Flash point	65 °C - closed cup
h) Evaporation rate	No data available
i) Flammability (solid, gas)	No data available
j) Upper/lower flammability or explosive limits	Upper explosion limit: 16,3 %(V) Lower explosion limit: 1,8 %(V)
k) Vapour pressure	7,3 hPa at 55 °C 0,7 hPa at 20 °C
l) Vapour density	3,39 - (Air = 1.0)
m) Relative density	1,135 g/cm <sup>3</sup> at 25 °C
n) Water solubility	No data available
o) Partition coefficient: n-octanol/water	log Pow: 0,3 at 25 °C
p) Auto-ignition temperature	No data available
q) Decomposition temperature	No data available
r) Viscosity	No data available
s) Explosive properties	No data available
t) Oxidizing properties	No data available

**9.2 Other safety information**

Relative vapour density	3,39 - (Air = 1.0)
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**SECTION 10: Stability and reactivity****10.1 Reactivity**

No data available

**10.2 Chemical stability**

Stable under recommended storage conditions.

**10.3 Possibility of hazardous reactions**

No data available

**10.4 Conditions to avoid**

Heat, flames and sparks.

**10.5 Incompatible materials**

Do not store near acids., Oxygen, Strong oxidizing agents

- 10.6 Hazardous decomposition products**  
 Other decomposition products - No data available  
 In the event of fire: see section 5

---

**SECTION 11: Toxicological information**

**11.1 Information on toxicological effects**

**Acute toxicity**

LD50 Oral - Rat - 177 mg/kg

Remarks: Behavioral:Excitement. Behavioral:Ataxia. Cyanosis

LC50 Inhalation - Rat - male and female - 4 h - > 0,82 - < 2,07 mg/l  
 (OECD Test Guideline 403)

LD50 Dermal - Rabbit - 400 mg/kg

Remarks: Behavioral:Convulsions or effect on seizure threshold.

**Skin corrosion/irritation**

No data available

**Serious eye damage/eye irritation**

Eyes - Rabbit

Result: Moderate eye irritation - 24 h

**Respiratory or skin sensitisation**

No data available

**Germ cell mutagenicity**

Ames test

Salmonella typhimurium

Result: negative

Mouse - male

Result: negative

**Carcinogenicity**

Carcinogenicity - Rat - Inhalation

Tumorigenic:Carcinogenic by RTECS criteria. Sense Organs and Special Senses (Nose, Eye, Ear, and Taste):Olfaction:Tumors.

Carcinogenicity - Mouse - Inhalation

Tumorigenic:Carcinogenic by RTECS criteria. Kidney, Ureter, Bladder:Kidney tumors.

Limited evidence of carcinogenicity in animal studies

IARC: No component of this product present at levels greater than or equal to 0.1% is identified as probable, possible or confirmed human carcinogen by IARC.

**Reproductive toxicity**

No data available

**Specific target organ toxicity - single exposure**

Inhalation - May cause respiratory irritation. - Nose

**Specific target organ toxicity - repeated exposure**

Inhalation - May cause damage to organs through prolonged or repeated exposure. - Nose

**Aspiration hazard**

No data available

**Additional information**

Repeated dose toxicity Rat - male - Oral - NOAEL : 53 mg/kg - OECD Test Guideline 408

RTECS: LU9100000



**15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

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**SECTION 16: Other information****Full text of H-Statements referred to under sections 2 and 3.**

H301	Toxic if swallowed.
H301 + H311	Toxic if swallowed or in contact with skin
H311	Toxic in contact with skin.
H315	Causes skin irritation.
H319	Causes serious eye irritation.
H330	Fatal if inhaled.
H335	May cause respiratory irritation.
H351	Suspected of causing cancer.
H373	May cause damage to organs (/S/*_ORG_REP_INHA/\$/) through prolonged or repeated exposure if inhaled.

