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Research Article

Optimizing of Temperature and Pressure in a Modified Plug Flow Reactor to Enhance Benzene Conversion with Process Simulation Software

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Abstract

The increase in industrial dependence on benzene demands a more efficient, high-conversion hydrodealkylation (HDA) process. The HDA of toluene is highly sensitive to temperature and pressure, and inaccuracies in operating conditions can cause side reactions and accelerate catalyst deactivation. This study determined optimal temperature–pressure conditions in a plug flow reactor through steady-state Aspen HYSYS simulation using the Peng–Robinson model and parameter interaction analysis in Design Expert. The results showed a synergistic effect, with temperature as the dominant factor and pressure enhancing conversion. Optimal conditions of 710.8 °C and 67.6 atm produced 90.39% conversion, while the lowest conditions resulted in < 5%. These findings confirm that precise control of operating parameters improves reactor performance and hydrogen utilization, supporting a more stable and energy-efficient HDA process.

Keywords: Process Optimization; Plug Flow Reactor; Benzene; Process Simulation Software

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1. Introduction

Benzene is a fundamental chemical feedstock that plays a crucial role in the petrochemical industry it is used as a precursor to produce polystyrene, nylon, detergents, and many other products [1]. The rising demand for benzene encourages the industry to optimize alternative production routes, one of which is hydrodealkylation (HDA) of toluene, which involves the removal of a methyl group from toluene to produce benzene in the presence of hydrogen and suitable catalysts/reactors. The HDA process is considered more economical than other methods because it utilizes toluene, which is relatively inexpensive and abundantly available [2]. In addition, this reaction produces hydrogen as a by-product that can be reused in industrial processes. Catalyst efficiency becomes a key factor in determining the quality and quantity of benzene produced.

Hydrodealkylation (HDA) of toluene is one of the principal industrial routes for producing benzene, a high-value aromatic compound that serves as a vital feedstock in petrochemical and basic chemical industries [3]. The continuously rising demand for benzene has driven the development of more efficient HDA processes in terms of conversion, selectivity, and energy consumption, particularly when the price differential between toluene and benzene makes process optimization economically attractive [4]. In industrial practice, the HDA process is also favored because it utilizes toluene, which is generally more abundant and less expensive than benzene, enabling producers to stabilize supply chains and reduce dependency on external

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benzene sources. [5]. However, achieving high conversion and selectivity remains a challenge due to competing side reactions, catalyst deactivation, and the necessity of operating under high temperature and pressure conditions. These challenges underscore the importance of reactor design and operational strategies, especially in systems constrained by heat and mass transfer phenomena that significantly influence reaction performance [6]. Consequently, researchers and industry practitioners continue to explore optimized reaction pathways, novel catalyst formulations, and more effective reactor configurations to enhance the overall efficiency of the HDA process [7].

The hydrodealkylation (HDA) process was first developed in the 1980s by James Merrill Douglas with the primary objective of producing benzene from heavier aromatic compounds, particularly toluene. The process proceeds through the reaction of aromatic hydrocarbons with hydrogen at elevated temperatures. The main reaction involves the dealkylation of the methyl group in toluene in the presence of hydrogen, yielding benzene as the principal product and methane as a by-product, as shown below:

$$C_6H_5CH_3 + H_2 \rightarrow C_6H_6 + CH_4 \quad \Delta H^o_{1,298K} = -50 \text{ kJ/mol} \quad (1)$$

This reaction is endothermic, requiring a continuous supply of heat to proceed. In addition to the desired pathway, a side reaction may occur in which two benzene molecules associate to form diphenyl and hydrogen, represented as:

$$2C_6H_6 \rightleftharpoons C_{12}H_{10} + H_2 \quad \Delta H^o_{2,298K} = +8.1 \text{ kJ/mol} \quad (2)$$

This secondary reaction is also endothermic and undesirable, as it consumes benzene that has already been formed, thereby reducing the overall benzene yield if not properly controlled. Consequently, careful regulation of operating conditions is essential in the HDA process to maximize benzene production while minimizing the formation of unwanted by-products.

