Matilda Lazić [47]
Technical College of Applied Sciences in Zrenjanin, Zrenjanin/Serbia
Dragan Halas [48]
Technical College of Applied Sciences in Zrenjanin, Zrenjanin/Serbia
Aleksandra Vasilić [49]
Luxol doo since 1884, Zrenjanin/Serbia

CALCULATION OF THE VOLUME OF TUBULAR REACTOR ON THE EXAMPLE OF CIS-TRANS CATALYTIC ISOMERIZATION OF 2-BUTENE

DOI: 10.5937/PIM26173L

Abstract:
This paper presents an example of reactor volume calculation for a system used in the cis–trans isomerization of 2-butene in catalytic processes in the petrochemical industry. The aim of this example is to demonstrate the application of tubular reactor design equations to calculate the required reactor volume as a fundamental design parameter. This parameter enables the achievement of the desired conversion of the reactant into the target product under the specified reaction conditions. Determining reactor volume as a key design variable facilitates effective control of catalyzed chemical reactions, which represents one of the primary objectives of chemical reaction engineering.

Keywords: *Tubular reactor, Catalytic processes, Chemical reaction engineering*

Introduction

The isomerization of cis-2-butene to trans-2-butene is a critical industrial process for producing high-octane gasoline, specialty chemicals, and optimizing petrochemical feedstock efficiency. The isomerization is catalyzed by materials like acid-exchanged clays, iodine, or noble metals (Pd, Pt). It involves breaking the π-bond to allow rotation, controlled by temperature and catalyst, to produce the more stable trans isomer [1].

The isomerization of cis-2-butene to trans-2-butene is a homogeneous, irreversible reaction with first-order kinetics. The reaction takes place in a plug-flow reactor PFR [2,3].

[47] matildalazic@outlook.com, ORCiD: 0009-0000-9174-554X
[48] draganhalas@gmail.com, ORCiD: 0009-0005-1426-0326
[49] aleksandra.stanic.vasilic@gmail.com

In addition to the continuous-stirred tank reactor (CSTR) and batch reactors, another type of reactor commonly used in chemical industry is the plug-flow reactors (PFRs). It consists of a cylindrical pipe and is normally operated at steady state. Tubular reactors are used most often for gas-phase reactions but they can also be used in the liquid phase [3,4,5].

Apart from the cis-trans isomerization of 2-butene, the PFRs are used in the petrochemical industry for the production of cumene by the process of catalytic alkylation of propylene and benzene as well as for the conversion of methanol into gaseous hydrocarbons [4-6].

This paper presents an example of calculating the volume of a tubular reactor, which is used for the cis-trans isomerization of 2-butene in the catalytic processes of the petrochemical industry. The example was intended to demonstrate the application of the design equations for tubular reactors, which are applied to dimension the reactor volume (as the basic design size of the reactor) required to achieve the specified conversion of the reactant to the desired product.

1. Key features and principles of tubular reactors

In the tubular reactors, the reactants are continually consumed as they flow down the length of the reactor. In modeling the tubular reactor, it is assumed that the concentration varies continuously in the axial direction through the reactor. Consequently, the reaction rate, which is a function of concentration for all but zero-order reactions, will also vary axially. For the purposes of the material presented here, we consider systems in which the flow field may be modeled by that of a plug-flow profile (e.g., uniform velocity as in turbulent flow) [3]. That is, there is no radial variation in reaction rate, and the reactor is referred to as a plug-flow reactors (PFRs) [3].

PFRs usage, advantages and disadvantages are shown in Table 1.

Table 1: *PFRs usage: advantages and disadvantages*

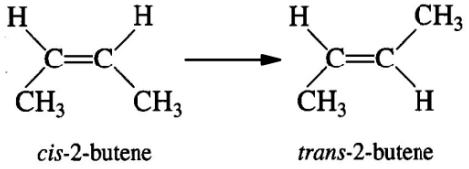
Usage	***Advantages***	Disadvantages
Large scale	High conversion per unit volume	Undesired thermal gradients may exist
Fast reaction	Low operating (labor) costs	Poor temperature control
Homogeneous reaction	Continuous operation	Shootdown and cleaning may be expensive
Heterogeneous reaction	Good heat transfer	/

Source: Tubular Reactos, Said Al-Qurri

2. Project problem

Derive an equation relating the tubular reactor volume to the entering and exiting concentrations of A, the rate constant - k, and the volumetric flow rate - v_0. Determine the reactor volume - V_1, necessary to reduce the exiting concentration to 10% of the entering concentration, i.e., $C_A = 0{,}1C_{A0}$ when the volumetric flow rate is10 dm^3/min, and the specific reaction rate - k, is 0,23 min^{-1} [3].

The catalytic reaction of the cis-trans isomerization of 2-butene is shown in Picture 1. [2-4].



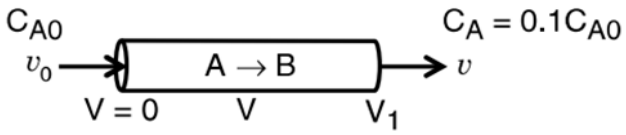
Picture 1*. Catalytic reaction of the cis-trans isomerization of 2-butene*

The reaction (Picture 1.) is kinetic, first-order and, in general, can be represented as follows:

$$A \longrightarrow B$$

Picture 2. *General presentation of the irreversible cis-trans isomerization reaction 2-butene*

A tubular reactor with input and output quantities, relevant for the calculation in this paper, is shown in Picture 3. [3].



