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Process Simulation of the Synthesis of Acetone from Isopropyl Alcohol

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ABSTRACT

This paper is focused on the synthesis of acetone from isopropyl alcohol (IPA). Acetone is a colourless, flammable, organic compound which finds applications as a solvent in the pharmaceutical industry and in the synthesis of fibres. Its usefulness could be further seen in preparing metal surface before coating or painting, in the area of biological research. In this work, the process route was simulated with Aspen HYSYS 8.8, using Peng-Robinson equation of state as the fluid package. Material and energy balances were carried out on the process route with the composition in each stream. The principal benefit of this process route is that the acetone synthetized does not contain benzene or any other aromatic compounds. Hence, it is useful in pharmaceutical outfits. The simulation results showed the feasibility of this process at 2 bar and 350 °C. A reactor conversion of 98% was achieved showing a good feasibility of the process and optimum process equipment arrangements. Conclusively, within the limit of this simulation, acetone product flow rate of approximately 10,000 tonnes/year was obtained from isopropyl alcohol feed rate of 12,000 tonnes/year. The feed rate of the raw materials could be predicted before real-time process via simulation. This would aid in optimizing costs and in the design of a pilot plant which could be further scaled up.

1. INTRODUCTION

Isopropyl alcohol (IPA) is regarded as a colorless, clear and volatile liquid substance that has a fruity odor and bitter taste like that of acetone (Richard and Lewis, 2012; Wang et al., 2020). Frequently, 70 % volume/volume water solution of IPA is found in rubbing alcohol. IPA is also an active ingredient in

synthesis of cosmetics products, drug preparations and solvents (Slaughter et al., 2014; Berardi et al., 2020; Bashir et al., 2021). The toxic effects of IPA, however, are observed frequently in alcoholics, who abuse it as a readily available alternative and cheap substitute for ethanol. So, ingesting IPA, otherwise known as rubbing alcohol, is not only intoxicating, it is dangerous to human health (Ford, 2001; Leikin and Paloucek, 2008; Dumollard et al., 2021).

Acetone is a colourless organic compound which is a liquid at room temperature, miscible with water, and almost all organic solvents, making it an essential solvent in the laboratory. The global demand for acetone was 7.44 million tons in 2020 and is estimated to reach 13.09 million tons by 2030 (ChemAnalyst, 2021). This overwhelming demand started at the beginning of the global COVID-19 pandemic, due to its application as a major feedstock for IPA. Acetone has multiple applications in industries such as pharmaceutical, automotive, personal care & household, rubber & leather and electronics. Acetone is also used in varnishes, paints, and lacquers industries, and most frequently in the formulation of nail polish removers.

One of the methods to synthesize acetone is called the cumene process, where benzene (C_6H_6) undergoes reaction with propylene (C_3H_6) to produce cumene (C_9H_{12}). The synthetized cumene is further oxidized to form acetone $(CH_3)_2CO$ and phenol (C_6H_6O) according to Equations (1) and (2) (Hsu and Alharthy, 2021). The limitation of this process is that it is highly capital intensive compared to isopropyl alcohol technique. Also, the reaction conversion to acetone is low, with unconverted benzene dangerous to some chemical processes, thereby requiring large number of separation processes which results to significantly high cost of production (Mushtaq et al., 2015).

$$C_6H_6 + C_3H_6 \rightarrow C_9H_{12} \quad (1)$$

$$C_9H_{12} + O_2 \rightarrow (CH_3)_2CO + C_6H_6O \quad (2)$$

The direct oxidation of propylene is another acetone production route and is an exothermic reaction process which occurs at 100 °C and moderate pressure, using air for the the direct oxidation of propylene as described in the stoichiometric reaction in Equation (3). Here, the catalyst is a solution of $CuCl_2$ containing small amounts of $PdCl_2$. The major limitation to this process is that the reactor conversion achieved is low.

