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Original Research

Isomerization of Cis-2-Butene to Trans-2-Butene in a Plug Flow Reactor: A Simulation Study Using Aspen HYSYS V14

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Abstract—*This study investigates the isomerization of cis-2-butene to trans-2-butene in a single-tube Plug Flow Reactor (PFR) using Aspen HYSYS V14 for process simulation. The reaction is modeled as a homogeneous, irreversible isomerization with first-order kinetics (rate constant k=0.003833 s−1). The objective was to determine the optimal reactor volume and channel diameter to achieve 95% conversion of cis-2-butene under specified conditions: 1 meter reactor length, 100 kgmol/h feed rate, 12 bar pressure, and 25°C. The Peng-Robinson fluid package was employed for thermodynamic calculations. Simulation results indicate that a reactor volume of 2.268 m³ and channel diameter of 1.699 m are required to achieve the target conversion. This study demonstrates the efficacy of Aspen HYSYS in reactor design optimization and provides valuable insights for industrial applications of butene isomerization. The methodology presented offers a robust framework for addressing similar chemical engineering challenges.*

Keywords: *aspen HYSYS, butene, isomerization, plug flow reactor, process simulation*

Abstrak—Penelitian ini menyelidiki isomerisasi cis-2-butena menjadi trans-2-butena dalam Reaktor Aliran Sumbat (PFR) tabung tunggal dengan menggunakan Aspen HYSYS V14 untuk simulasi proses. Reaksi dimodelkan sebagai isomerisasi homogen irreversible, dengan kinetika orde pertama (konstanta kecepatan reaksi k = 0,003833 s^{-1}). Tujuan penelitian ini adalah menentukan volume reaktor dan diameter saluran yang optimal untuk mencapai konversi cis-2-butena sebesar 95% di bawah kondisi yang telah ditentukan: panjang reaktor 1 meter, laju umpan 100 kgmol/jam, tekanan 12 bar, dan suhu 25°C. Paket fluida Peng-Robinson digunakan untuk perhitungan termodinamika. Hasil simulasi menunjukkan bahwa volume reaktor sebesar 2,268 m³ dan diameter saluran sebesar 1,699 m diperlukan untuk mencapai konversi yang ditargetkan. Penelitian ini menunjukkan efektivitas Aspen HYSYS dalam optimasi desain reaktor dan memberikan wawasan berharga untuk aplikasi industri isomerisasi butena. Metodologi yang dipresentasikan menawarkan kerangka kerja yang kuat untuk mengatasi tantangan rekayasa kimia serupa.

Kata kunci: *aspen HYSYS, butena, isomerisasi, plug flow reaktor, simulasi proses*

INTRODUCTION

Aspen HYSYS is a pivotal tool in chemical process simulation, widely recognized for its ability to model and optimize complex chemical processes (Junior et al. 2022; Valverde et al. 2023). The software is instrumental in designing and simulating reactors, such as Continuous Stirred-Tank Reactors (CSTRs), Plug Flow Reactors (PFRs), and equilibrium reactors (Wasalathilake KC 2014; Tuluc et al. 2015; Riaz et al. 2023). Its application spans various industrial processes, providing accurate predictions and optimization strategies.

Several recent studies have demonstrated the effectiveness of Aspen HYSYS in process simulation. For instance, a detail analysis of the CO_2 removal process from natural gas using MEA and the application of Aspen HYSYS for modeling and simulation (Olugbenga 2024). Another study on the hydrodealkylation of toluene using HYSYS on conversion reactor (Agustriyanto et al. 2024) leads to process modification and heat integration strategies for substantial energy savings in chemical manufacturing process (Maulana et al. 2024).

Moreover, Aspen HYSYS has been used to simulate and optimize chemical processes and reactor designs without extensive physical experimentation (Agustriyanto et al. 2023). Similarly, the software's application in a study by Ahmed et.al (Ahmed et al. 2024) made the researchers able to conduct a comprehensive study of hydrate formation under various conditions without the need for extensive physical experiments, which can be costly and time-consuming in this field. The software's capabilities in modeling complex thermodynamic systems made it an ideal tool for this type of research.

