World Scientific Research Journal
Volume 7 Issue 6, 2021
ISSN: 2472-3703
DOI: 10.6911/WSRJ.202106_7(6).0041

Process Dynamics and Modelling in Chemical and Biological Systems Design of a Continuous Stirred-Tank Reactor in an Ethylene Glycol Factory

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Abstract

Continuous-stirred tank reactors (CSTRs), also known as back-mix reactors, are widely used to optimize feasible bioprocess system. It is also designed to fulfill commercial requirements of ethylene glycol company. The company annually produces 400 million pounds of ethylene glycol and the production process achieves a reaction conversion of 85%. The dimensions of the tank CSTR is calculated to be 7.5 ft in diameter and approximately 12 ft in height. Five 800 gal CSTRs in series was designed to refining the process. The CSTRs are assumed to run at steady state with well mixed content in each unit and fixed inlet and outlet flow rate and composition in this design.

Keywords

Continuous stirred-tank reactors; Reactor design; Ethylene glycol; Steady state.

1. INTRODUCTION

CSTRs are developed from basic batch reactors. They are more commonly used in industry for continuous industrial processing. In petrochemical industry depuration process, the continuous flow reactors are used to treat petroleum hydrocarbon-rich liquid effluents. According to the results of a 225-day experiment carried out in a petroleum refinery industry north of Tunisia, CSTRs are highly efficient in eliminating the wastewater pollutants and reduce Chemical Oxygen Demand (COD). The COD rates were reduced up to 95% after the water treatment process and the residual total petroleum hydrocarbon (TPH) decreased to 1/40 of the original. The bioremediation process was also successfully developed and the System design of the aerobic CSTR used in the experiments is shown below in Figure 1.

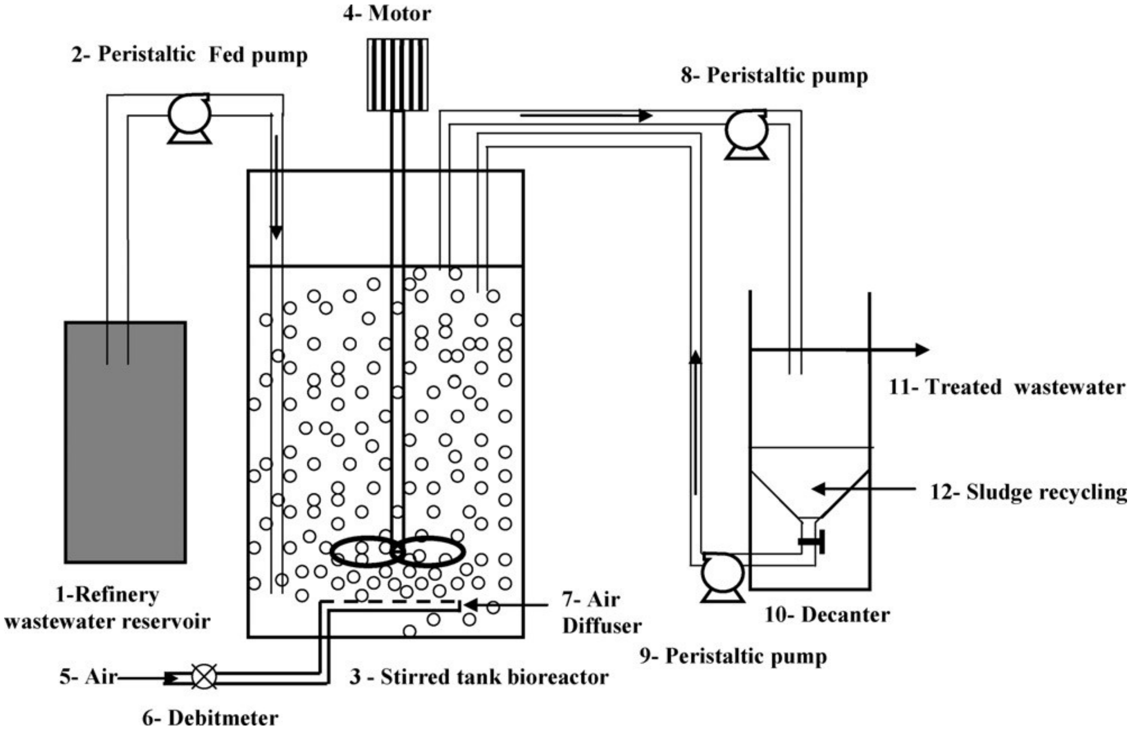

Figure 1. Schematic diagram of the aerobic continuously stirred tank bioreactor (CSTR) used for continuous experiments [1]

Aside from petroleum processing, backmix reactors can be frequently seen in a variety of industries, fermentation, water treatment, and even in farms. Since CSTRs can be very large in size, it is adequate to deal with crude flow that contains solid suspension. Furthermore, in a CSTR type digester, the material is well stirred to evenly distribute the solution so as to avoid stratification and this increases the chance of contact between material and microorganism [2]. CSTRs can be also used in slaughterhouse wastewater treatment [3], livestock manure treatment of cattle, pigs, chickens and other farms [4], biogas production and power generation projects [5, 6], and high concentration organic wastewater treatment projects with more suspended solids such as urban domestic sludge [7].