**Further information**

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The above information is believed to be correct but does not purport to be all inclusive and shall be used only as a guide. The information in this document is based on the present state of our knowledge and is applicable to the product with regard to appropriate safety precautions. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

## 1-Butanol information:



## SAFETY DATA SHEET

Creation Date 21-Jan-2009

Revision Date 15-Jul-2013

Revision Number 6

**SECTION 1: IDENTIFICATION OF THE SUBSTANCE/MIXTURE AND OF THE COMPANY/UNDERTAKING**
**1.1. Product identifier**

<b>Product Description:</b>	<b>1-Butanol</b>
<b>Cat No.</b>	232080000; 232080010; 232080025; 232080250
<b>Synonyms</b>	n-Butanol; n-Butyl alcohol, Butan-1-ol
<b>CAS-No</b>	71-36-3
<b>EC-No.</b>	200-751-6
<b>Molecular Formula</b>	C4 H10 O
<b>Reach Registration Number</b>	01-2119484630-38

**1.2. Relevant identified uses of the substance or mixture and uses advised against**

<b>Recommended Use</b>	Laboratory chemicals
<b>Uses advised against</b>	No information available

**1.3. Details of the supplier of the safety data sheet**

<b>Company</b>	Acros Organics BVBA Janssen Pharmaceuticaaan 3a 2440 Geel, Belgium
<b>E-mail address</b>	bege1.sdsdesk@thermofisher.com

**1.4. Emergency telephone number**

For information US call: 001-800-ACROS-01 / Europe call: +32 14 57 52 11  
 Emergency Number US:001-201-796-7100 / Europe: +32 14 57 52 99  
 CHEMTREC Tel. No.US:001-800-424-9300 / Europe:001-703-527-3887

**SECTION 2: HAZARDS IDENTIFICATION**
**2.1. Classification of the substance or mixture****CLP Classification - Regulation (EC) No 1272/2008**

<b>Physical hazards</b>	
Flammable liquids	Category 3

**Health hazards**

Acute oral toxicity	Category 4
Skin Corrosion/Irritation	Category 2
Serious Eye Damage/Eye Irritation	Category 1
Specific target organ toxicity - (single exposure)	Category 3

**Environmental hazards**

Based on available data, the classification criteria are not met

Classification according to EU Directives 67/548/EEC or 1999/45/EC  
 Symbol(s) Xn - Harmful

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**SECTION 2: HAZARDS IDENTIFICATION**

R-phrases(s)	R10 - Flammable R22 - Harmful if swallowed R41 - Risk of serious damage to eyes R67 - Vapors may cause drowsiness and dizziness R37/38 - Irritating to respiratory system and skin
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For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16

**2.2. Label elements**

Signal Word

Danger

**Hazard Statements**

H226 - Flammable liquid and vapor  
H315 - Causes skin irritation  
H302 - Harmful if swallowed  
H336 - May cause drowsiness or dizziness  
H318 - Causes serious eye damage  
H335 - May cause respiratory irritation

**Precautionary Statements**

P280 - Wear protective gloves/ protective clothing/ eye protection/ face protection  
P305 + P351 + P338 - IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing  
P301 + P312 - IF SWALLOWED: Call a POISON CENTER or doctor/ physician if you feel unwell  
P304 + P340 - IF INHALED: Remove to fresh air and keep at rest in a position comfortable for breathing  
P210 - Keep away from heat/sparks/open flames/hot surfaces. - No smoking  
P303 + P361 + P353 - IF ON SKIN (or hair): Remove/ Take off immediately all contaminated clothing. Rinse skin with water/ shower

**2.3. Other hazards**

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB)

**SECTION 3: COMPOSITION/INFORMATION ON INGREDIENTS****3.1. Substances**

Component	CAS-No.	EC-No.	Weight %	CLP Classification - Regulation (EC) No	DSD Classification - 67/548/EEC
n-Butyl alcohol	71-36-3	EEC No. 200-751-6	99	1722/2008 Flam. Liq. 3 (H226) Acute Tox. 4 (H302) Skin Irrit. 2 (H315) Eye Dam. 4 (H318) STOT SE 3 (H335) STOT SE 3 (H336)	R10 Xn; R22 Xi; R37/38-41 R67

Reach Registration Number

01-2119484630-38

For the full text of the R-phrases and H-Statements mentioned in this Section, see Section 16



