Fundamental insights into propane aromatization: understanding the essential principles

Davron Hamidov[1]*, *Normurod* Fayzullayev[2], *Sadoqat* Nomozova[1], *Ra'no* Norboyeva[1], *Gulnoza* Tursunova[1], *Chinigul* Bobilova[1], *Ma'mura* Do'stmurodova[1], and *Sardor* Samiyev[1]

[1]Karshi Engineering Economics Institute, 180100 Karshi, Uzbekistan
[2]Samarkand State University, 140101, Samarkand, Republic of Uzbekistan

Abstract. This article explores the catalytic reaction mechanisms of propane aromatization using catalysts containing 2% Zr, 2% Zn, and 7% Mo supported on mesoporous silica (MPS). Prior to catalytic testing, the samples underwent hydrogen treatment at a flow rate of 2500 h^{-1} for two hours. The experiments were conducted at a consistent volumetric velocity of 500 h^{-1}, employing a standardized methodology. The study evaluates key parameters of the propane aromatization process on the 2%Zr-2%Zn-7%Mo/MPS catalyst, with and without hydrogen pre-treatment, as well as on a catalyst with a 5% Zr concentration prepared through impregnation. The findings offer insights into the catalytic behaviour and effectiveness of the propane aromatization process on these specific catalyst formulations.

1 Introduction

The aromatization of light alkanes, particularly propane and butane, has been a focal point of research for nearly three decades due to its significant economic and strategic implications [1,2]. Among the catalysts studied, the ZSM-5 catalyst, enhanced by the work of P. Zhang, L. Tan, G. Yang, and N. Tsubaki, stands out as an effective bifunctional catalyst for propane aromatization [3,4,5,6]. The process of transforming light hydrocarbons into aromatic compounds is not only crucial from a scientific perspective but also highly relevant for industrial applications. Aromatization of lower alkanes yields aromatic hydrocarbons like benzene, toluene, and xylenes, which are valuable feedstocks for the chemical and petrochemical industries. Additionally, understanding the mechanism of hydrocarbon conversion through this reaction is of considerable scientific interest. The conversion of low molecular weight paraffinic hydrocarbons into aromatic compounds is a complex process, involving both target reactions and several side reactions. Achieving selective conversion of lower alkanes to aromatic hydrocarbons requires a catalyst with high selectivity. Previous studies on the aromatization of C2-C4 hydrocarbons demonstrate the effectiveness of bifunctional catalytic systems, which feature both acidic sites from the

* Corresponding author: fer.sapedu@gmail.com

© The Authors, published by EDP Sciences. This is an open access article distributed under the terms of the Creative Commons Attribution License 4.0 (https://creativecommons.org/licenses/by/4.0/).

sorbent carrier and active metal-containing sites introduced by dehydrating promoters [7,8,9].

In recent decades, there has been significant advancement in converting light hydrocarbons into more valuable products. This has underscored the importance of converting light alkanes into aromatic compounds within the industry. Aromatic hydrocarbons such as benzene, toluene, and xylenes, produced through the aromatization of light alkanes, are highly valued as intermediates in the chemical and petrochemical sectors [10,11,12]. Extensive research has been conducted on synthesizing these aromatic compounds from propane-butane fractions and petroleum gases using catalysts based on high-silicon sorbents [13,14,15,16]. Additionally, studies have explored the synthesis of ethylene from methane [17,18], and the production of hydrocarbons from synthesis gas, methanol, and dimethyl ether using catalysts derived from high-silicon sorbents [19,20].