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Aspen HYSYS has been shown in numerous studies to be successful in reactor modeling (Kartal et al. 2022; Yandrapu and Kanidarapu 2022), especially when developing and optimizing chemical reactors under various situations. Aspen HYSYS has been extensively used to simulate reactors such as Plug Flow Reactors (PFRs) (Arefi et al. 2008) , Continuous Stirred-Tank Reactors (CSTRs) (Guedes et al. 2023), and other systems essential to effectively accomplishing desired reaction conversions. As an illustration of Aspen HYSYS's adaptability in handling intricate thermodynamic and kinetic systems, studies have used it to model CO_2 removal procedures, toluene hydrodealkylation, and hydrate formation. These examples demonstrate how Aspen HYSYS makes it possible to model accurately while reducing the need for expensive experimental rigs. When it comes to simulating isomerization reactions, such as butene isomerization, which is crucial for the production of high-octane fuels and other petrochemical products, Aspen HYSYS has shown to be an indispensable tool.

Despite these advancements, a gap remains in the application of Aspen HYSYS for specific processes, such as the isomerization of 1-butene to 2-butene under various operating conditions. Existing studies primarily focus on general applications or well-established reactions, leaving a significant gap for specific process optimizations.

From an industrial perspective, the isomerization of butene is crucial in producing high-octane gasoline and other petrochemical products (Hidalgo et al. 2014; Dhar et al. 2018; Naqvi et al. 2018; Abdellatief et al. 2020; Qiu et al. 2023). Optimizing this process can significantly enhance yield and efficiency, thereby improving the overall profitability and sustainability of petrochemical operations. By providing a detailed simulation and optimization framework, this study contributes valuable insights that can be directly applied to industrial settings, advancing chemical process engineering and industrial practices.

The simulation of cis-2-butene to trans-2-butene isomerization in a plug flow reactor (PFR) using Aspen HYSYS is crucial due to its significant impact on the petrochemical industry, especially in the production of high-octane fuels. This process enhances the octane rating of fuels, which is vital for meeting contemporary fuel performance standards. Given the industry's focus on efficiency and optimization, Aspen HYSYS provides notable benefits, such as the precise modeling of process conditions without the need for costly and time-consuming physical experiments. By using Aspen HYSYS, reactor parameters can be adjusted to achieve high conversion rates with minimal energy consumption, thereby improving efficiency and reducing operating costs.

This study aims to bridge this gap by offering a comprehensive simulation and optimization of the isomerization of cis-2-butene (INCHEM [no date][a]; PubChem [no date][a]) to trans-2-butene (INCHEM [no date][b]; PubChem [no date][b]) using Aspen HYSYS. This research is novel as it integrates kinetic aspects, and economic considerations, providing a holistic approach to process optimization.

METHODS

Problem Statement

The isomerization of cis-2-butene to trans-2-butene is a homogeneous, irreversible reaction with first-order kinetics.

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The reaction takes place in a PFR, and the rate equation is given by: rA=k·CA. where k=0.003833 s^{-1} (Aspen Technology 2012).

According to Arrhenius: $k = Ae^{-E_a/RT}$,

where $R = 8.314 J/mol.K$ and $T = 25^oC = 298K$.

$E_a \approx 95 kJ/mol$ (a mid-range estimate for similar isomerization process) (Satterfield 1991). Therefore $A = 1.72 \times 10^{14} s^{-1}$.

Given Data

- Conversion rate: 95%
- PFR length: 1 m (this length is an initial assumption, the reactor diameter will be calculated by HYSYS)
- Feed rate of cis-2-butene: 100 kgmol/h
- Operating pressure: 12 bar
- Operating temperature: 25°C
- Assumptions: steady-state, isothermal operation, 100% cis-2-butene feed, no pressure drop.