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**SECTION 4: FIRST AID MEASURES****4.1. Description of first aid measures**

<b>Eye Contact</b>	Rinse immediately with plenty of water, also under the eyelids, for at least 15 minutes. Obtain medical attention.
<b>Skin Contact</b>	Wash off immediately with plenty of water for at least 15 minutes. Get medical attention if symptoms occur..
<b>Ingestion</b>	Do not induce vomiting. Rinse mouth. Drink plenty of water. Call a physician or Poison Control Center immediately.
<b>Inhalation</b>	Move to fresh air. If breathing is difficult, give oxygen. Do not use mouth-to-mouth resuscitation if victim ingested or inhaled the substance; induce artificial respiration with a respiratory medical device. Obtain medical attention.
<b>Protection of First-aiders</b>	Ensure that medical personnel are aware of the material(s) involved, take precautions to protect themselves and prevent spread of contamination

**4.2. Most important symptoms and effects, both acute and delayed**

Breathing difficulties. . Causes eye burns. Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

**4.3. Indication of any immediate medical attention and special treatment needed**

**Notes to Physician** Treat symptomatically. Symptoms may be delayed.

**SECTION 5: FIREFIGHTING MEASURES****5.1. Extinguishing media****Suitable Extinguishing Media**

Use water spray, alcohol-resistant foam, dry chemical or carbon dioxide. Cool closed containers exposed to fire with water spray.

**Extinguishing media which must not be used for safety reasons**

Do not use a solid water stream as it may scatter and spread fire.

**5.2. Special hazards arising from the substance or mixture**

Flammable. Risk of ignition. Containers may explode when heated. Vapors may form explosive mixtures with air. Vapors may travel to source of ignition and flash back.

**Hazardous Combustion Products**

Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).

**5.3. Advice for firefighters**

As in any fire, wear self-contained breathing apparatus pressure-demand, MSHA/NIOSH (approved or equivalent) and full protective gear. Thermal decomposition can lead to release of irritating gases and vapors.

**SECTION 6: ACCIDENTAL RELEASE MEASURES****6.1. Personal precautions, protective equipment and emergency procedures**

Wear protective gloves and eye/face protection. Ensure adequate ventilation. Remove all sources of ignition. Take precautionary measures against static discharges.

**6.2. Environmental precautions**

Should not be released into the environment. Prevent spreading of vapors through sewers, ventilation systems and confined areas..

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**6.3. Methods and material for containment and cleaning up**

Soak up with inert absorbent material. Keep in suitable, closed containers for disposal. Remove all sources of ignition. Use spark-proof tools and explosion-proof equipment. Take precautionary measures against static discharges.

**6.4. Reference to other sections**

Refer to protective measures listed in Sections 8 and 13.

**SECTION 7: HANDLING AND STORAGE****7.1. Precautions for safe handling**

Wear personal protective equipment. Do not get in eyes, on skin, or on clothing. Do not breathe vapors or spray mist. Keep away from open flames, hot surfaces and sources of ignition. Use only non-sparking tools. Use explosion-proof equipment. Take precautionary measures against static discharges.

**7.2. Conditions for safe storage, including any incompatibilities**

Keep containers tightly closed in a dry, cool and well-ventilated place. Keep away from heat and sources of ignition. Flammables area.

**7.3. Specific end use(s)**

Use in laboratories

**SECTION 8: EXPOSURE CONTROLS/PERSONAL PROTECTION****8.1. Control parameters****Exposure limits**

List source(s):

UK - EH40/2005 Containing the workplace exposure limits (WELs) for use with the Control of Substances Hazardous to Health Regulations (COSHH) 2002 (as amended). Updated by September 2006 official press release and October 2007 Supplement.  
IRE - 2010 Code of Practice for the Safety, Health and Welfare at Work (Chemical Agents) Regulations 2001. Published by the Health and Safety Authority.