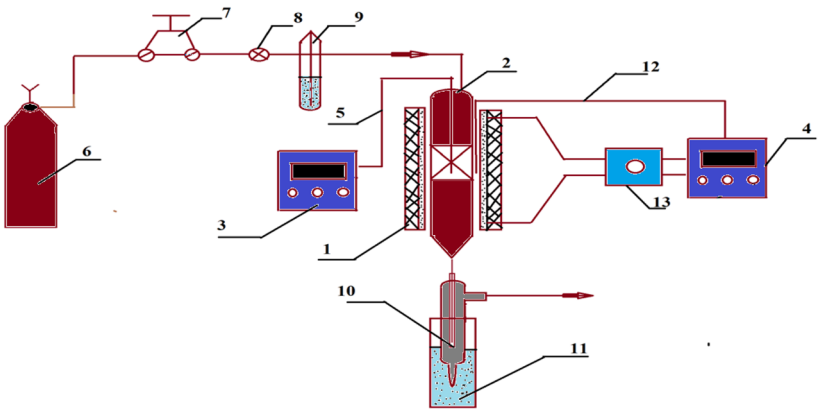
2 Experimental part

High-purity gases were used in the study, including propane (99.9%), hydrogen (99.9%), helium (99.9%), and nitrogen (98.8%). Catalysts were prepared using two methods: solid-phase modification and impregnation. For solid-phase modification, mesoporous sorbent powder was mixed with zirconium oxide for 2 hours. In the impregnation method, a calculated amount of $ZrO(NO_3)_2 \cdot 8H_2O$ was dissolved in distilled water, then the solution was added to a measured amount of sorbent. The mixture was evaporated on a water bath with constant stirring and subsequently calcined in an oven at 200°C for 3 hours. A zirconium aluminosilicate sample with a MPS structure was synthesized hydrothermally at high pressure, using a mixture of aluminosilicate and zirconium nitrate, designed for propane catalytic dehydroaromatization. Before conducting experiments, the catalyst powder was ground, sieved to a 1-2 mm particle size, pressed, and formed into tablets. To enhance heat transfer during reactions, the catalyst was diluted with quartz of the same particle size in a 1:1 ratio. All samples were pre-treated at 550°C in either air or hydrogen flow for 2 hours prior to catalytic testing. The catalyst regeneration in hydrogen flow (1 l/h) was carried out as follows:

- Heating from 25°C to 350°C at a rate of 4°C/min, followed by a 1-hour hold at 350°C.
- Further heating from 350°C to 550°C at the same rate, with a 1-hour hold at 550°C.

After activation, the catalyst was purged with helium for 15 minutes at the experimental temperature to remove any residual water.

The catalytic aromatization of propane was performed in a fixed-bed flow reactor under atmospheric pressure. A schematic diagram of the laboratory setup is illustrated in Figure 1.



1- quartz furnace, 2- quartz reactor, 3- relay RES-10, 4- thermocouple for temperature control, 6- gas cylinder, 7- reducer, 8- valve, 9- rheometer, 10- catalytic dehydroaromatization reaction of liquid propane holder for collecting products, 11- Liquid nitrogen container, 12 - thermocouple (temperature regulator), 13- Thermometer

Fig. 1. Schematic diagram of the experimental device

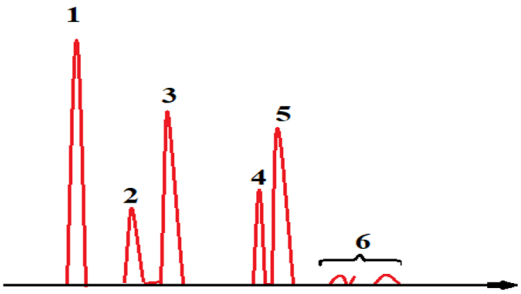
2.1 Laboratory Equipment and Experimental Procedure

The laboratory setup includes a vertical quartz furnace (1), shaped as a hollow cylinder, heated by nichrome wire with asbestos insulation. A quartz reactor (2) with an inner diameter of 21 mm is positioned within the furnace. The heating rate and temperature are precisely controlled by RES-10 (3) and TRM-1 (4) devices, with an accuracy of ±1°C. The temperature in the catalytic dehydroaromatization reaction zone was varied between 350°C and 650°C, monitored by a chrome-aluminum thermocouple (5) encased in a quartz housing with a diameter of 1 mm. Gases, including propane, helium, or hydrogen, were supplied from cylinders (6) through a regulator (7). The gas flow rate was adjusted with a valve (8) and measured using a rheometer (9) pre-calibrated for the specific gas. Propane was delivered at a volumetric rate of 500 h^{-1}, with experiments typically lasting 2.5 hours. The products of the catalytic dehydroaromatization reaction were collected in a liquid nitrogen-cooled trap (10) (11) twice for 40 minutes, then degassed for 15-20 minutes at room temperature before being weighed and analyzed. Gaseous products and starting materials were collected in a gasometer for chromatographic analysis of component concentrations. After each experiment, the catalyst was purged with helium for 15 minutes to remove adsorbed reaction products. Helium was supplied from a cylinder at a rate of 5 l/h, regulated by a fine-adjustment valve on the rheometer. The catalyst was then regenerated by treating it with air at 550°C for two hours.