$$2CH_3 - CH = CH_2 + O_2 \rightarrow 2CH_3 - CO - CH_3 \quad (3)$$

The dehydrogenation of isopropyl alcohol is one of the most efficient methods for acetone production and involves the decomposition of IPA as illustrated by Mushtaq et al. (2015). In this process, an aqueous solution of IPA is fed into the reactor, where vaporization of steam occurs over a Cu/C catalyst. The reaction stoichiometry is given in Equation (4).

$$(CH3)_2CHOH \rightarrow (CH_3)_2CO + H_2 \quad (4)$$

The major advantage of this process is that the synthetized acetone is free from trace of benzene and some other aromatic compounds. This process is also characterized with higher purity and conversion, and lower cost of production compared to cumene process and direct oxidation process (Mushtaq et al., 2015). In addition, IPA dehydrogenation has been reported to be more economical compared to other techniques (Ulrich, 1984; Tremoulet et al., 2022). Therefore, simulation work is performed in this study in order to assess the feasibility higher acetone synthesis by dehydrogenation process. Simulation designates the rough imitation of a chemical process that characterizes its operational conditions over time. Simulation is frequently used with scientific modeling of chemical systems to have an insight to the function or behavior of the particular system. Aspen HYSYS process simulator, used for conceptual design with good applications in industries and academics, has the capacity to simulate steady and dynamic state processes, as demonstrated in our previous publication (Akintola et al., 2020). Hence, this paper presents an integrated process route for higher reaction conversion of IPA to Acetone via Aspen simulation.

2. METHODOLOGY

2.1. Process Description

The synthesis of acetone from isopropyl alcohol had earlier been presented in the previous work of Mohamed et al. (2017). The synthesis process uses isopropyl alcohol and water as the feed material, and sequence of unit operations, such as vaporization, heating, reaction, cooling and separation was followed. However, the simulation work in this study follows the block diagram of the process route presented in Figure 1, with the exception of vaporization, as the feed material only contain isopropyl alcohol.

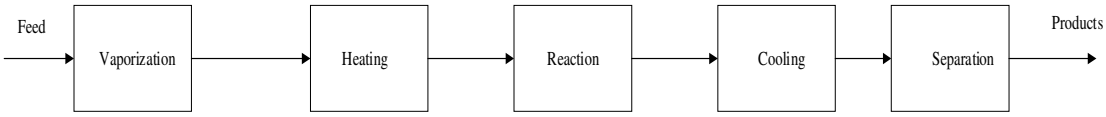

Figure 1: Block diagram for the syntheis of acetone from dehydrogenation of isopropyl alcohol (Mohamed et al., 2017)

2.2. Simulation Basis

As defined in the stoichiometric reaction in Equation 4, the components used in the simulation as added in the component list are IPA, acetone and hydrogen. Peng-Robinson (PR) was selected as the fluid package in the simulation basis environment. The choice of Peng-Robinson in this process simulation is due to its versatility to handle hydrocarbons (oil, gas and petrochemicals). For simplicity of the model, a conversion reaction which uses only the stoichiometry of the components (reactants and products) was used. Here, the stoichiometry of IPA took value of -1, while that of acetone and hydrogen took +1 each.. Within the reaction set environment, IPA was selected as the reactant, while acetone and hydrogen were selected as the products. For convergence of the global reaction set, IPA was selected as the base component, as it is the only reactant decomposing in the reaction. On completion of the simulation basis, the main simulation process began by switching to "simulation environment" where all necessary equipment were added.

2.3. Process Simulation

Aspen HYSYS 8.8 was used for the simulation. IPA was heated from 25 °C to 350 °C, as this is the required temperature for the reaction to take place. The heated IPA was sent to the reactor. It was observed that acetone appears at both top and bottom products of the reactor. The reactor products were channeled to a mixer, further heated from 49.82 °C to 120 °C. The heated product was then separated to have over 96 % composition of acetone and a total flow rate of acetone-rich stream is 10,418.76 tonnes/year. Hence, within the simulation work, owing to the composition of acetone in the final product stream, a total flow rate of 9,941 tonnes/year of acetone was produced, reaching a final reactor conversion of 98%, thereby showing the feasibility of the process and optimum process equipment arrangements. The simulated process route is presented in Figure 2.