Component	European Union	The United Kingdom	France	Belgium	Spain
n-Butyl alcohol		50ppm STEL; 154mg/m <sup>3</sup> STEL	STEL / VLCT: 50 ppm. STEL / VLCT: 150 mg/m <sup>3</sup> .	50ppm VLE; 154mg/m <sup>3</sup> VLE	STEL / VLA-EC: 50 ppm (15 minutos). STEL / VLA-EC: 154 mg/m <sup>3</sup> (15 minutos). Piel
Component	Italy	Germany	Portugal	The Netherlands	Finland
n-Butyl alcohol		100ppm TVA; 310mg/m <sup>3</sup> TVA	TWA: 20 ppm 8 horas	15ppm STEL; 45mg/m <sup>3</sup> STEL	TWA: 50 ppm 8 tuntaina TWA: 150 mg/m <sup>3</sup> 8 tuntaina STEL: 75 ppm 15 minuutteina STEL: 230 mg/m <sup>3</sup> 15 minuutteina Skin
Component	Austria	Denmark	Switzerland	Poland	Norway
n-Butyl alcohol	STEL: 200 ppm 15 Minuten STEL: 600 mg/m <sup>3</sup> 15 Minuten TWA: 50 ppm 8 Stunden TWA: 150 mg/m <sup>3</sup> 8 Stunden	Ceiling: 50 ppm Ceiling: 150 mg/m <sup>3</sup> Skin	STEL: 50 ppm 15 Minuten STEL: 150 mg/m <sup>3</sup> 15 Minuten MAK: 50 ppm 8 Stunden MAK: 150 mg/m <sup>3</sup> 8 Stunden	NDSCR: 150 mg/m <sup>3</sup> 15 minulach TWA: 50 mg/m <sup>3</sup> 8 godzinach Skóra	Skin Ceiling: 25 ppm Ceiling: 75 mg/m <sup>3</sup>

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Component n-Butyl alcohol	<b>Bulgaria</b> TWA: 100.0 mg/m <sup>3</sup> STEL : 150.0 mg/m <sup>3</sup>	<b>Croatia</b> Skin notation STEL: 50 ppm 15 minutama. STEL: 154 mg/m <sup>3</sup> 15 minutama.	<b>Ireland</b> STEL: 25 ppm 15 min STEL: 75 mg/m <sup>3</sup> 15 min Skin	<b>Cyprus</b>	<b>Czech Republic</b> TWA: 300 mg/m <sup>3</sup> 8 hodinich. Potential for cutaneous absorption Ceiling: 600 mg/m <sup>3</sup>
	<b>Estonia</b> Skin notation TWA: 15 ppm 8 tundides. TWA: 45 mg/m <sup>3</sup> 8 tundides. Ceiling: 30 ppm Ceiling: 90 mg/m <sup>3</sup>	<b>Gibraltar</b>	<b>Greece</b> skin - potential for cutaneous absorption STEL: 100 ppm STEL: 300 mg/m <sup>3</sup> TWA: 100 ppm TWA: 300 mg/m <sup>3</sup>	<b>Hungary</b> STEL: 90 mg/m <sup>3</sup> 15 percenkben. TWA: 45 mg/m <sup>3</sup> 8 oraban. potential for cutaneous absorption	<b>Iceland</b> STEL: 50 ppm STEL: 150 mg/m <sup>3</sup> TWA: 25 ppm 8 klukkustundum. TWA: 80 mg/m <sup>3</sup> 8 klukkustundum. Skin notation Ceiling: 50 ppm Ceiling: 160 mg/m <sup>3</sup>
Component n-Butyl alcohol	<b>Latvia</b> TWA: 10 mg/m <sup>3</sup>	<b>Lithuania</b> Ceiling: 30 ppm Ceiling: 90 mg/m <sup>3</sup> TWA: 15 ppm TWA: 45 mg/m <sup>3</sup> Skin notation	<b>Luxembourg</b>	<b>Malta</b>	<b>Romania</b> TWA: 33 ppm 8 ore TWA: 100 mg/m <sup>3</sup> 8 ore STEL: 66 ppm 15 minute STEL: 200 mg/m <sup>3</sup> 15 minute
	<b>Russia</b> STEL: 30 mg/m <sup>3</sup> vapor	<b>Slovak Republic</b> Ceiling: 310 mg/m <sup>3</sup> TWA: 100 ppm TWA: 310 mg/m <sup>3</sup>	<b>Slovenia</b> TWA: 100 ppm 8 urah TWA: 310 mg/m <sup>3</sup> 8 urah STEL: 100 ppm 15 minutah STEL: 310 mg/m <sup>3</sup> 15 minutah	<b>Sweden</b> LLV: 15 ppm 8 timmar. LLV: 45 mg/m <sup>3</sup> 8 timmar. Skin notation CLV: 30 ppm CLV: 90 mg/m <sup>3</sup>	<b>Turkey</b>