In stark contrast to batch reactors, CSTRs are designed to be run at a well mixed steady state with fixed inlet and outlet flow rate and composition. In ideal situations, the reactants and the products of the reactor should be well stirred and evenly distributed. Upon achieving steady state, the entire system will not change with respect to time. (Temperature, composition, reaction rate, etc.) In reality, the CSTR's performance deviates from ideal mixed model due to its size. In these cases, new adequate models should be developed to address these deviations. In other cases, which are not the highly non-ideal condition, the spatial variations in reactants composition, liquid and gas phase temperature are assumed to be negligible. At the same time, the reaction rate throughout the reacting space can be considered to be the same as well. Therefore, the outlet stream and the vessel content share the same physical properties.

2. BACKGROUND

"The global ethylene market size was USD 166,529 million in 2019 and is projected to reach USD 245,005 million by 2027, exhibiting a CAGR of 5.6% during the forecast period [8]."

Ethylene glycol is used in many commercial and industrial applications [9, 10, 11, 12]. It is the raw material for making polyester, polyester resin, synthetic fiber, cosmetics and explosives. Additionally, ethylene glycol also acts as a solvent for dyes, inks and can be used like a condensing agent such as water. In daily life, this chemical is also a common anti-freezing agent for engine preparation and a gas dehydrating agent. It is also used for the transportation of industrial cooling capacity, which is generally called refrigerant.

Taking a small factory as an example to design a CSTR ethylene glycol reactor [13], assume that 400 million pounds per year of ethylene glycol is required by the commercial market. To meet this production goal, an isothermal CSTR is designed in this paper to convert ethylene oxide in water into ethylene glycol. The reaction requires two streams to be mixed and fed to the reactor. The conversion can achieve 85% in the reactor using H_2SO_4 as the catalyst for the reaction. Required materials include 1 lb. mol/ft3 of ethylene oxide solution and equal volumetric solution of water containing 0.9 wt. % of the catalyst H2SO4. The reactor is to be operated isothermally and the necessary reactor volume and form will be determined and discussed.

3. CALCULATION AND DESIGN SPECIFICATIONS

3.1. The Reactor Design Equation in CSTR

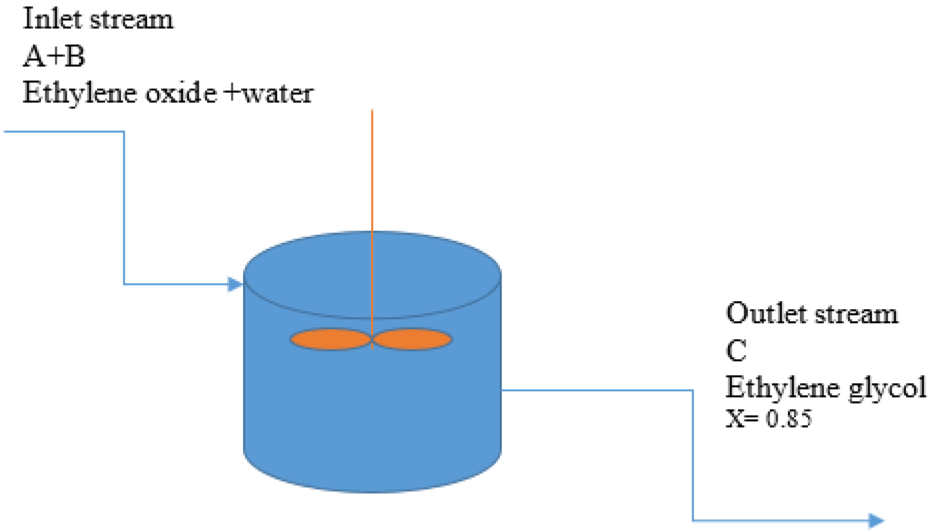

Figure 2. Illustration of CSTR reactor model in ethylene glycol factory

The reaction can be shown as,

Ethylene oxide + water → ethylene glycol

(with H_2SO_4 to be the catalyst)

A+B → C (with the catalyst)

Assuming that the ethylene glycol (C) is the only reaction product formed.

The generation of species C in the vessel (G_C), should be calculated as the rate of generation integrated by the total volume of the vessel.

$$G_C = \int_0^v r_C \, dV$$

For general mole balance in the CSTR reactor,

$$F_{C0} - F_C + \int_0^v r_C \, dV = \frac{dN_C}{dt}$$

In this equation, V(volume) is the volume, r is the reaction rate, NC (moles) is the total accumulation of species C in the system, and F (moles / time) is the molar rate of species C in the inlet (FC_0) and outlet flow (F_C).

