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Simulation Of The Optimum Operating Conditions For A Propylene Glycol Production Unit Using Aspen Hysys Software

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ABSTRACT

Commercially, propylene glycol is produced by the direct hydrolysis of propylene oxide with water. This first-order, irreversible, exothermic reaction is performed in a glass-lined Continuous Stirred Tank Reactor (CSTR). In this study, the initiation of a CSTR was modelled from first principles and simulated using Aspen Hysys 3.2 to obtain concentration and temperature profiles. It is often very important how these profiles approximate the steady-state values. For example, when approaching a steady state the temperature may rise too high and this leads to degradation of the reactant or product, or the altitude may be unacceptable for safe operation. If either condition occurs, the system will exceed its practical stability limit. The practical stability limit represents the temperature above which it is undesirable to operate due to undesirable side reactions or equipment damage. Therefore, the best-operating conditions were obtained in terms of the flow rate of the raw material and the temperature of the reactor at 345 Kgmol/h and 82.2 °C on straight. The production of propylene glycol in the presence of an acid catalyst in an isothermal tank reactor is presented using advanced process simulation software. The effect of temperature was also calculated using the principle of energy balance on the reactor. The reactor operates optimally at a fractional conversion of 0.995 to obtain optimal values for the most important variables/parameters [reactor volume 7.92 m3, reactor length 2.83 m, reactor diameter 1.89 m, and amount of heat required for cooling per unit volume of the reactor 1205 kw].

محاكاة ظروف التشغيل المُثلى لوحدة إنتاج البروبيلين جليكول بإستخدام برنامج Aspen Hysys

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محاكاة

الملخص

تجاريا ، يتم إنتاج البروبيلين غليكول عن طريق التحلل المائي المباشر لأكسيد البروبيلين بالماء. يتم إجراء هذا التفاعل الطارد للحرارة من الدرجة الأولى وغير معكوس في مفاعل خزان التقليب المستمر مبطن بالزجاج (CSTR). في هذه الدراسة ، تم نمذجة بدء CSTR من المبادئ الأولى ومحاكاة باستخدام ASPEN HYSYS 3.2 للحصول على ملامح التركيز ودرجة الحرارة. غالبًا ما يكون من المهم جدًا كيف تقترب هذه المعاملات من قيم الحالة الثابتة. على سبيل المثال ، عند الاقتراب من حالة مستقرة ، قد ترتفع درجة الحرارة بشكل كبير مما يؤدي إلى تدهور المادة المتفاعلة أو المنتج ، أو قد يكون الإرتفاع غير مقبول للتشغيل الآمن. في حالة حدوث أي من الشرطين ، سيتجاوز النظام حد الثبات العملي. يمثل حد الثبات العملي درجة الحرارة التي يكون فوقها غير مرغوب فيه للعمل بسبب التفاعلات الجانبية غير المرغوب فيها أو تلف المعدات. لذلك ، تم الحصول على أفضل ظروف التشغيل من حيث معدل تدفق المادة الخام ودرجة حرارة المفاعل عند 345 كجم مول / ساعة و 82.2 درجة مئوية على التوالي. يتم تقديم إنتاج البروبيلين جليكول في وجود محفز حمضي في مفاعل خزان المتساوي الحرارة بإستخدام برنامج محاكاة عملية متقدم. تم حساب تأثير درجة الحرارة أيضًا باستخدام مبدأ توازن الطاقة في المفاعل. يعمل المفاعل على النحو الأمثل عند التحويل الجزئي 0.995 للحصول على القيم المثلى لأهم المتغيرات / المعاملات [حجم المفاعل 7.92 م 3 ، طول المفاعل 2.83 م ، قطر المفاعل 1.89 م ، كمية الحرارة المطلوبة للتبريد لكل وحدة حجم للمفاعل 1205 كيلو واط].