**Biological limit values**

List source(s):

Component n-Butyl alcohol	<b>European Union</b>	<b>United Kingdom</b>	<b>France</b>	<b>Spain</b>	<b>Germany</b> 1-Butanol: 10 mg/g urine end of shift measured as mg/g Creatinine 1-Butanol: 2 mg/g urine before beginning of next shift measured as mg/g Creatinine

**Monitoring methods**

BS EN 14042:2003 Title Identifier: Workplace atmospheres. Guide for the application and use of procedures for the assessment of exposure to chemical and biological agents.

MDHS70 General methods for sampling airborne gases and vapours

MDHS 58 Volatile organic compounds in air. Laboratory method using diffusive samplers, solvent desorption and gas chromatography

MDHS 56 Volatile organic compounds in air - Laboratory method using pumped solid sorbent tubes, solvent desorption and gas chromatography

**Derived No Effect Level (DNEL)** See table for values

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Route of exposure	Acute effects (local)	Acute effects (systemic)	Chronic effects (local)	Chronic effects (systemic)
Oral				
Dermal				
Inhalation				310 mg/m <sup>3</sup> 100 ppm

**Predicted No Effect Concentration (PNEC)** See values below.

Fresh water	0.082 mg/l
Fresh water sediment	0.178 mg/kg
Marine water	0.0082 mg/l
Marine water sediment	0.0178 mg/kg
Soil (Agriculture)	0.015 mg/kg

**8.2. Exposure controls****Engineering Measures**

Ensure that eyewash stations and safety showers are close to the workstation location. Ensure adequate ventilation, especially in confined areas. Use explosion-proof electrical/ventilating/lighting/equipment. Wherever possible, engineering control measures such as the isolation or enclosure of the process, the introduction of process or equipment changes to minimise release or contact, and the use of properly designed ventilation systems, should be adopted to control hazardous materials at source.

**Personal protective equipment**

**Eye Protection** Goggles (European standard - EN 166)

**Hand Protection** Protective gloves

Glove material	Breakthrough time	Glove thickness	EU standard	Glove comments
Butyl rubber	> 480 minutes	0.35 mm	EN 374	As tested under EN374-3 Determination of Resistance to Permeation by Chemicals
Nitrile rubber	> 480 minutes	0.38 mm	Level 6	
Neoprene	> 480 minutes	0.45 mm		
Viton (R)	> 480 minutes	0.7 mm		

Inspect gloves before use.

Please observe the instructions regarding permeability and breakthrough time which are provided by the supplier of the gloves. (Refer to manufacturer/supplier for information)

Ensure gloves are suitable for the task: Chemical compatibility, Dexterity, Operational conditions, User susceptibility, e.g. sensitisation effects, also take into consideration the specific local conditions under which the product is used, such as the danger of cuts, abrasion. Remove gloves with care avoiding skin contamination.

**Skin and body protection** Wear appropriate protective gloves and clothing to prevent skin exposure

**Respiratory Protection** When workers are facing concentrations above the exposure limit they must use appropriate certified respirators  
To protect the wearer, respiratory protective equipment must be the correct fit and be used and maintained properly.

**Large scale/emergency use** Use a NIOSH/MSHA or European Standard EN 136 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended Filter type:** Organic gases and vapours filter, Type A, Brown, conforming to EN14387.

**Small scale/Laboratory use** Use a NIOSH/MSHA or European Standard EN 149:2001 approved respirator if exposure limits are exceeded or if irritation or other symptoms are experienced.  
**Recommended half mask:-** Valve filtering: EN405 or Half mask: EN140 plus filter, EN 141  
When RPE is used a face piece Fit Test should be conducted.