2.2 Product Analysis and Calculation of Process Indicators

The products from propane catalytic aromatization include both gaseous and liquid hydrocarbons. The liquid products are a mixture of aromatic hydrocarbons formed during the reaction, using a 2%Zr-2%Zn-7%Mo/MPS catalyst, while the gaseous products consist of methane, ethane, ethylene, propane, and propylene. The gaseous hydrocarbons were analysed using an LXM-2000M chromatograph equipped with a thermal conductivity detector (catharometer). The analysis was conducted isothermally in a column filled with Porapak Q (column length 2.4 m, diameter 4 mm) at 70°C. The carrier gas flow rate (Ne)

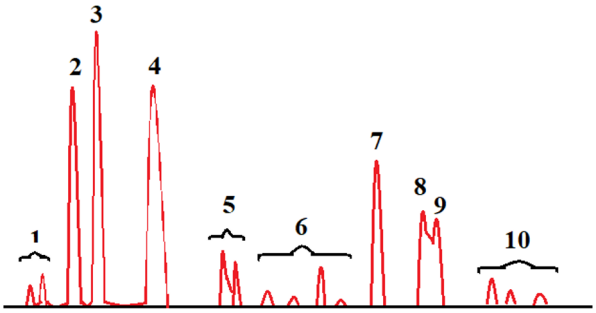
was maintained at 30 cm³/min. The composition of the components was calculated using the absolute calibration method. An example chromatogram is presented in Figure 2.



Component comparison procedure:1- methane. 2- ethylene, 3-ethane, 4-propylene, 5-propane, 6-C4+-hydrocarbons

Fig. 2. Chromatogram of gaseous hydrocarbons

Aromatic hydrocarbons produced from the catalytic aromatization of propane using a Mo/MPS-containing catalyst were analyzed with an LXM-2000M chromatograph. This chromatograph featured a 5% SE-30 column (1.5 m in length, 3 mm in diameter) with nitrogen as the carrier gas. The analysis was conducted by gradually increasing the temperature from 50°C to 160°C, using a flame ionization detector, and subsequently under isothermal conditions with temperature programming. The composition of the hydrocarbons was determined through the internal normalization method. A representative chromatogram is shown in Figure 3.



1- dissolved gases, 2-solvent,3-benzene. 4- toluene, 5- xylene and ethylbenzene, 6 - C9 hydrocarbons, 7-naphthalene, 8 - 9 - C10 -hydrocarbons 10- C12 -hydrocarbons

Fig. 3. Chromatogram of aromatic hydrocarbons produced during the catalytic aromatization of propane using a 2%Zr-2%Zn-7%Mo/MPS catalyst.

To assess the overall catalytic activity in the aromatization of propane with the 2%Zr-2%Zn-7%Mo/MPS catalyst, the propane conversion rate (K_C_3H_8) was calculated. The aromatization activity of the catalyst samples was evaluated based on the yield of aromatic hydrocarbons (B_ArH) produced during the reaction. The selectivity (S) for the formation of aromatic and gaseous hydrocarbons was calculated using the following formula:

$$S = \frac{B}{KC_3H_8} \times 100\%$$

B - product productivity (%),
KC_3H_8 - conversion (%) of propane in catalytic dehydroaromatization

3 Results and discussion

The reaction temperature for the catalytic dehydroaromatization of propane was varied between 500°C and 650°C at a constant volumetric rate (V = 500 h^{-1}) using an MPS sorbent. The key process indicators are summarized in Table 1. Figure 4 illustrates how conversion, efficiency, and selectivity for aromatic products change with temperature during the catalytic dehydroaromatization of propane. At 500°C, the yield of aromatic hydrocarbons (ArH) produced with the 2%Zr-2%Zn-7%Mo/MPS catalyst was 17.8%. As the temperature increased, the yield of aromatic hydrocarbons also rose, reaching 38.6% at 600°C. The propane conversion rate also accelerated with temperature, increasing from 65.4% at 500°C to 95.9% at 650°C. The yield of gaseous products from the catalytic aromatization of propane is strongly influenced by the reaction temperature. As shown in Table 1, the methane yield increased by almost 50%, from 20.5% to 30.8%, and the yield of C_2 hydrocarbons rose from 21.8% to 27.4% as the temperature increased from 500°C to 650°C.

