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Simulation of cyclohexane production using free software DWSIM

Simulación de la producción de ciclohexano mediante la utilización del software libre DWSIM

SOTO-CASTRO, Luis[1]†, CORTÉS-CAMPOS, M. de Lourdes[2]*, MARTÍNEZ-VÁZQUEZ, J. Merced and RODRÍGUEZ-ORTIZ, Gabriel[1]

[1]*Universidad Politécnica de Juventino Rosas, Ingeniería Metalúrgica. Hidalgo 102, Comunidad de Valencia, Santa Cruz de Juventino Rosas, Gto. 38253.*
[2]*Universidad Politécnica de Guanajuato, Ingeniería Agroindustrial. Avenida Universidad Norte s/n, Cortazar, Gto. 38294*

ID 1st Author: *Luis, Soto-Castro* / **ORC ID**: 0000-0002-6230-3846, **CVU CONACYT ID**: 93450

ID 1st Co-author: *M. de Lourdes, Cortés-Campos* / **ORC ID**: 0000-0003-1267-2560

ID 2nd Co-author: *J. Merced, Martínez-Vázquez* / **ORC ID**: 0000-0002-3702-4853, **CVU CONACYT ID**: 48565

ID 3rd Co-author: *Gabriel, Rodríguez-Ortiz* / **ORC ID**: 0000-0001-9967-0642, **CVU CONACYT ID**: 100227

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Abstract

Cyclohexane is mainly used as a precursor to cyclohexanol and cyclohexanone. Caprolactam and adipic acid are obtained from them, which are used to produce nylon-6 and nylon-66. Cyclohexane is a volatile, colorless, flammable, non-corrosive, non-polar liquid whose most notable physical property is its insolubility in water and the azeotropes it forms with a variety of chemical products. The most common method of obtaining cyclohexane is the hydrogenation of benzene. The production of cyclohexane in the current market is closely linked to the demand for such a product, as well as the importance of the raw material from which it is obtained, specifically benzene. In the present work, the design of a cyclohexane production plant from the hydrogenation of benzene is presented. For the simulation and modeling of the plant, the DWSIM tool has been used. The starting data was taken from the Aspen Plus Costing manual of 1988, with this simulation the results obtained from the free software DWSIM and the commercial software ASPEN Plus were compared.

Simulation, DWSIM, Cyclohexane

Resumen

El ciclohexano se emplea principalmente como precursor del ciclohexanol y la ciclohexanona. De ellos se obtienen caprolactama y ácido adípico, que sirven para producir nylon-6 y nylon-66. El ciclohexano es un líquido volátil, incoloro, inflamable, no corrosivo, no polar cuya propiedad física más destacable es la insolubilidad en agua y los azeótropos que forma con variedad de productos químicos. El método más común para obtener ciclohexano es la hidrogenación de benceno. La producción de ciclohexano en el mercado actual está íntimamente ligada con la demanda que presenta tal producto, así como con la importancia que posee la materia prima de la cual se obtiene, en concreto el benceno. En el presente trabajo se presenta el diseño de una planta productora de ciclohexano a partir de la hidrogenación de benceno. Para la simulación y modelado de la planta se ha hecho uso de la herramienta DWSIM. Los datos de partida fueron tomados del manual Aspen Plus Costing de 1988, con esta simulación se compararon los resultados obtenidos del software libre DWSIM y el software comercial ASPEN Plus.

Simulación, DWSIM, Ciclohexano

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*Correspondence to Author (e-mail: mcortes@upgto.edu.mx)
† Researcher contributing as first Author.

Introducción

It is known that the methodological procedure to solve a problem in engineering consists of representing it in a correct and precise way, to obtain a substitution of the real system by a more adequate one for the formal treatment. In general, the logical-mathematical tools provide a useful framework to represent by means of a system of symbols and rules, the behavior of real systems.

The scientific method helps us to consolidate laws and theories in different areas of knowledge, which are understandable by means of differential equations, for example. In other words, we are able to recreate a new system, of which we know its rules and symbols, such as of which we know its rules and symbols, as the result of a process of abstraction from the environment [1].

Process simulation using computer software has become popular among researchers today. However, publications related to this field using open source as its simulation platform have not yet been seen [2], so the present work shows the results obtained with the free simulation software DWSIM and compares them with those obtained using ASPEN Plus.

The existing processes for obtaining cyclohexane comprise all those developed at the industrial level to meet market demands. These processes differ mainly in several aspects: nature of the catalyst, operating conditions, reactor design, heat dissipation, extractant agent [3].

Regarding their production, there are two commercial alternative methods:

1. Extraction of cyclohexane from crude oil streams.

Cyclohexane can be distilled directly from naphtha. The starting concentration of cyclohexane in the naphtha fraction of crude oil is in the range of 0.5% to 5% by volume. The presence of several hydrocarbons with a boiling point in the same range, such as n-hexane, isohexanes, methylcyclopentane, benzene and dimethylpentanes, makes the recovery of cyclohexane from crude oil by fractional distillation or recrystallization difficult and expensive.

The difficulty of separating cyclohexane from naphtha is highlighted by the fact that in 1991 only one company, Phillips Petroleum, produced cyclohexane by distillation. Despite this, cyclohexane is manufactured through simple distillation with 85% purity by weight in commercial quantities by fractionation of naphtha from natural gasoline, then this stream can finally be treated in extractive distillation columns, where it is possible to obtain cyclohexane with a purity of 98% purity.

2. Hydrogenation of benzene.

It is based on the catalytic hydrogenation of benzene, forming cyclohexane as a product. Benzene hydrogenation is not only of great interest to the petroleum industry but also to the environment. The U.S. Environmental Protection Agency (EPA) under the Clean Air Act requires that gasoline contain less than 1.0% by volume of benzene. To comply with this regulation, refiners have implemented various techniques to reduce benzene levels in gasoline, which otherwise contains approximately 2 to 3% benzene [4].