**Hygiene Measures** Handle in accordance with good industrial hygiene and safety practice

**Environmental exposure controls** No information available.

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**SECTION 9: PHYSICAL AND CHEMICAL PROPERTIES****9.1. Information on basic physical and chemical properties**

Appearance	Colorless	
Physical State	Liquid.	
Odor	Alcohol-like	
Odor Threshold	No data available	
pH	No information available.	
Melting Point/Range	-89°C / -128.2°F	
Softening Point	No data available	
Boiling Point/Range	117.8°C / 243.7°F	
Flash Point	35°C / 95°F	Method - Closed cup
Evaporation Rate	0.46	(Butyl Acetate = 1.0)
Flammability (solid, gas)	Not applicable	Liquid
Explosion Limits	Lower 1.4 Vol% Upper 11.2 Vol%	
Vapor Pressure	6.7 mbar @ 20 °C	
Vapor Density	2.6	(Air = 1.0)
Specific Gravity / Density	0.810	
Bulk Density	Not applicable	Liquid
Water Solubility	80 g/L (20°C)	
Solubility in other solvents	No information available.	
Partition Coefficient (n-octanol/water)	Component n-Butyl alcohol	log Pow 0.785
Autoignition Temperature	340°C / 644°F	
Decomposition temperature	No data available	
Viscosity	2.95 mPa.s (20 °C)	
Explosive Properties	No information available.	explosive air/vapour mixtures possible
Oxidizing Properties	No information available.	

**9.2. Other information**

Molecular Formula	C4 H10 O
Molecular Weight	74.12
Refractive index	1.390 - 1.400

**SECTION 10: STABILITY AND REACTIVITY**

**10.1. Reactivity** None known, based on information available.

**10.2. Chemical stability** Stable under normal conditions.

**10.3. Possibility of hazardous reactions**

**Hazardous Polymerization** Hazardous polymerization does not occur.  
**Hazardous Reactions** None under normal processing.

**10.4. Conditions to avoid**

Incompatible products, Heat, flames and sparks, Keep away from open flames, hot surfaces and sources of ignition.

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**10.5. Incompatible materials**

Strong oxidizing agents. Reducing agents. Acid chlorides. copper. Copper alloys. Acid anhydrides.

**10.6. Hazardous decomposition products**Carbon monoxide (CO), Carbon dioxide (CO<sub>2</sub>).**SECTION 11: TOXICOLOGICAL INFORMATION****11.1. Information on toxicological effects****Product Information****(a) acute toxicity;**Oral  
Dermal  
Inhalation

Category 4

Based on available data, the classification criteria are not met  
Based on available data, the classification criteria are not met

Component	LD50 Oral	LD50 Dermal	LC50 Inhalation
n-Butyl alcohol	790 mg/kg ( Rat )	3400 mg/kg ( Rabbit )	8000 ppm ( Rat ) 4 h 17.7 mg/L ( Rat ) 4 h

**(b) skin corrosion/irritation;**

Category 2

**(c) serious eye damage/irritation;**

Category 1

**(d) respiratory or skin sensitization;**Respiratory  
SkinBased on available data, the classification criteria are not met  
Based on available data, the classification criteria are not met**(e) germ cell mutagenicity;**

Based on available data, the classification criteria are not met

Mutagenic effects have occurred in experimental animals.

**(f) carcinogenicity;**

Based on available data, the classification criteria are not met

There are no known carcinogenic chemicals in this product

**(g) reproductive toxicity;**Reproductive Effects  
Developmental Effects  
TeratogenicityBased on available data, the classification criteria are not met  
Experiments have shown reproductive toxicity effects on laboratory animals.  
Developmental effects have occurred in experimental animals.  
Teratogenic effects have occurred in experimental animals..**(h) STOT-single exposure;**

Category 3

**(i) STOT-repeated exposure;**

Based on available data, the classification criteria are not met

Target Organs

Skin, Respiratory system, Eyes.