Table 1. Key parameters of the propane aromatization process on the MPS catalyst

T, °C	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
500	65.4	20.6	21.8	1.7	2.8	46.9	17.8
550	79.4	25.4	23.4	2.2	1.8	52.5	27.8
600	94.6	30.8	25.6	2.5	1.7	60.6	38.6
650	95.9	31.9	27.4	2.8	0.0	62.1	40.6
T, °C	KC_3H_8	Product selectivity, %					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
500	62.4	32.9	33.4	2.4	3.9	72.4	27.6
550	79.4	31.7	29.4	2.8	1.9	65.4	35.4
600	96.6	31.8	25.6	2.5	1.4	61.4	39.4
650	99.4	31.2	25.8	2.4	0.4	59.42	40.8

At a constant volumetric rate (V = 500 h^{-1}), the temperature for the catalytic dehydroaromatization of propane was varied between 450°C and 500°C. The primary process indicators are summarized in Table 2. Figure 5 illustrates how conversion, efficiency, and selectivity for aromatic products depend on temperature during the reaction. At 450°C, the yield of aromatic hydrocarbons using the 2%Zr-2%Zn-7%Mo/MPS catalyst was 15.8%. As the temperature increased, the yield of aromatic hydrocarbons rose significantly, reaching 53.8% at 600°C. At the initial temperature of 450°C, the propane conversion rate was relatively low, at 36.4%.

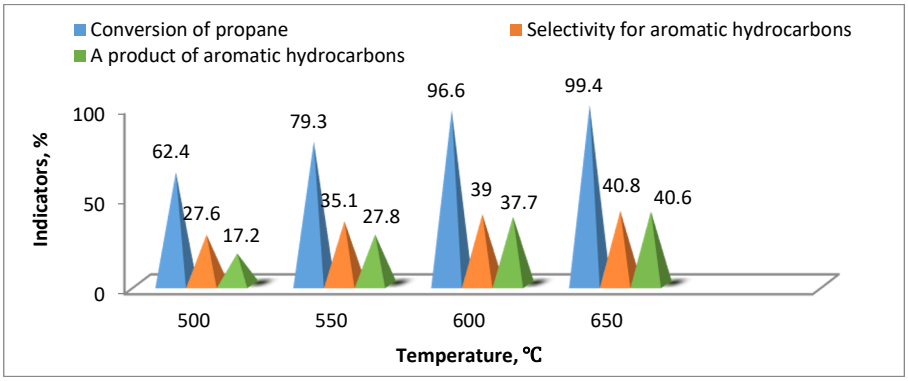


Fig. 4. Temperature dependence of key parameters for the propane aromatization process using the 2%Zr-2%Zn-7%Mo/MPS catalyst.

The yield of gaseous products from the catalytic aromatization of propane with a 2%Zr-2%Zn-7%Mo/MPS catalyst is highly temperature-dependent. As demonstrated, increasing the temperature from 450°C to 600°C led to a rise in methane yield from 9.8% to 23.6%.

Table 2. Performance metrics for the propane aromatization process using the 2%Zr-2%Zn-7%Mo/MPS catalyst prepared via the impregnation method without prior hydrogen treatment.

T, ℃	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	36.4	9.8	10.4	0.5	1.6	21.4	15.8
500	68.4	14.8	16.6	0.8	0.6	32.9	35.6
550	87.8	19.0	21.2	1.5	0.4	42.0	45.9
600	99.4	23.6	22.0	1.5	0.0	46.2	53.8
T, ℃	KC_3H_8	Product selectivity, %					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	36.4	24.4	28.5	1.4	4.4	58.4	41.7
500	68.4	21.6	24.4	1.4	0.9	48.0	52.0
550	87.8	21.6	24.0	1.7	0.5	47.8	52.4
600	99.4	22.7	22.4	1.6	0.0	46.5	53.5

Prior to conducting the catalytic experiments, the samples were exposed to a hydrogen flow (2500 h^{-1}) for 2 hours. The experiments were then performed at a constant volumetric rate (V = 500 h^{-1}) using the same procedure. Key process indicators are summarized in Table 3. Figure 6 illustrates how temperature affects the conversion, efficiency, and selectivity during the catalytic dehydroaromatization of propane to produce aromatic products. At a temperature of 450°C, the yield of aromatic hydrocarbons using the 2%Zr-2%Zn-7%Mo/MPS catalyst was 17.4%.