Most of the cyclohexane is obtained by hydrogenation of benzene. Therefore, in this work, this process is analyzed. The 90% of the cyclohexane produced that is obtained by hydrogenation of benzene is used in the production processes of nylon 6 and nylon 66, although it is also used to produce esters, plasticizers, synthetic lubricants, polyurethanes and as a food acidulant, but the quantities of total cyclohexane produced in the world for these uses is low [5].

Since the last century, several industrial processes using this method have been invented; all of them are based on provoking the hydrogenation reaction, and then purifying and conditioning the final product [6].

Process description

In the cyclohexane production process, one of the most important parameters is the starting feedstock. The hydrogenation of benzene requires a high purity of the feedstock, benzene. Nowadays, the purity of the raw material is not an impediment to the development of the reaction since sufficiently advanced technologies are available to obtain benzene of very high purity.

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Catalytic hydrogenation is a reversible, highly exothermic reaction, as shown below:

$$C_6H_6 + 3H_2 \leftrightarrow C_6H_{12} \quad (1)$$

This benzene hydrogenation process comprises two main phases:

1. Reaction phase for the transformation of the feedstock into the process of interest.

2. Purification and conditioning process of the final product obtained.

For the simulation, data collected from a plant presented in a course on Modeling and Simulation of Chemical Processes (DIQUIMICA, 2012-2013) and by the Aspen Plus Costing manual of 1988 [7] will be taken.

The process is composed of the equipment necessary to carry out the basic reaction and separation operations. The benzene fed to the plant can come from the following sources:

1. Catalytic reforming of naphtha.

2. Desalkylation of toluene

3. Recovery of gasoline from pyrolysis plant ethylene pyrolysis, coke oven

4. Selective disproportionation of toluene [8].

In the feed enters a first stream of hydrogen (H) rich gas with a minimum amount of impurities, such as nitrogen and methane, with a molar flow of 313 kmol/h; a second stream of pure liquid benzene, with a molar flow of 100 kmol/h; both streams enter a mixer at a pressure of 330 psi, the mixture of the streams is preheated to the reaction temperature and pass through a conversion reactor, as observed in Figure 1. A conversion of 99.8 % benzene was established.

Figure 1 Schematic of the benzene hydrogenation process

The reactor product is taken to a separator, at a temperature of 120ºF, where the purification of the product begins, with the separation of the liquid stream and the gas stream. What comes out in the vapor phase is hydrogen, and the liquid phase is processed to obtain a cyclohexane of higher purity.

Methodology

In the simulation, the hydrogen-rich gas stream was considered to have a purity level of less than 100%, the impurities are formed by two components, nitrogen (N) and methane (CH4). The mole fractions of the input components were: 97.5% H2, 2% CH4 and 0.5% N2.

The steps followed were:

1. Determine the components in the plant along the process:

2. Choice of the thermodynamic method; it represents the crucial part, since an erroneous selection leads to deviations in the estimation of the properties of the substances that correlates with important perturbations in the global calculation of the process. In this case the thermodynamic method chosen is the Soave-Redlich-Kwong (SRK).

3. Equipment specifications, at this point the process input variables were selected.

Results

The components that were present during the simulation are shown in Table 1.

Compounds
Benzene (C_6H_6)
Hydrogen (H_2)
Nitrogen (N_2)
Methane (CH_4)
Cyclohexane (C_6H_{12})

Table 1 Compounds used in the simulation

The simulated equipment and their input specifications are shown in Table 2.

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Equipment	Specifications
Mixer	Input current Output current
Heat exchanger	Heater Spray pressure: 0 Pa Efficiency: 100%. Outlet temperature: 330 °F
Reactor	Co-inversion reactor Conversion reaction Base component: benzene Phase: mixture
Flash Separator	Type: adiabatic Temperature: 120 °F Pressure: 310 psi

Table 2 Equipment specifications

The simulation results are shown in Table 3.

Property	Vapor	Product	H_2	C_6H_6
Temperature (°F)	120	120	120	100
Pressure (psi)	310	310	335	15
Molar flow (kmol/h)	10.112	103.48	313	100
Mole fraction H_2	0.4986	0.007	0.975	0
Mole fraction C_6H_6	0.0006	0.002	0	1
Mole fraction C_6H_{12}	0.0203	0.9623	0	0

Table 3 Simulation results

Table 4 shows the comparison of the results obtained with DWSIM and ASPEN Plus.

Component	DWSIM	ASPEN Plus
Benzene	0.002	0.0013
Hydrogen	0.007	0.004
Cyclohexane	0.9623	0.9679

Table 4 Comparison of the results obtained with DWSIM and ASPEN Plus, shown in mole fraction

The input parameters in both simulations were the same: comparing the results shows a difference of 5.79% in the mole fraction of cyclohexane in the output stream; therefore, considering that both programs are an approximation of reality, the difference is not significant.

Conclusions

In this work the simulation of a plant that produces cyclohexane by the hydrogenation of benzene was carried out, for the simulation real data obtained from the bibliography were taken.

In addition the results of the simulations were compared with the programs DWSIM and ASPEN plus, the first one is a free use software and the second one is commercial. The results obtained are similar.

The advantages of DWSIM, besides having no cost, is that the interface is more user-friendly, which allowed the simulation to be carried out step by step and to instantly correct the exact point where the error is generated and to continue editing until completing the simulation, a situation that cannot be done in ASPEN Plus, since it is necessary to carry out the entire simulation, compile the project and then look for the errors.

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