Simulation Steps

1. **Component Entry**: Input all relevant chemical components into the component list in Aspen HYSYS.
2. **Fluid Package Selection**: Select the Peng-Robinson fluid package, suitable for the given operating conditions.
3. **Reaction Setup**: Add the isomerization reaction under the kinetics section, including stoichiometric coefficients.
4. **Reaction Constant Entry**: Input the rate constant k.
5. **Fluid Package Assignment**: Add the reaction to the fluid package, ensuring the system is ready for simulation.
6. **Simulation Environment**: Select and place the PFR in the simulation canvas.
7. **Parameter Adjustment**: Label the inlet, outlet, and energy requirements, and set pressure drop and duty to zero.
8. **Reactor Sizing**: Input the PFR length and provide an initial guess for the reactor volume for iteration purposes.
9. **Feed Data Entry**: Input feed stream data, assuming 100% cis-2-butene.
10. **Reaction Set Application**: Apply the reaction set to the simulation.
11. **Simulation Execution**: Run the simulation, adjusting parameters to achieve the target conversion of 95%.
12. **Iterative Adjustment**: Use the "Adjust" function to iterate the reactor volume until the desired conversion is achieved.
13. **Verification**: Check the product composition to ensure it matches the expected conversion rate.
14. **Final Results**: Record the reactor volume and channel diameter.

RESULTS

The simulation results for the isomerization of cis-2-butene to trans-2-butene in a plug flow reactor (PFR) are presented in this section. A 95% conversion of cis-2-butene was targeted under specific conditions, including a reactor length of 1 meter, a feed rate of 100 kgmol/h, an operating pressure of 12 bar, and a temperature of 25°C. Therefore the diameter of the reactor should be 1.699 m (calculated automatically). Figure 1 presents the process flow diagram, providing a clear visual representation of the plug flow reactor setup and the overall isomerization process.

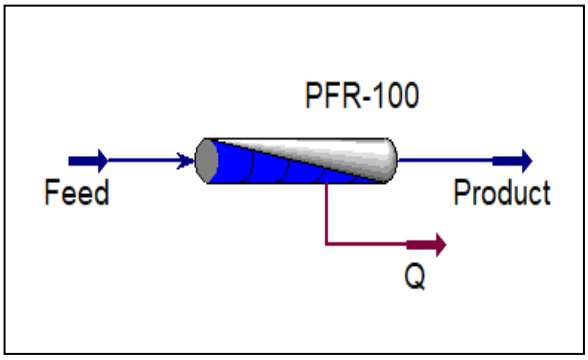

Figure 1. Process flow diagram.

Reactor Volume and Conversion Efficiency:

To achieve the desired conversion efficiency, the optimal reactor volume was found to be 2.268 m^3. Figure 2 shows the relationship between the reactor volume and the percentage conversion, demonstrating the effectiveness of the PFR design in achieving the conversion goal.

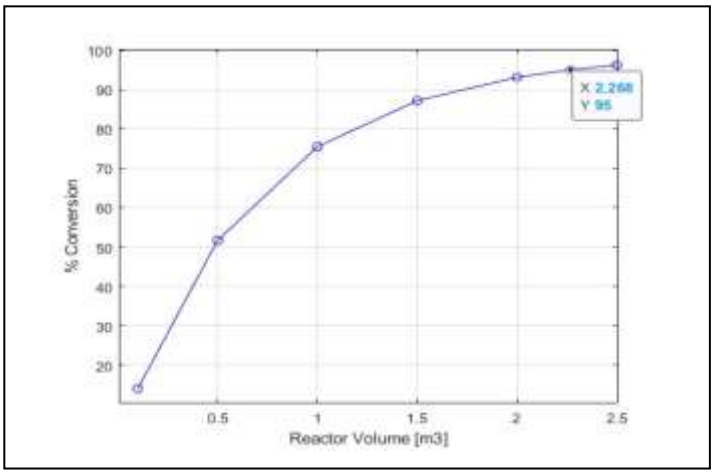

Figure 2. Plot of reactor volume vs % conversion.

Effect of Temperature on Conversion:

The simulation also evaluated the effect of temperature on the conversion efficiency. As shown in Table 1 and Figure 3, the optimal conversion (95%) was achieved at 25°C. When the temperature increased, the conversion efficiency decreased significantly, with values dropping to 66.74% at 75°C and to 6.83% at 90°C.