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Introduction

Modern technological developments are developing rapidly. Everything has harnessed the power of computers, from equipment, services, and factory requirements to lessons. In the discipline of chemical engineering, its use is very broad, ranging from simple effects to more complex situations to illustrate the process of modeling and simulating a reactor-like process system or tool. Propylene glycol is used in processes similar to other glycols. Propylene glycol is an important raw material for unsaturated polyesters, epoxies, and polyurethane resins. The level of use in this region represents approximately 45% of the total propylene glycol consumption. A similar unsaturated polyester is commonly used for reinforced plastics and surface coatings. Propylene glycol is characterized by excellent density, hygroscopicity, and non-toxicity, so it is widely used as a hygroscopic agent, antifreeze, lubricant, and cleaning agent in food, medicine, and decoration auxiliaries. When ingested, propylene glycol reacts with fatty acids to form propylene esters of fatty acids and is mainly used as a food emulsifier; Propylene glycol is a suitable detergent for flavoring and coloring. Propylene glycol is generally used as a cleaning agent, humectants, incipient, etc. In pharmaceutical auxiliaries for the preparation of colored ointments and bandages. Propylene glycol is also used as a cosmetic cleaner and softener due to its good group solubility with multiple flavors. Propylene glycol is also used as a wetting agent for tobacco, an antifungal agent, a food processing lubricant, and a cleaning agent for food marking items. The anhydrous result of propylene glycol is an effective antifreeze [1].

Propylene glycol is one of the most commonly used moisturizers with high hydrophilicity and a stabilizing effect on the water content of the material. It is used in some medicines and cosmetics to absorb excess water and retain moisture. The growing use of propylene glycol is in the area of dust removal and antifreeze in automobiles. Propylene glycol is produced from propylene oxide by hydrolysis in the liquid phase with excess water in the presence of sulfuric acid of little interest as a catalyst [2].

Synthesis method

It can be obtained by hydrolysis of Propylene oxide:

Direct hydration reaction

$$C_3H_6O \quad + \quad H_2O \quad \xrightarrow{H_2SO_4} \quad C_3H_6(OH)_2$$

Propylene oxide and water react in a molar ratio of 1:15, the reaction is carried out at 150-2000 ° C, pressure 1.2-1.4 MPa for 30 minutes, obtaining a 16% aqueous solution of propylene glycol, which is evaporated to obtain the final product. Catalytic Hydrolysis: The reaction begins with catalysis using sulfuric acid or hydrochloric acid. Add 0.5-1.0% sulfuric acid diluted with a 10-15% aqueous solution of propylene oxide and the mixture decomposes at 50-70 °C; The hydrolysis is neutralized, concentrated under reduced pressure, and purified to give the final products. The production method is a method in which propylene oxide is decomposed into propylene glycol, which can be implemented in a liquid phase. There are catalytic and non-catalytic processes in manufacturing processes. The catalytic method is a method in which hydrolysis occurs in the presence of 0.5-1% sulfuric acid at 50-70 °C. The non-catalytic process is carried out at high temperatures and pressures (150 to 300 °C, 980 to 2940 kPa) and is used for domestic production [2].

The selection of reactors to be used based on chemical reactions and various hydrodynamic factors that exist to determine the size of the reactor and how to determine the best-operating conditions are the problems faced in planning to increase production from the laboratory scale to the industrial scale. The scale-up process has traditionally been carried out in stages from a laboratory scale to a pilot scale to finally a larger scale. However, this experiment requires considerable cost, time, and energy to obtain the results of excellent or optimum operating conditions. Using models and simulations can reduce the risk of danger, and save time and money in analyzing reactor performance [3].

Mathematical model of CSTR

Subsequent assumptions were made in formulating the model.

1. Differences in heat of reaction, density, heat capacity, and UA are neglected
reaction temperature ranges.
2. Under the prevailing conditions of concentrations and temperature of the side reactor
Negligible feedback.
3. The casing fluid flow rate and temperature are treated as constants [4].