**(j) aspiration hazard;**

Based on available data, the classification criteria are not met

**Symptoms / effects,  
both acute and delayed**

Symptoms of overexposure may be headache, dizziness, tiredness, nausea and vomiting.

**SECTION 12: ECOLOGICAL INFORMATION****12.1. Toxicity**

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**SECTION 12: ECOLOGICAL INFORMATION****Ecotoxicity effects**

Component	Freshwater Fish	Water Flea	Freshwater Algae	Microtox
n-Butyl alcohol	1740 mg/L LC50 96 h 1910000 µg/L LC50 96 h 100000-500000 µg/L LC50 96 h 1730-1910 mg/L LC50 96 h	1983 mg/L EC50 = 48 h 1897 - 2072 mg/L EC50 = 48 h	500 mg/L EC50 > 96 h 500 mg/L EC50 > 72 h	EC50 = 2041.4 mg/L 5 min EC50 = 2186 mg/L 30 min EC50 = 3980 mg/L 24 h EC50 = 4400 mg/L 17 h

**12.2. Persistence and degradability**

**Persistence** Soluble in water, Persistence is unlikely, based on information available.

Component	Degradability
n-Butyl alcohol	70 %

**12.3. Bioaccumulative potential**

Does not bioaccumulate

Component	log Pow	Bioconcentration factor (BCF)
n-Butyl alcohol	0.785	0.64

**12.4. Mobility in soil**

The product is water soluble, and may spread in water systems. . Will likely be mobile in the environment due to its water solubility. Highly mobile in soils.

**12.5. Results of PBT and vPvB assessment**

Substance is not considered persistent, bioaccumulative and toxic (PBT) / very persistent and very bioaccumulative (vPvB).

**12.6. Other adverse effects****Endocrine Disruptor Information**

This product does not contain any known or suspected endocrine disruptors

**Persistent Organic Pollutant**

This product does not contain any known or suspected substance

**Ozone Depletion Potential**

This product does not contain any known or suspected substance

**SECTION 13: DISPOSAL CONSIDERATIONS****13.1. Waste treatment methods****Waste from Residues / Unused Products**

Waste is classified as hazardous. Dispose of in accordance with the European Directives on waste and hazardous waste. Dispose of in accordance with local regulations.

**Contaminated Packaging**

Dispose of this container to hazardous or special waste collection point. Empty containers retain product residue, (liquid and/or vapor), and can be dangerous. Keep product and empty container away from heat and sources of ignition.

**European Waste Catalogue (EWC)**

According to the European Waste Catalogue, Waste Codes are not product specific, but application specific.

**Other Information**

Waste codes should be assigned by the user based on the application for which the product was used. Do not dispose of waste into sewer. Can be incinerated, when in compliance with local regulations. Do not empty into drains.

**SECTION 14: TRANSPORT INFORMATION****IMDG/IMO****14.1. UN number**

UN1120

**14.2. UN proper shipping name**

BUTANOLS

**14.3. Transport hazard class(es)**

3

**14.4. Packing group**

III

**ADR**

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14.1. UN number	UN1120
14.2. UN proper shipping name	BUTANOLS
14.3. Transport hazard class(es)	3
14.4. Packing group	III
<b>IATA</b>	
14.1. UN number	UN1120
14.2. UN proper shipping name	BUTANOLS
14.3. Transport hazard class(es)	3
14.4. Packing group	III
14.5. Environmental hazards	No hazards identified
14.6. Special precautions for user	No special precautions required
14.7. Transport in bulk according to Annex II of MARPOL73/78 and the IBC Code	Not applicable, packaged goods

**SECTION 15: REGULATORY INFORMATION****15.1. Safety, health and environmental regulations/legislation specific for the substance or mixture**

International Inventories X = listed

Component	EINECS	ELINCS	NLP	TSCA	DSL	NDSL	PICCS	ENCS	CHINA	AICS	KECL
n-Butyl alcohol	200-781-6	-		X	X	-	X	X	X	X	X

**National Regulations**

Component	Germany - Water Classification (Vw/VwS)	Germany - TA-Luft Class
n-Butyl alcohol	WGK 1	