Catalyst deactivation due to coke formation remains one of the major challenges in continuous reaction processes. The accumulation of coke can cover the active surface of the catalyst, thereby reducing the number of available active sites for the reaction to proceed. Research on catalyst stability has shown that suboptimal operating conditions can accelerate the formation of carbon deposits [8]. These deposits ultimately lower reactant conversion and diminish overall process efficiency. Modifications in catalyst composition can reduce the tendency for coke formation. In addition, adjustments to operating conditions have been proven to enhance reaction performance while simultaneously maintaining catalyst stability over the long term [9].

The optimization of temperature and pressure combinations is crucial for achieving maximum process performance. Recent studies in flow chemistry have emphasized the importance of optimizing operating conditions in continuous reactors. For example, the integration of flow chemistry with a design of experiments approach has proven effective in identifying optimal combinations of reaction parameters, such as temperature, residence time, and flow rate to maximize yield. Furthermore, the use of micro flow reactors with simulated temperature and conversion profiles along the reactor channel enables precise estimation of conversion and temperature distribution, thereby providing a robust foundation for operating condition optimization [10]. In addition, data-rich approaches through dynamic flow experiments have recently been introduced as efficient methods for systematic chemical process optimization [11]. Given the sensitivity of hydrodealkylation (HDA) reactions to operating conditions, optimizing temperature and pressure in flow or plug-flow reactor (PFR) systems is particularly relevant. However, while optimization of temperature and pressure has been extensively studied in other flow reactions, limited research has systematically investigated the HDA of toluene in PFR systems. This study seeks to address this gap by optimizing operating temperature and pressure in a PFR to maximize benzene conversion from toluene, while simultaneously maintaining catalyst stability and minimizing side reactions.

2. Methods

2.1. Basic Chemical Process of Hydrodealkylation of Toluene

In this process, toluene and hydrogen react to produce benzene, which can further convert into biphenyl through a side reaction. The hydrodealkylation method is widely used to obtain high-purity benzene by promoting the hydrodealkylation of toluene. The primary reaction leading to benzene formation is presented in Equation (1), with its corresponding kinetic model shown in Equation (2). Meanwhile, the side reaction is illustrated in Equation (3), accompanied by its kinetic equation in Equation (4) [12]. Main reaction of Hydrodealkylation process:

$$C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4 \quad (3)$$

$$R_1 = 1.9580\times10^8 \exp(-25616/T) \quad (4)$$

Side Reaction of Dimer of benzene:

$$2C_6H_6 \leftrightarrow C_{12}H_{10} + H_2 \quad (5)$$

$$R_2 = 1.2115\times10^6 \exp(-25616/T) - 5.1662\times10^6 \exp(-25616/T) \quad (6)$$

Simulation of this production process was carried out using the Aspen HYSYS application. The two reactions described earlier were incorporated as Reaction Set 1 (kinetic) and Reaction Set 2 (kinetic). Both reaction sets were assigned to the selected fluid package. All components involved in the reactions were already available in the HYSYS component list. The Peng–Robinson Equation of State (PR-EOS) was used as the thermodynamic model to accurately represent the vapor–liquid equilibrium behavior of the hydrocarbon–hydrogen system [13]. The overall production process consists of a mixer, a plug flow reactor, a heat exchanger, and a compressor.