Mole balance: application of the law of conservation of mass to all species present in the reaction system,

Rate of accumulation Rate of Rate of
Rate of production /
of mass within the = mass flow – mass flow +
depletion of mass
reactor in out

Species A $$\frac{dN_A}{dt} = V_0 C_{A_0} - V_0 C_A + \left(-r_A\right)V$$

$$\frac{dC_A}{dt} = \frac{V_0}{V}(C_{A_0} - C_A) + \left(-r_A\right)$$

$$\frac{dC_A}{dt} = \frac{1}{\tau}(C_{A_0} - C_A) + \left(-r_A\right), \text{ where } \quad \tau = \frac{V}{V_0}$$

$$V_0 = \sum \frac{F_{i\,0} M_i}{\rho_{i\,0}} \qquad C_{i_0} = \frac{F_{i\,0}}{V_0}$$

Similarly for other species

$$\frac{dC_B}{dt} = \frac{V_0}{V}(C_{B_0} - C_B) + \left(-r_B\right)$$

$$\frac{dC_C}{dt} = \frac{1}{\tau}(C_{C_0} - C_C) + r_C$$

$$\frac{dC_M}{dt} = \frac{1}{\tau}(C_{M_0} - C_M)$$

Energy Balance: Applying law of conservation of energy to the reacting system,

Rate of Rate of Rate of Rate of
Rate of heat accumulation of = energy into – energy out of +
enthalpy – removal
energy within the system the system change due to
through jacket
the reactor reaction

$$\left[N_A C_{P_A}\frac{dT}{dt} + N_B C_{P_B}\frac{dT}{dt} + N_C C_{P_C}\frac{dT}{dt} + N_M C_{P_M}\frac{dT}{dt}\right]$$

$$= \left[F_{A_0} C_{P_A}\left(T_0 - T_r\right) + F_{B_0} C_{P_B}\left(T_0 - T_r\right) + F_{M_0} C_{P_{P_M}}\left(T_0 - T_r\right)\right]$$

$$-\left[F_A C_{P_A}\left(T - T_r\right) + F_B C_{P_B}\left(T - T_r\right) + F_C C_{P_C}\left(T - T_r\right) + F_M C_{P_M}\left(T - T_r\right)\right]$$

$$+\left[\Delta H_{R_X}\left(r_A V\right)\right] - \left[UA\left(T - T_j\right)\right]$$

Now, Taking T = Tr (Exit temperature = Reference temperature)

$$\left[\sum_i N_i C_{P_i}\right]\frac{dT}{dt} = F_{A_0}\left(T_0 - T\right)\left[C_{P_A} + \frac{F_{B_0}}{F_{A_0}} C_{P_B} + \frac{F_{M_0}}{F_{A_0}} C_{P_M}\right] + \left[\Delta H_{R_X}\left(r_A V\right)\right] - \left[UA\left(T - T_j\right)\right]$$

$$\frac{dT}{dt}=\frac{\left(UA\left(T_j-T\right)-F_{A_0}\left(T_0-T\right)\sum_i\theta_i C_{P_i}+\Delta H_{R_X}\left(r_A V\right)\right)}{\sum_i N_i C_{P_i}}$$

Where: $\theta_i=\frac{F_{i0}}{F_{A0}}$ and $N_i=C_iV$

Problem Statement

A liquid phase reaction between propylene oxide and water at room temperature catalyzed by H_2SO_4 in an encapsulated CSTR is considered. at 24 °C (T_0) and 0.1 wt% of H_2SO_4 in a 7.92 cubic meter reactor (V). The feed stream consisted of 68 kmol/h (FA_0) propylene oxide (A), 2300 kmol/h (FB_0) water (B) containing 0.1 wt% H_2SO_4, and 10 kmol/h (FM_0) methanol (M).

Table 1: Parameter values [5].