Table 1
Conversion Efficiency at Different Temperatures

Temperature (°C)	Conversion (%)
25	95
50	94.23
75	66.74
85	33.66
90	6.83

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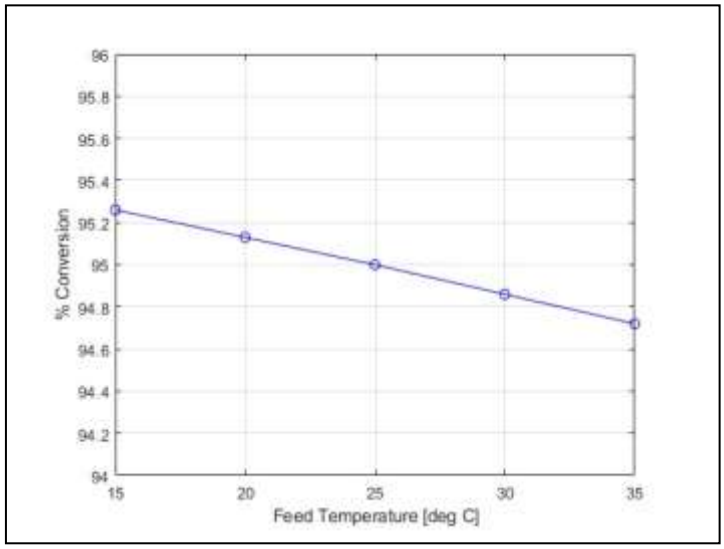

Figure 3. Plot of feed temperature vs % conversion.

Effect of Pressure on Conversion:

The effect of pressure on the isomerization process is depicted in Figure 4. The results indicate that higher pressures initially enhance the conversion rate, but beyond a certain threshold, further pressure increases lead to diminishing returns and higher operational costs.

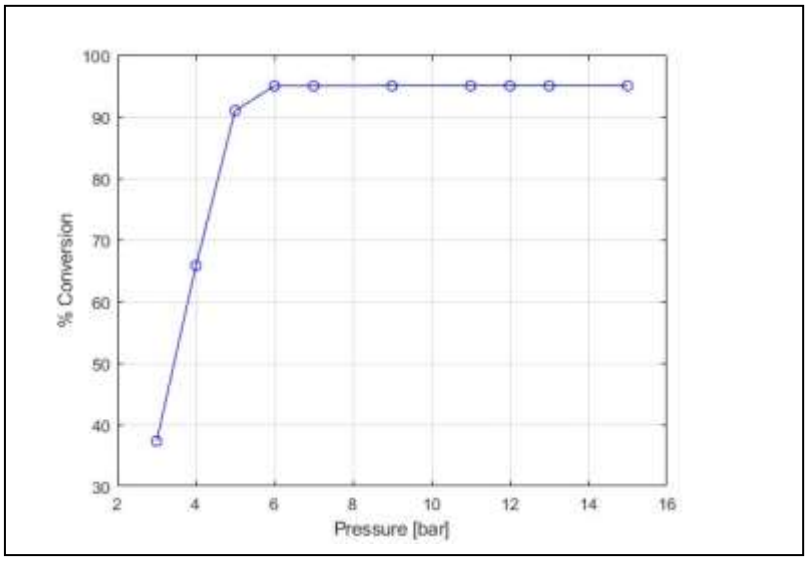

Figure 4. Plot of pressure vs % conversion.

Reactor Performance:

Figure 5 illustrates the reaction rate along the reactor's length, while Figure 6 shows the mole fraction of cis-2-butene and trans-2-butene along the reactor length. These figures validate the efficiency of the plug flow reactor in progressively converting cis-2-butene to trans-2-butene.

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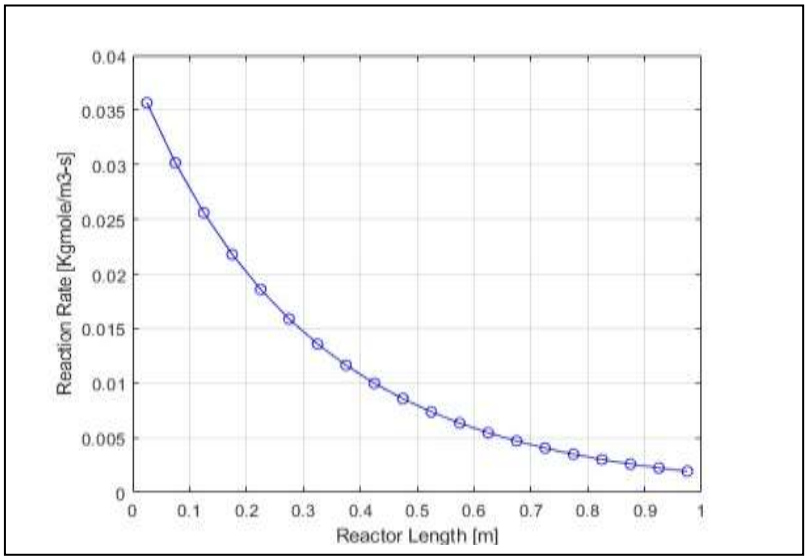

Figure 5. Performance of reaction rate.