2.2. Basic Process Flow Diagram(PFD)

Figure 1 illustrates the simplified process flow diagram of the toluene hydrodealkylation (HDA) process, in which benzene is produced via the hydrodealkylation of toluene. The process begins with the feed preparation and mixing stage, where the fresh feed is combined with recycled gas and liquid streams in the MIX-100 unit to ensure a homogeneous composition and a stable flow rate prior to thermal conditioning. The mixed stream is subsequently directed to the E-100 heat exchanger, where its temperature is increased by the external heat input Q1 to approach the desired reactor operating conditions while simultaneously reducing the thermal duty required in the downstream heating stage. Following this initial preheating step, stream S1 enters the K-100 compressor, where its pressure is elevated to meet the reactor operating pressure and to compensate for pressure losses associated with the recycle loop. The energy requirement for the compression process is represented by OKOM . The pressurized stream is then routed to the E-101 heater/heat exchanger, where additional heat input Q2 is supplied to precisely control the reactor inlet temperature at its optimal value. Finally, stream S3, having satisfied the required temperature and pressure specifications, is introduced into the plug flow reactor (PFR-100), in which the primary chemical reactions occur, resulting in the formation of the product stream S4.

2.3. Process Optimization

In this study, the production process was optimized with an emphasis on reactor operating conditions, specifically temperature and pressure. The toluene hydrodealkylation process typically operates within a temperature range of 500–650 °C and a pressure range of 20–60 atm [12]. The optimization was conducted using Design Expert, with the detailed variables presented in Table 1, while the fixed parameters of Feed Pressure is 20 atm, Feed Flow Rate of 40689.8 kg/h, and the constraints of the optimization of Temperature is in range 600-750 °C and Pressure is in range 30-80 atm. The variables were then simulated in the reactor to obtain the reaction conversion for each condition. The simulation process was supported by the case study feature that available in Aspen HYSYS.

Table 1. Independent variables used for optimization in Design Expert.

Run	Temperature (℃)	Pressure (atm)
1	600	30
2	800	30
3	600	80
4	800	80
5	600	55
6	800	55
7	700	30
8	700	80
9	700	55
10	650	42.5
11	750	42.5
12	650	67.5
13	750	67.5

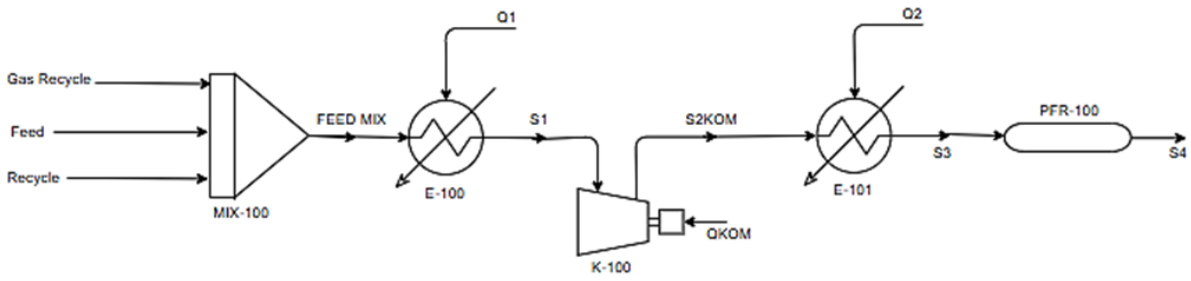

Figure 1. Process flow diagram of the toluene hydrodealkylation process.

3. Results and Discussion

Optimization was performed to obtain the most optimal reactor temperature and pressure in the benzene production simulation using the hydrodealkylation process of toluene. The simulation performed with Aspen HYSYS is shown in Figure 2. The Figure 2 illustrates the steady-state simulation of the benzene production process. The fresh feed, consisting of toluene and hydrogen, is combined with the recycle stream and subsequently heated in heater (E-100 and E-101) to reach the required operating conditions before entering the Plug Flow Reactor (PFR-100). Within the PFR-100, the primary hydrodealkylation reaction proceeds exothermically. Once the base-case model achieved successful convergence, a parametric study (case study) and optimization were performed to assess the reactor's sensitivity to variations in key operating variables temperature and pressure to obtain maximum conversion.

The combined effects of temperature and pressure on toluene conversion were systematically evaluated using a Design Expert optimization framework, as summarized in Table 2 and illustrated by the three-dimensional response surface that shown in Figure 3. The results clearly demonstrate that both variables significantly influence reactor performance, with temperature exhibiting a more pronounced effect compared to pressure.