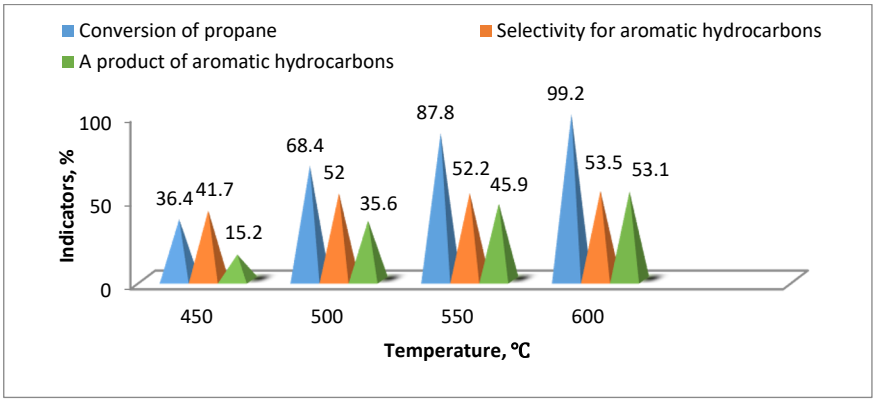


Fig. 5. Temperature dependence of the main process parameters for catalyst 2%Zr-2%Zn-7%Mo/MPS (soaking without hydrogen treatment)

As the temperature increased, the yield of aromatic hydrocarbons during the catalytic aromatization of propane with the 2%Zr-2%Zn-7%Mo/MPS catalyst also rose, reaching 54.5% at 600°C. At the initial temperature of 450°C, propane conversion was relatively low at 37.5%. However, with increasing temperature from 450°C to 600°C, the conversion rate accelerated significantly, achieving 99.4% at 600°C. Similarly, the methane yield increased from 8.8% to 21.5% as the temperature was raised from 450°C to 600°C.

Table 3. Key performance of propane aromatization over 2%Zr-2%Zn-7%Mo/MPS catalyst prepared by hydrogen impregnation

T, °C	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ApH
450	37.5	8.8	9.5	0.5	2.0	20.4	17.4
500	71.6	16.4	16.2	0.9	0.7	33.9	37.7
550	89.6	20.2	20.0	1.2	0.0	41.4	48.4
600	99.4	21.5	20.9	1.4	0.0	42.6	54.5
T, °C	KC_3H_8	Product selectivity, %					
		CH4	ΣC2	C3H8	ΣC4	ΣC1-C4	ArU
450	36.5	23.0	26.0	1.4	5.4	56.0	44.0
500	71.6	22.7	22.5	1.4	1.0	47.4	52.6
550	89.6	22.4	22.4	1.4	0.0	46.2	53.9
600	99.2	20.7	21.2	1.4	0.0	43.0	57.0

At a constant volumetric rate (V = 500 h^{-1}), the temperature for the catalytic dehydroaromatization of propane was varied between 450°C and 500°C. Key process indicators are detailed in Table 4. Figure 7 illustrates how temperature affects the conversion, yield, and selectivity of aromatic products in the catalytic dehydroaromatization of propane. At 450°C, the yield of aromatic hydrocarbons using the 2%Zr-2%Zn-7%Mo/MPS catalyst was 15.4%. As the temperature increased, the yield of aromatic hydrocarbons also rose, reaching 53.4% at 600°C.

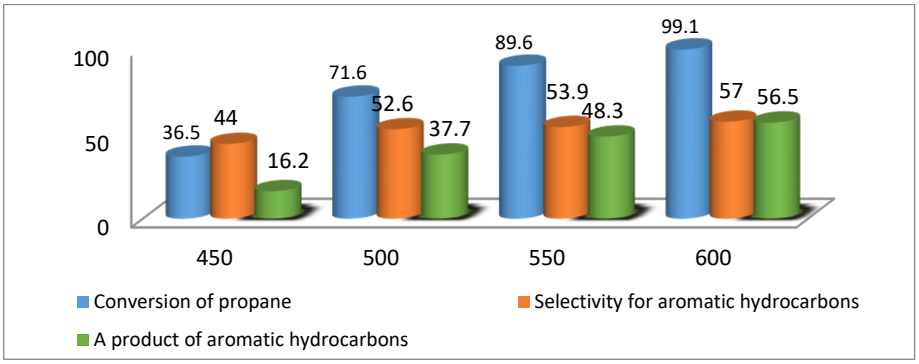


Fig. 6. Temperature dependence of the main process parameters for catalyst 2%Zr-2%Zn-7%Mo/MPS (impregnation with hydrogen treatment)