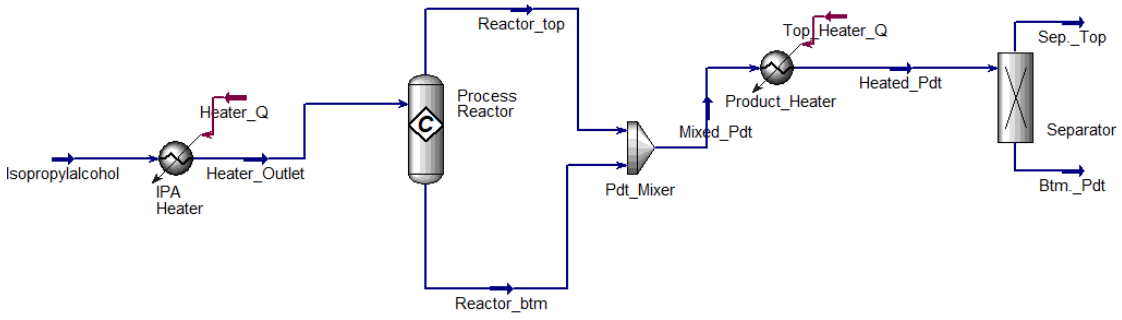

Figure 2: Aspen HYSYS simulated process route for the synthesis of acetone from isopropyl alcohol

3. RESULTS AND DISCUSSION

Table 1 is the equipment design parameters used for achieving a converged simulated process route. This gives the actual process conditions in the simulation environment, which could be used in a real-time process for developing a pilot plant as well as a scaled up plant. Table 2 is the material and energy stream flow for the synthesis of 10,000 tonnes/year of acetone and 2,000 tonnes/year for the trace of unreacted IPA and hydrogen from 12,000 tonnes/year of IPA feed rate. The mass balance, also termed material balance in this research paper uses the principle of application of conservation of mass for the analysis of the physical system (Chen and Yang, 2021), as applicable to the simulation of the process for the synthesis of acetone from IPA using Aspen HYSYS 8.8. The conservation of the chemical system analyzed in the process flow diagram of Figure 2 clearly reveals that for the simulated steady state process route, the mass entering the system will equal mass leaving the system, and this conforms to the early study of Smith and Peters (2013). This approach has helped to formulate the required product, acetone to a specified composition of 96.47 % in the final product stream, indicating a total flow rate of 10,000 tonnes/year from feed rate of 12,000 tonnes/year of IPA. The heat energy, presented as heat flow describes the quantity of heat energy available, using variables such as heat, measured in (kcal/h); or the temperature measured in (°C). From the simulation result, a final reactor conversion of 98 % and selectivity of 99.98 % was achieved, which is in agreement with the previous study of Llyas et al. (1994). Hence, this research paper has justified the earlier comments of Fadayini et al. (2018) and Akintola et al. (2020) that computer-based simulation is a state in which a particular set of conditions is generated artificially in order to investigate process that could really exist in reality. The final composition of the acetone-rich stream was 0.018 (1.8%), 0.9647 (96.47 %) and 0.0335 (3.35%) for IPA, hydrogen and acetone, respectively. Hence, the product stream reveals high purity acetone, implying that the stream can be described majorly in terms of Acetone product.