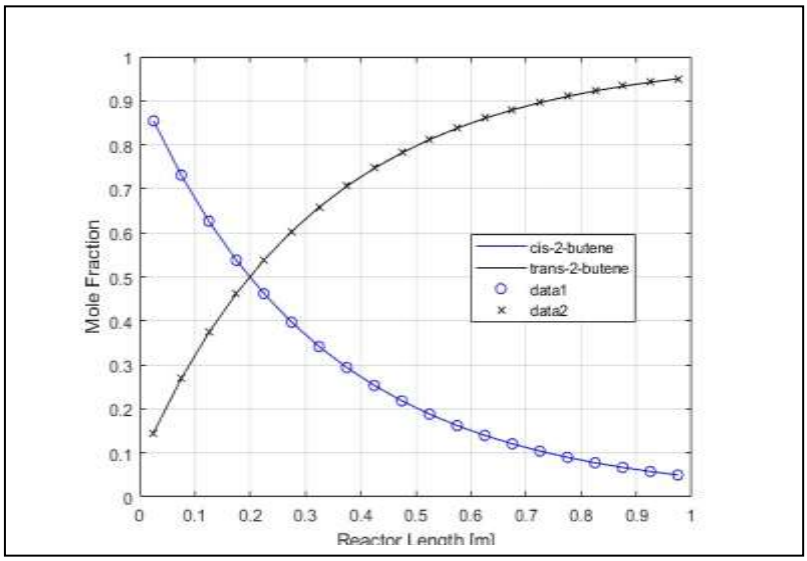

Figure 6. Plot of reactor performance: Mole fraction vs reactor length.

DISCUSSION

The results confirm that the selected reactor design and operational conditions are effective in achieving high conversion rates for the isomerization of cis-2-butene to trans-2-butene. The optimal reactor volume of 2.268 m^3 at 25°C demonstrates the efficiency of the plug flow reactor, particularly in scenarios where high conversion rates are required.

Temperature Sensitivity:

The simulation results highlight the sensitivity of the isomerization process to temperature variations. The sharp decline in conversion efficiency at higher temperatures (75°C and 90°C) indicates equilibrium limitations in the reaction. This behavior aligns with the expected thermodynamic behavior of exothermic reactions, where higher temperatures shift the equilibrium toward the reactants, reducing conversion.

Pressure Optimization:

The impact of pressure on conversion efficiency further emphasizes the need to balance operating pressure and economic considerations. Although higher pressures enhance conversion rates, the benefits diminish beyond a certain point, increasing operational costs without a corresponding increase in conversion efficiency.

Reactor Performance:

The reaction rate and mole fraction profiles along the reactor length provide valuable insights into the reaction dynamics. The progressive conversion of cis-2-butene to trans-2-butene suggests that the plug flow reactor is well-suited for this type of isomerization reaction, allowing for efficient conversion within the reactor's length.

CONCLUSION

This study successfully demonstrated the simulation and optimization of the isomerization process of cis-2-butene to trans-2-butene using Aspen HYSYS V14 in a single-tube plug flow reactor. The optimal conditions for achieving a 95% conversion efficiency were identified, with a reactor volume of 2.268 m^3 at a temperature of 25°C.

Our findings underscore the sensitivity of the isomerization process to temperature variations, where higher temperatures significantly reduce the conversion efficiency due to equilibrium constraints. The analysis also highlighted the critical balance required in pressure settings to enhance conversion while maintaining economic viability.

The comprehensive data presented in the figures and tables validate the efficiency of the plug flow reactor design for this isomerization process. The insights gained from the mole fraction distributions and reaction rates along the reactor length provide a deeper understanding of the reaction dynamics, which are crucial for industrial applications.

In conclusion, the optimized conditions and reactor design proposed in this study offer a robust framework for industrial butene isomerization, ensuring high conversion efficiency and economic feasibility. Future work should focus on exploring further optimization parameters and scaling up the process for commercial applications.

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