At the initial temperature, propane conversion in the catalytic dehydroaromatization process was relatively low, at 33.7%. As the temperature increased from 450°C to 600°C, the conversion rate rose significantly, reaching 96.9% at 600°C. These values are slightly lower compared to those achieved with the catalyst prepared by the impregnation method. The yield of gaseous products from the catalytic aromatization of propane with the 2%Zr-2%Zn-7%Mo/MPS catalyst is influenced by a less pronounced temperature effect compared to the impregnation method. Specifically, as the temperature increased from 450°C to 600°C, the methane yield rose from 9.8% to 18.4%.

Table 4. Key process parameters for propane aromatization over 2%Zr-2%Zn-7%Mo/MPS catalyst prepared by solid-phase modification method without hydrogen pretreatment

T, °C	KC_3H_8	Product yield,%					
		CH4	ΣC2	C3H8	ΣC4	ΣC1-C4	ArU
450	33.7	9.8	8.4	0.5	1.5	19.4	15.4
500	68.2	14.8	17.0	1.2	0.5	33.4	34.7
550	86.4	15.5	21.9	1.4	0.4	39.4	47.4
600	96.9	18.4	23.7	1.4	0.0	42.5	53.4
T, °C	KC_3H_8	Product selectivity, %					
		CH4	ΣC2	C3H8	ΣC4	ΣC1-C4	ArU
450	32.7	27.0	25.5	1.7	4.7	59.4	40.7
500	68.2	21.7	24.9	1.6	0.7	49.0	51.0
550	86.4	18.0	25.4	1.6	0.4	45.4	54.7
600	95.9	18.0	24.7	1.5	0.0	44.4	55.7

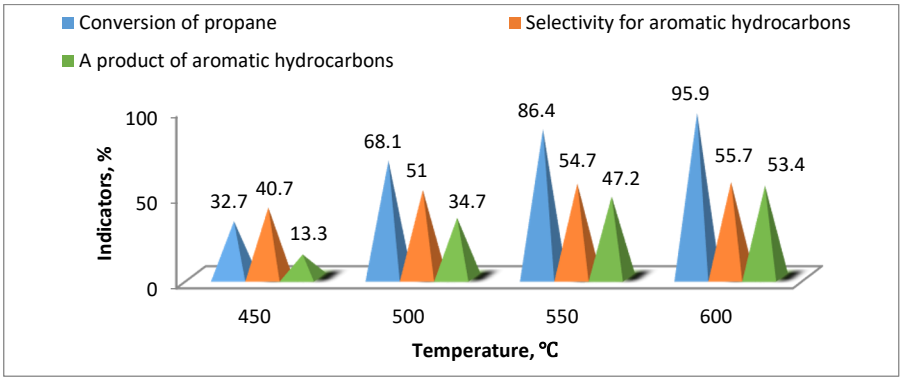


Fig. 7. Temperature dependence of key process parameters for 2%Zr-2%Zn-7%Mo/MPS catalyst (solid phase modification, without hydrogen treatment)

Prior to the catalytic experiments, the samples were treated in a hydrogen flow (2500 h^{-1}) for 2 hours. Following this, the experiments were conducted at a constant volumetric rate (V = 500 h^{-1}) using the same method. Key process indicators are detailed in Table 5. Figure 8 illustrates how temperature affects the conversion, efficiency, and selectivity in the catalytic dehydroaromatization of propane for aromatic products. At 450°C, the yield of aromatic hydrocarbons using the 2%Zr-2%Zn-7%Mo/MPS catalyst was 13.8%.