Component	France - INRS (Tables of occupational diseases) Tableaux des maladies professionnelles (TMP) - RG 84
n-Butyl alcohol	

Take note of Control of Substances Hazardous to Health Regulations (COSHH) 2002 and 2005 Amendment

Take note of Dir 94/33/EC on the protection of young people at work

Take note of Directive 98/24/EC on the protection of the health and safety of workers from the risks related to chemical agents at work

**15.2. Chemical safety assessment**

A Chemical Safety Assessment/Report (CSA/CSR) has been conducted by the manufacturer/importer

**SECTION 16: OTHER INFORMATION****Full text of R-phrases referred to under sections 2 and 3**

R10 - Flammable  
 R22 - Harmful if swallowed  
 R41 - Risk of serious damage to eyes  
 R67 - Vapors may cause drowsiness and dizziness  
 R37/38 - Irritating to respiratory system and skin

**Full text of H-Statements referred to under sections 2 and 3**

H228 - Flammable liquid and vapor  
 H302 - Harmful if swallowed  
 H315 - Causes skin irritation  
 H318 - Causes serious eye damage  
 H335 - May cause respiratory irritation  
 H336 - May cause drowsiness or dizziness

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**Legend**

CAS - Chemical Abstracts Service	TSCA - United States Toxic Substances Control Act Section 8(b) Inventory
EINECS/ELINCS - European Inventory of Existing Commercial Chemical Substances/EU List of Notified Chemical Substances	DSL/NDSL - Canadian Domestic Substances List/Non-Domestic Substances List
PICS - Philippines Inventory of Chemicals and Chemical Substances	ENCS - Japan Existing and New Chemical Substances
IECS - China Inventory of Existing Chemical Substances	AICS - Australian Inventory of Chemical Substances
KECL - Existing and Evaluated Chemical Substances	NZIC - New Zealand Inventory of Chemicals
WEL - Workplace Exposure Limit	TWA - Time Weighted Average
ACGIH - American Conference of Industrial Hygiene	IARC - International Agency for Research on Cancer
DNEL - Derived No Effect Level	PNEC - Predicted No Effect Concentration
RPE - Respiratory Protective Equipment	LD50 - Lethal Dose 50%
LC50 - Lethal Concentration 50%	EC50 - Effective Concentration 50%
NOEC - No Observed Effect Concentration	POW - Partition coefficient Octanol/Water
PBT - Persistent, Bioaccumulative, Toxic	vPvS - very Persistent, very Bioaccumulative
ADR - European Agreement Concerning the International Carriage of Dangerous Goods by Road	ICAO/IATA - International Civil Aviation Organization/International Air Transport Association
IMO/IMDG - International Maritime Organization/International Maritime Dangerous Goods Code	MARPOL - International Convention for the Prevention of Pollution from Ships
OECD - Organisation for Economic Co-operation and Development	ATE - Acute Toxicity Estimate
BCF - Bioconcentration factor	VOC - Volatile Organic Compounds

**Key literature references and sources for data**

Suppliers safety data sheet,  
Chemadvisor - LOLI,  
Merck index,  
RTECS

**Training Advice**

Chemical hazard awareness training, incorporating labelling, Safety Data Sheets (SDS), Personal Protective Equipment (PPE) and hygiene.  
Use of personal protective equipment, covering appropriate selection, compatibility, breakthrough thresholds, care, maintenance, fit and standards.  
First aid for chemical exposure, including the use of eye wash and safety showers.  
Fire prevention and fighting, identifying hazards and risks, static electricity, explosive atmospheres posed by vapours and dusts.  
Chemical incident response training.

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Revision Summary	
Reason for revision	Update to Format, (M)SDS sections updated, 8, 11, 15, 16.

**This safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006****Disclaimer**

The information provided on this Safety Data Sheet is correct to the best of our knowledge, information and belief at the date of its publication. The information given is designed only as a guide for safe handling, use, processing, storage, transportation, disposal and release and is not to be considered as a warranty or quality specification. The information relates only to the specific material designated and may not be valid for such material used in combination with any other material or in any process, unless specified in the text.

**End of Safety Data Sheet**