From the experimental data, conversion increases consistently with rising temperature across all pressure levels. At a low pressure of 30 atm, increasing the temperature from 600 °C to 700 °C enhances conversion from 45.2% to 78.5%, while a further increase to 800 °C results in a more moderate improvement to 62.5%, indicating diminishing returns at excessively high

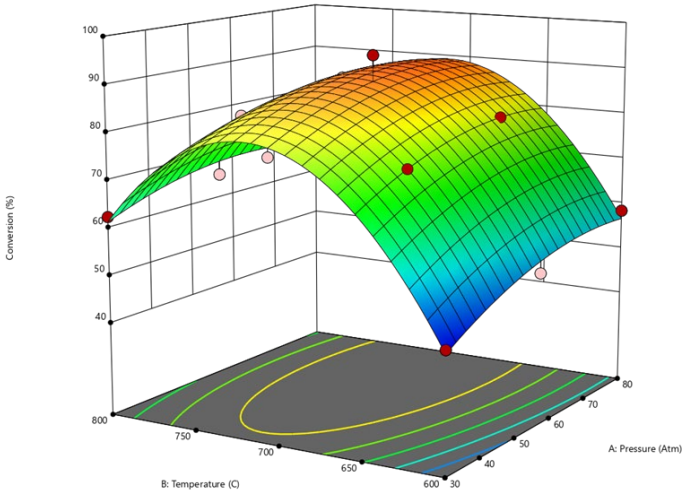

Figure 3. Result of simulation hydrodealkylation toluene process using Aspen HYSYS.

Table 2. Result of simulation hydrodealkylation toluene process using Aspen HYSYS.

Run	Temperature (℃)	Pressure (atm)	%Conversion
1	600	30	45.2
2	800	30	62.5
3	600	80	58.4
4	800	80	68.8
5	600	55	52.1
6	800	55	65.3
7	700	30	78.5
8	700	80	85.4
9	700	55	94.5
10	650	42.5	74.98
11	750	42.5	82.65
12	650	67.5	80.24
13	750	67.5	86.19

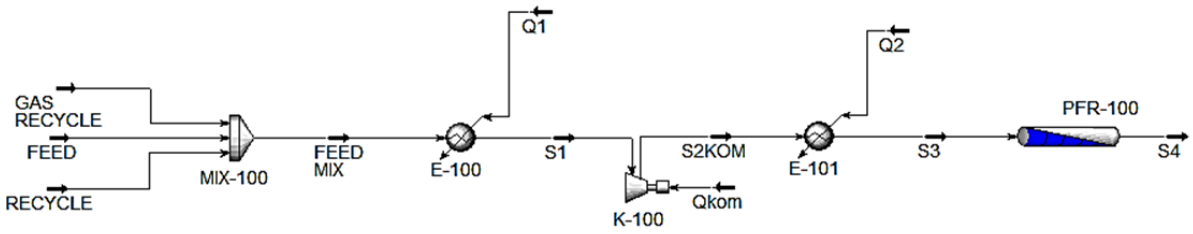

Figure 2. Simulation of hydrodealkylation toluene using Aspen HYSYS.

temperatures. A similar trend is observed at higher pressures, where conversion reaches its maximum values within the intermediate-to-high temperature range rather than at the extreme upper limit.

Pressure also contributes positively to conversion, particularly at moderate and high temperatures. For instance, at 700 °C, increasing pressure from 30 atm to 55 atm raises conversion from 78.5% to 94.5%, indicating that elevated pressure enhances hydrogen availability and promotes the hydrodealkylation reaction. However, further pressure increases beyond this range yield marginal improvements, suggesting that the reaction becomes kinetically rather than mass-transfer limited.