$C_{P_A}=146$ J/mol-K	$\rho_{A_0}=0.859$ g/cc	$M_A=58.08$	$A=16.96\times10^{12}$ hr^{-1}
$C_{P_B}=75$ J/mol-K	$\rho_{B_0}=0.9941$ g/cc	$M_B=18$	$E=18$ kcal/mol
$C_{P_C}=193$ J/mol-K	$\rho_{M_0}=0.7914$ g/cc	$M_M=32.04$	$UA=133$ MJ/hr-K
$C_{P_M}=82$ J/mol-K	$\Delta H_{Rx}=-83740$ J/mol of propylene oxide reacted		$t_0=0$; $t_f=4$hr

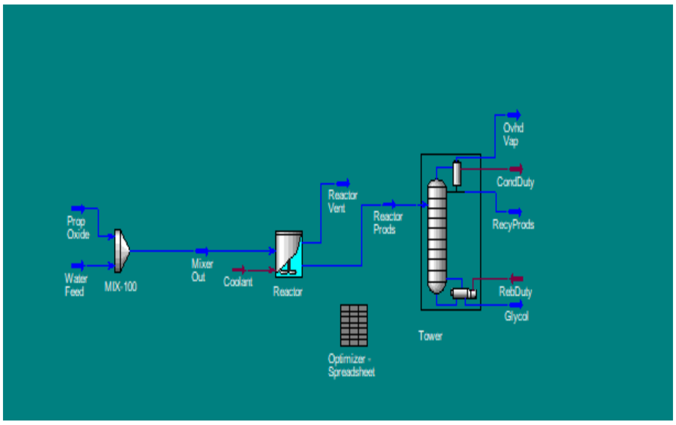

Fig. 1: PFD of the propylene glycol production process[5].

Simulation Results and Discussion

While running the simulation program and after entering the necessary data to perform the simulation, a flow chart of the production process was created as shown in Figure 1 and Table 1. Table 2 shows the balancing result of the substance on the distillation column. The result of the molar fraction of the produced glycol was about (0.995).

Table 2: Mole balance on the tower.

Streams Comp.	Reactor Prods, Mole%	Ovhd Vap, Mole%	RecyProds, Mole%	Glycol, Mole%
1-2-C_3Oxide	1.29E-02	0.69612	1.67E-02	4.25E-14
1-2-C_3diol	0.22965	1.37E-09	2.02E-07	0.995001
H_2O	0.757496	0.30388	0.983289	5.00E-03

Figure 2 shows the relationship between the fraction of The concentration of the products and the reactants and the temperature of the distillation column, i.e. with a decrease in the water concentration with an increase in the concentration of the glycol produced.

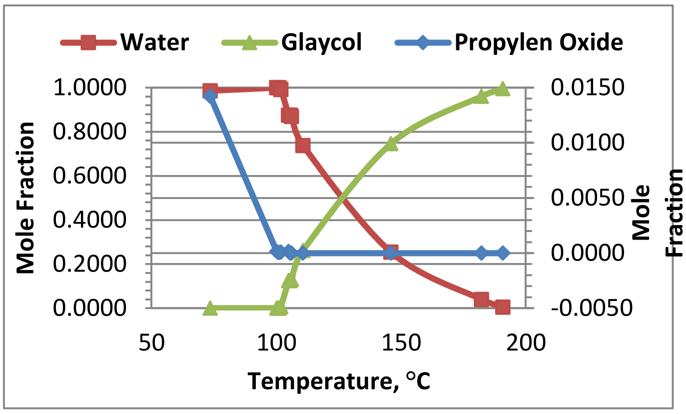

Fig. 2: Temperature vs Mole fraction of materials

Figure 3 is quite similar to Figure 2 and shows the relationship between the tower operating pressure and the concentration of materials, that is, with an increase in the glycol concentration, the water concentration decreases, as well as propylene oxide.