Table 1: Equipment design parameter

Pdt. Mixer	Elevation (Base) (m)	Elevation (Ground) (m)	Diameter (m)				
	1.00	2.00	2.00				
Process Reactor	Delta P (bar)	Vessel volume(m^3)	Liquid level (%)	Liquid volume (m^3)	Reaction heat (kCal/kgmole)	React. Conv. (%)	React. Extent
	0.0000	3.00	50.00	150.00	1.3×10^4	92.00	20.97
IPA Heater	Delta P (bar)	Delta T (°C)	Duty (kCal/h)				
	-1.00	325.0	465,795				
Product Heater	Delta P (bar)	Delta T (°C)	Duty (kCal/h)				
	-0.2.00	70.18	113,798				
Separator	Products	Vapour Fraction	Temperature (°C)	Enthalpy	Pressure (kPa)		
	Sep_Top	1.000	130.00	-5.045×10^4	230		
	Btm_Pdt	0.961	135.00	-2.481×10^4	1755		

Table 2: Material and energy stream flow

Material streams								
Name	Isopropyl alcohol	Heater_Outlet	Reactor_top	Reactor_Btm	Mixed_Pdt	Heated_Pdt.	Sep._Top	Btm_Pdt
Vapor fraction	0.0000	1.0000	1.0000	0.0000	0.7814	1.0000	1.0000	0.9610
Temperature (°C)	25.00	350.0	49.82	49.82	49.82	120.0	130.0	135.0
Pressure (kPa)	100.00	200.0	200.0	200.0	200.0	220.0	230.0	1,755
Mass flow (tonne/year)	1.2×10^4	1.2×10^4	7,116	4,884	1.2×10^4	1.2×10^4	1,162	1.084×10^4
Total feed rate (tonne/year)	1.2×10^4					Total product rate (tonne/year)	1.2×10^4	
Heat flow (kcal/h)	-1.733×10^6	-1.267×10^6	-6.887×10^5	-5.781×10^5	-1.267×10^6	-1.020×10^6	-1.325×10^5	-1.267×10^6
Composition								
Name	Isopropyl alcohol	Heater_Outlet	Reactor_top	Reactor_Btm	Mixed_Pdt	Heated_Pdt.	Sep._Top	Btm_Pdt
IPA mole frac.	1.0000	1.0000	0.0217	0.1130	0.0417	0.0417	0.6806	0.018
Acetone mole frac.	0.0000	0.0000	0.3652	0.8867	0.4792	0.4792	0.1597	0.9647
Hydrogen mole frac.	0.0000	0.0000	0.6131	0.0004	0.4792	0.4792	0.1597	0.0335
Energy streams			Conversion	98 %		Selectivity	99.98 %	
Name	Heater_Q	Top_Heater_Q						
Heat flow (kCal/h)	4.658×10^5	1.138×10^5						

4. CONCLUSION

This study has effectively investigated the simulation of the synthesis of acetone from isopropyl alcohol, using a process simulator, Aspen HYSYS 8.8. The aim is targeted towards synthetizing from isopropyl alcohol feed rate of 12,000 tonnes/year. The simulation results gave significantly high conversion and selectivity values, thereby revealing the feasibility of this process route. Hence, it can be concluded that high product flow rate of acetone is achievable using isopropyl alcohol as a starting raw material.

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6. CONFLICT OF INTEREST

There is no conflict of interest associated with this work.

REFERENCES

Akintola, J. T., Odunlami, M. O., Akintola, O. E. and Abdulkareem, Y. T. (2020). Statistical Analysis and Optimization of the Synthesis of Vinyl Chloride from Acetylene via Simulation. *International Journal of Latest Technology in Engineering, Management & Applied Science (IJLTEMAS),* 9(8), pp. 6 - 12.

Bashir, M. H., Hollingsworth, A., Thompson, J. D., Shortridge, D., Lake, S. P., Deeken, C. R. and Zook, E. C. (2021). Antimicrobial performance of two preoperative skin preparation solutions containing iodine and isopropyl alcohol. *American Journal of Infection Control,* 50(7), pp. 792-798

Berardi, A., Perinelli, D. R., Merchant, H. A., Bisharat, L., Basheti, I. A., Bonacucina, G. and Palmieri, G. F. (2020). Hand sanitisers amid CoViD-19: A critical review of alcohol-based products on the market and formulation approaches to respond to increasing demand. *International Journal of Pharmaceutics*, *584*, p. 119431.