The 3D response surface further confirms the existence of an optimal operating region rather than a monotonic increase in conversion with temperature and pressure. The surface exhibits a dome-shaped profile, with the highest conversion occurring at approximately 700–750 °C and 55–70 atm. Beyond this region, conversion declines, particularly at very high temperatures, which can be attributed to the increasing dominance of side reactions and possible thermal degradation effects. This observation is consistent with selectivity analysis, where excessive temperatures were shown to favor undesired hydrocracking reactions at the expense of the primary hydrodealkylation pathway [14].

From a kinetic perspective, the strong temperature dependence aligns with the Arrhenius relationship, where higher temperatures significantly increase reaction rates by overcoming the activation energy barrier [15]. Meanwhile, increased pressure shifts the reaction equilibrium and enhances hydrogen partial pressure, favoring benzene formation. Nevertheless, excessively severe conditions accelerate secondary reactions, reducing the effective conversion to the desired product.

Overall, the optimization results demonstrate that the highest conversion is achieved under moderate-to-high temperatures combined with intermediate pressures, rather than at extreme operating conditions. This finding underscores the importance of balancing kinetic enhancement with selectivity control. The identified optimal region provides a practical operating window that maximizes conversion while mitigating the formation of undesired by-products, thereby offering valuable guidance for reactor design and industrial-scale operation. The contour plot projection reinforces this interpretation by highlighting an elliptical optimal zone, indicating strong interaction effects between temperature and pressure. The non-linear nature of the surface implies that optimizing one variable independently is insufficient; instead, simultaneous optimization is required to achieve maximum conversion. Based on these data trends, numerical optimization was performed using Design-Expert to determine the precise operating point that maximizes conversion, with constraints set for temperature between 600−800 °C and pressure between 30−80 atm.

Table 3. Optimization results of operating conditions to achieve desirability.

Temperature (°C)	Pressure (atm)	Conversion (%)	Desirability
710.8	67.6	90.39s	0.917

The optimization results presented in Table 3 which selected as the best operating condition. The solver recommends operating at the middle point parameters, specifically at a temperature of 710.8 °C and a pressure of 67.6 atm. Under these conditions, the predicted conversion is 90.39% with a desirability value of 0.917. A desirability value approaching 1.0 indicates that this operating condition is technically ideal for meeting the desired production targets, balancing the need for fast reaction kinetics with equipment operational limits.

4. Conclusions

This study aimed to determine the optimal reactor operating conditions for maximizing benzene conversion in the toluene hydrodealkylation (HDA) process, using Aspen HYSYS simulation and Design-Expert optimization. Within the defined ranges of independent variables, temperature (600–750 °C) and pressure (30–80 atm), reactor temperature was identified as the primary factor influencing conversion. The simulation results showed that increasing temperature significantly enhanced conversion due to the high activation energy of the HDA reaction, while pressure had a secondary but positive effect by increasing reactant concentration in the gas phase. Numerical optimization indicated that the best operating conditions were at the upper limits of the studied range, specifically 710.8 °C and 67.6 atm, yielding a predicted conversion of 90.39 % with a desirability value of 0.917. These findings suggest that operating the HDA reactor at high temperature and pressure within the specified ranges is crucial to achieving near-maximum toluene conversion, with temperature exerting a stronger influence on reaction kinetics than pressure.

CRedit Author Statement

Author Contributions: A. R. H. Sitio: Conceptualization, Methodology, Investigation, Resources, Data Curation, Writing, Review, Software and Editing, Supervision. A. W. Hutabarat: Conceptualization, Methodology, Formal Analysis, Data Curation, Writing Draft Preparation, Visualization, Project Administration; A. R. I. Zahkia: Validation, Writing Draft, Review and Editing, Data Curation; A. E. Damanik: Validation, Investigation, Resources, Writing Draft, Review and Editing, Validation; M. D. Huda: Validation, Investigation, Software Resources, Data Curation, Writing Draft, Review and P. U. Pulungan: Investigation, Resources, and Data Curation. All authors have read and agreed to the published version of the manuscript.

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