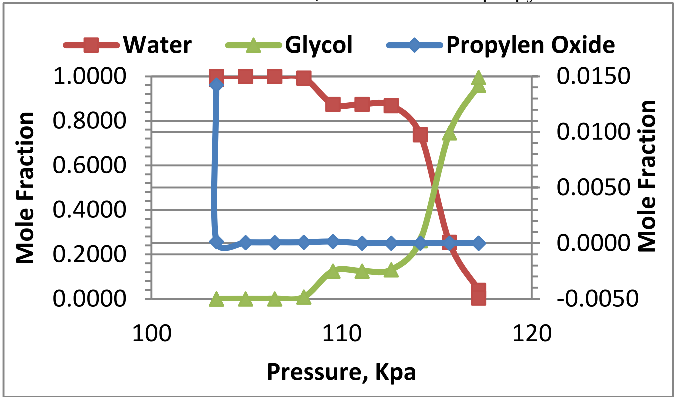

Fig. 3: Pressure vs Mole fraction of materials

Figure 4 shows the relationship between the operating temperature of the reactor and the conversion rate of propylene oxide in the normal operating condition and the optimal operating condition. We note that the optimal operating conditions are better than the normal operation in terms of operating costs, yield ratio, and equipment safety. This is based on the objective function used, which is shown as the highest profit. It is equal to the price of the product minus the cost of raw materials and operating expenses.

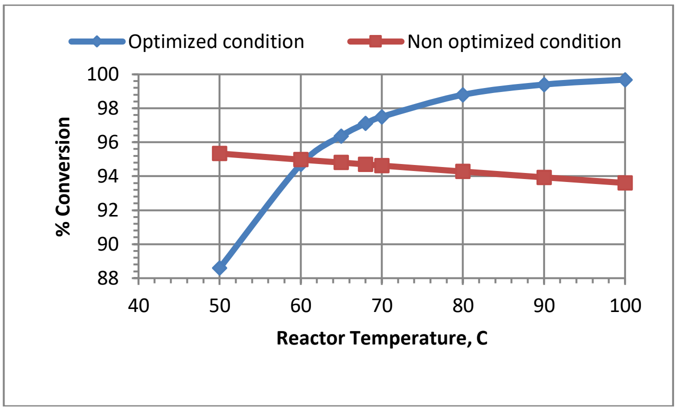

Fig. 4: Reactor temperature vs conversion ratio

Conclusion

This simulation model is for the production of propylene glycol. A continuously stirred tank reactor was used to create a product stream containing approximately 20% propylene glycol, and then a distillation column was designed to produce a product stream with a purity of 99.5% propylene glycol. The column also recovers all propylene glycol fed into the column. The steady-state simulation results show that the feed flow rate, temperature, and pressure affect the efficiency of the continuously stirred tank reactor. It was also concluded that the best safe operating conditions and the most significant profit from the yield are obtained by adjusting the temperature of the reactor Which is 82.2 °C by applying the objective function necessary for that and fixing the rest of the reactor operating variables. Thus we get the highest profitability and in the safe operation mode of the equipment.

Nomenclature

C_A, C_B, C_C, C_M Concentrations of A,B,C and M respectively, kmol/m^3
$C_{A0}, C_{B0}, C_{C0}, C_{M0}$ Initial concentrations of A,B,C and M respectively, kmol/m^3
N_A, N_B, N_C, N_M Moles of A, B, C and M respectively
F_{A0} ,F_{B0} ,F_{C0} ,F_{M0} Molar feed rates of A,B,C and M respectively, kmol/hr
M_A, M_B, M_C, M_M Molecular weights of A,B,C and M respectively
$C_{PA}, C_{PB}, C_{PC}, C_{PM}$ Heat capacities of A,B,C and M respectively, J/mol-K
ρ_{A0}, ρ_{B0}, ρ_{C0}, ρ_{M0} Densities of A, B, C and M respectively, g/cc
ΔH_{Rx} Heat of reaction, J/mol
U Overall heat transfer coefficient, MJ/m2-hr-K

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