In an ideal CSTR model, the reaction rate should be the same in the entire vessel.

$$\int_0^v r_C \, dV = V r_C$$

When it is applied to a CSTR in steady state, the composition for species does not change with time.

$$\frac{dN_C}{dt} = 0$$

Plug in CSTR model into the mole balance, we will get the following equation to set the volume.

$$\mathrm{V} = \frac{\mathrm{F_{C0} - F_C}}{\mathrm{-r_C}}$$

When there is no product C in the inlet flow, $F_c0 = 0$

$$V = \frac{F_C}{r_C}$$

The reaction stoichiometry shows,

$$r_C = -r_A$$

$$F_C = F_{A0} X$$

The design equation becomes,

$$V = \frac{F_C}{r_C} = \frac{F_{A0} X}{-r_A}$$

The rate law gives,

$$-r_A = k C_A$$

And for liquid phase, the volume does not change during reaction, so does the volumetric flow rate, $v = v_0$

$$C_A = C_{A0}(1 - X)$$

Thus, the calculation of the volume can be determined by,

$$V = \frac{F_{A0} X}{k C_{A0}(1 - X)} = \frac{v_0 X}{k(1 - X)}$$

3.2. Vessel Volume Calculation

The Specified production rate in lb. mol / min is

$$F_C = 4e8\ lb\ /year * 1\ yr\ /365 days * 1 day/24h * 1h/60min * 1\ lb\ mol\ /62\ lb$$
$$= 12.273\ lbmol/min$$

The required molar flow rate of ethylene oxide (A) is

$$F_{A0} = \frac{F_C}{X} = \frac{12.2748}{0.85} = 14.44 \frac{\mathrm{lbmol}}{min}$$

With a concentration of 1 mol /L, the reactant A volumetric flow entering the reactor is,

$$v_{A0} = \frac{F_{A0}}{C_{A0}} = \frac{14.44\ lbmol/min}{1\ lb \frac{mol}{ft^3}} = 14.44\ ft^3/min$$

Equal volumetric flow for species A and B,

$$v_0 = 2 v_{A0} = 28.88\ ft^3/min$$

The reaction constant, k=0.311 min-1 for this reaction, plug in,

$$V=\frac{v_0X}{k(1-X)}=28.88ft^3/\min*\frac{0.85}{0.311min^{-1}(1-0.85)}=526.22\ ft^3=14.90\ \ m^3$$
$$=3936\ gal$$

A tank of 7.5 ft in diameter and approximately 12 ft tall is necessary to achieve 85% conversion.

3.3. CSTR in Parallel and CSTR in Series Comparison

If 800gal of reactor are used, 5 reactors in total will be needed.

For parallel CSTRs, the resistance time

$$\tau=\frac{V}{v_0/5}=\left(800*\frac{1ft^3}{7.48gal}\right)*\frac{5}{14.44\frac{ft^3}{min}}=37.03\,min$$

The Conversion is to be,

$$X=\frac{\tau k}{1+\tau k}=37.03*\frac{0.311}{1+37.03*0.311}=0.92$$

For CSTRs in Series,

The resistance time τ can be determined as

$$\tau=\frac{V_1}{v_0}=800*\frac{1ft^3}{7.48gal}*\left(\frac{1}{28.88\,ft^3/min}\right)=\ 3.70\,min$$

The conversion after 5 CSTRs can be calculated as

$$X=1-\frac{1}{(1+\tau k)^n}=1-\frac{1}{(1+3.70)^5}=0.9996$$

4. CONCLUSION

This study proposes the application of a steady state CSTR in an ethylene glycol company. From the result, the single CSTR size can be relatively large. In a large CSTR, the steady state might be hard to achieve due to the insufficient and inefficient stirring. In order achieve more stable output flow and the concentration in the reactor of the ethylene glycol products, CSTRs of smaller size are suggested to be set in series. 5 of 800 gal CSTRs will give a 1.17 times higher conversion. These encouraging results give strong evidence that CSTR in series are more efficient in decreasing the single reactor size and increasing the reaction rate at the same time. The stirring in reality can be achieved using a higher speed stirrer and in situ concentration monitor.

The design of the CSTR in this paper is assumed to be in isothermal condition. However, the temperature may change due to natural climate change and reaction process. A cooling and heating system is necessary to achieve the conversion rate in the discussion. If CSTRs in series are used in the production process, the temperature control system would be relatively simpler. Notice that the conversion rate is high and approaching to 1 for 5 of 800 gal CSTRs in series. The composition change step by step in the reactor and the size of the reactor are smaller compared to the single tank CSTR. As a result, the heat exchange will also be lesser for each reactor.

ACKNOWLEDGMENTS

Deepest appreciation to Shuyan Jin (jinshuyan1999@gmail.com) for analyzing and vetting this paper and those who supported me when I was writing this paper.

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