Picture 3. *A tubular reactor with input and output quantities, relevant for the calculation [3]*

3. Problem solving

The set project problem is solved in two steps, which are presented in this paper.

1. Derive an equation relating: V, v_0, k, C_{A0}, and C_A. For a tubular reactor, the mole balance can be represented by equation (1) [3]:

$$\frac{dF_A}{dV} = r_A \tag{1}$$

For a first-order reaction, the rate law is [3]:

$$-r_A = kC_A \tag{2}$$

Because the volumetric flow rate - v, is constant ($v = v_0$), as it is for most all liquid-phase reactions [3]:

$$\frac{dF_A}{dV} = \frac{d(C_A \cdot v)}{dV} = \frac{d(C_A \cdot v_0)}{dV} = v_0 \frac{dC_A}{dV} = r_A \tag{3}$$

Multiplying both sides of equation (3) by minus one and then substituting equation (2) yields [3]:

$$-\frac{v_0\, dC_A}{dV} = -r_A = kC_A \tag{4}$$

Separating the variables and rearranging equation (4) gives the following (equation 5) [3]:

$$-\frac{v_0}{k}\left(\frac{dC_A}{C_A}\right) = dV \tag{5}$$

Using the conditions at the entrance of the reactor that when $V = 0$, then, $C_A = C_{A0}$ [3] the following is obtained:

$$-\frac{v_0}{k}\int_{C_{A0}}^{C_A}\left(\frac{dC_A}{C_A}\right)=\int_0^V dV \qquad (6)$$

Carrying out the integration of Equation (6) gives the following result:

$$V=\frac{v_0}{k}ln\frac{C_{A0}}{C_A} \qquad (7)$$

We can also rearrange equation (7) to solve for the concentration of A as a function of reactor volume to obtain:

$$C_A=C_{A0}\,e^{(-kV/v_0)} \qquad (8)$$

2. Calculate V. We want to find the volume, V_1, at which $C_A=\frac{1}{10}C_{A0}$, for k =0,23 min^{-1} and $v_0=10\ dm^3/min$.

Substituting C_{A0}, C_A, v_0, and k, equation (7), we have [3]:

$$V_1=\frac{10\ dm^3/min}{0{,}23\ min^{-1}}ln\frac{C_{A0}}{0{,}1\ C_{A0}}=\frac{10\ dm^3}{0{,}23}ln\ 10=100\ dm^3 \qquad (9)$$

We see that a reactor volume of 0,1 m^3 is necessary to convert 90% of species A entering into product B for the parameters given.

If one were to analyze the concentration profile of reactant A along the length of the reactor (equation (8)) it would be observed that the concentration of the reactant decreases exponentially down the length (i.e., volume V) of the reactor [3].

The purpose of the example was to give a vision of the types of calculations we will be carrying out as we study chemical reaction engineering (CRE).

It should be emphasized that the input, specified variables, numerically correspond to the volume values for semi-industrial reactors and are given only as an example for calculation.

4. Conclusion

In this work, a classic chemical-engineering volume calculation was performed, as a key parameter for sizing a tubular reactor. The presented example shows how to apply the design equations for the calculation of the reactor volume, which would make it possible to achieve the set performance and manage the catalytic reaction. The calculated volume

of the reactor (corresponds to the values of semi-industrial reactors) enables the reduction of the input concentration of the reactant to the set level in accordance with the specified reaction conversion; obtaining a given reaction product concentration for a first-order catalytic reaction taking place in a tubular reactor.
Calculating the volume as a basic design quantity for achieving the desired conversion enables the management of a catalyzed chemical reaction, which is one of the basic goals of applying chemical reaction engineering.

The problem can be transferred to the industrial level by describing the concentration profile along the length of the reactor, which could represent a further work flow.

REFERENCES

[1] Moronta, A., Luengo, J., Ramirez, Y., Quiñónez, J, González, E., and Sanchez, J. (2004). Isomerization of cis-2-butene and trans-2-butene catalyzed by acid- and ion-exchanged smectite-type clays. *Applied Clay Science 29*(2), 117-123.

[2] Agustriyanto, R., Mochni E.S., Edy Purwanto, E., Setyopratomo, P. (2024). Isomerization of Cis-2-Butene to Trans-2-Butene in a Plug Flow Reactor: A Simulation Study Using Aspen HYSYS V14. Keluwih: Jurnal Sains dan Teknologi *5* (2).

[3] Fogler, S.H. (2016). *Elements of Chemical Reaction Engineering*, Fifth Edition. USA: Pearson/Prentice Hall.

[4] Rodgers, T. (2013). *Chemical Reaction Engineering*. UK: The University of Mančester.

[5] Rawlings, J.B., Ekerdt, J.G. (2025). *Chemical Reactor Analysis and Design Fundamentals*, 2nd Edition. USA: Nob Hill Publishing.

[6] Wosu, C.O. (2024). Plug Flow Reactor (PFR) Design for the Production of 100,000 tons per year of Cumene from the Catalytic Alkylation of Propylene and Benzene. *Journal of Engineering Research Innovation and Scientific Development, 2*(2), 24-33.