ChemAnalyst (2021). Global Acetone Market Analysis: Plant Capacity, Production, Operating Efficiency, Demand and & Supply, End Use, Application, Sales Channel, Region, Competition, Trade, Customer & Price Intelligence Market Analysis, 2015-2030. (https://www.marketresearch.com/ChemAnalyst-v4204/Global-Acetone-Plant-Capacity-Production). Date accessed – May 27, 2022.

Chen, C. and Yang, A. (2021). Power-to-methanol: The role of process flexibility in the integration of variable renewable energy into chemical production. *Energy Conversion and Management*, *228*, p. 113673.

Dumollard, C., Wiart, J. F., Hakim, F., Demarly, C., Morbidelli, P., Allorge, D. and Gaulier, J. M. (2021). Putatively lethal ingestion of isopropyl alcohol-related case: interpretation of post mortem isopropyl alcohol and acetone concentrations remains challenging. *International Journal of Legal Medicine*, *135*(1), pp. 175-182.

Fadayin, O., Madu, C., Oso, A. O., Ugba, E., Ajayi, S. J. and Akintola, J. T. (2018). Simulation and Synthesis of Toluene by Dehydrogenation of N-heptane. *Journal of Industrial Research and Technology,* 7(2), pp. 110 - 120.

Ford, M. (2001). *Isopropanol.* In: Clinical toxicology. Philadelphia: W B Saunders Company, pp. 769–773.

Hsu, H.L. and Alharthy, R. D. (2021). Enhanced Room-Temperature Catalytic Decomposition of Cumene Hydroperoxide into Phenol and Acetone. *Science of Advanced Materials*, *13*(7), pp. 1246-1252.

Llyas, M., Shah, S., Nigar, R. and Khan, H. (1994). Conversion of lsopropyl Alcohol to Acetone Catalysed by Cr,O, at 473 K: Role of Molecular Oxygen. *Journal of Chemical Society, Faraday Transactions.* 90(16), pp. 2413-2415.

Leikin, J. and Paloucek, F. (2008). *Poisoning & Toxicology Handbook.* 4 Ed. Boca Raton: CRC Press.

Mohamed, M. E., Alghanai, M. F., Abdullah, A. M. and Ali, M. A. (2017). *Production of Acetone from isopropanol.* Sebha, Libya: Ministry of Higher Education and Scientific Research.

Mushtaq, U. M., Shafique, M., Khan, Z. and Shah, H. H. (2015). *Production of Acetone from Isopropyl Alcohol.* Wah Cantt: Wah Engineering College.

Richard, J. and Lewis, S. (2012). *Sax's dangerous properties of industrial materials,* Vol. 1–5, 12 Ed. New York: Wiley.

Slaughter, R., Mason, R. W., Beasley, D. and Vale JA, S. (2014). Isopropanol poisoning. *Clinical Toxicology, 52(5)*, pp. 470–8.

Smith, R. and Peters, C. (2013). *Introduction to Supercritical Fluids.* Edinburg: Elsevier B.V.

Tremoulet, M., Unton, M. and Feng, E. (2022, May 25). *Production ofAcetone Using Catalytic Dehydrogenation of Isopropyl Alcohol.* Retrieved from www.owlnet.rice.edu: http://www.owlnet.rice.edu/~ceng403/gr1998/acetone.html

Ulrich, G.D. (1984). *A Guide to Chemical Engineering Process Design and Economics.* 1 Ed. New York: Wiley.

Wang, Y., Guldiken, B., Tulbek, M., House, J. D. and Nickerson, M. (2020). Impact of alcohol washing on the flavour profiles, functionality and protein quality of air classified pea protein enriched flour. *Food Research International*, *132*, p. 109085.