Table 5. Key process parameters for propane aromatization over 2%Zr-2%Zn-7%Mo/MPS catalyst prepared by solid-phase modification method with hydrogen pretreatment

T, °C	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	30.4	7.8	7.4	1.4	1.6	17.2	13.8
500	64.2	10.4	14.7	1.4	1.4	27.8	36.4
550	86.4	15.4	19.6	1.5	0.4	36.8	49.5
600	94.0	17.2	21.4	1.6	0.0	39.6	55.4
T, °C	KC_3H_8	Product selectivity, %					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArU
450	30.4	23.4	24.4	4.0	5.4	56.8	43.4
500	64.2	16.4	23.0	2.4	2.2	43.4	56.6
550	86.4	17.8	22.8	1.7	0.4	42.6	57.4
600	94.0	17.6	22.8	1.7	0.0	42.4	57.8

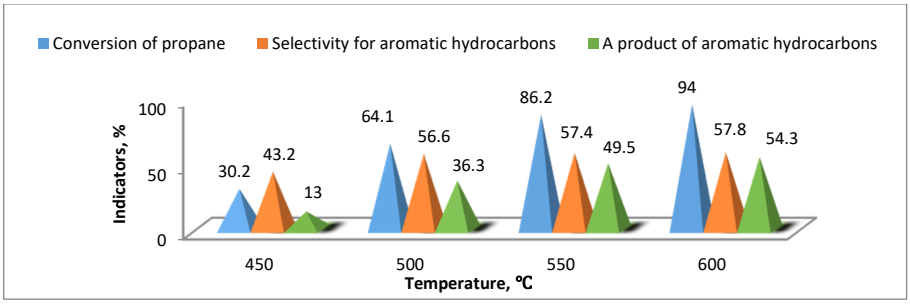


Fig. 8. Temperature dependence of key process parameters for 2%Zr-2%Zn-7%Mo/MPS catalyst (solid phase modification, with hydrogen treatment) Aromatization on 5%Zr-2%Zn-7%Mo/MPS catalyst.

As the temperature increased, the yield of aromatic hydrocarbons in the catalytic aromatization of propane using the 2%Zr-2%Zn-7%Mo/MPS catalyst also rose, reaching 55.4% at 600°C. At the starting temperature of 450°C, the propane conversion was relatively low, at 30.4%. However, as the temperature increased from 450°C to 600°C, the conversion rate increased rapidly, reaching 94.0% at 600°C. Compared to the previous experiment, these results show similar trends in temperature dependence. The yield of gaseous products, including methane, also exhibited a comparable pattern; it increased from 7.8% to 17.4% as the temperature was raised from 450°C to 600°C. In another series of experiments, the temperature for catalytic dehydroaromatization of propane was varied between 450°C and 650°C at a constant volumetric rate (V = 500 h^{-1}). Key process indicators are summarized in Table 6. Figure 9 displays how conversion, productivity, and selectivity of aromatic hydrocarbons vary with temperature when using a 5%Zr-2%Zn-7%Mo/MPS catalyst.

Table 6. The main parameters of the propane aromatization process in the 5%Zr-2%Zn-7%Mo/MPScatalyst prepared by the soaking method

T, °C	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	39.8	9.9	11.2	0.4	2.0	23.2	16.8
500	68.2	11.4	19.0	1.2	1.0	32.4	35.7
550	83.6	11.6	21.4	1.5	0.6	35.2	48.5
600	88.6	13.4	22.4	1.9	0.4	36.8	52.4
T, °C	KC_3H_8	Product selectivity, %					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	39.0	24.6	28.4	1.2	5.0	59.2	40.9
500	68.2	16.6	27.9	1.6	1.5	47.5	52.5
550	83.6	13.9	25.5	1.9	0.7	42.0	58.0
600	87.9	13.9	25.4	2.2	0.5	41.9	58.2

At 450°C, the yield of aromatic hydrocarbons using the 5%Zr-2%Zn-7%Mo/MPS catalyst was 16.8%. As the temperature increased, the yield of aromatic hydrocarbons rose, reaching 52.4% at 600°C. Initially, the conversion of propane at 450°C was 39.8%. As the temperature increased from 450°C to 600°C, conversion improved substantially, but at 600°C, it reached 88.6%, which was lower compared to earlier experiments. The yield of gaseous products from propane catalytic aromatization was also lower compared to previous experiments. Specifically, the methane yield increased only from 9.9% to 13.4% over the temperature range of 450°C to 600°C. Additionally, the proportion of C9-C10 hydrocarbons in the aromatic product mixture significantly increased, while the proportions of benzene and toluene decreased.

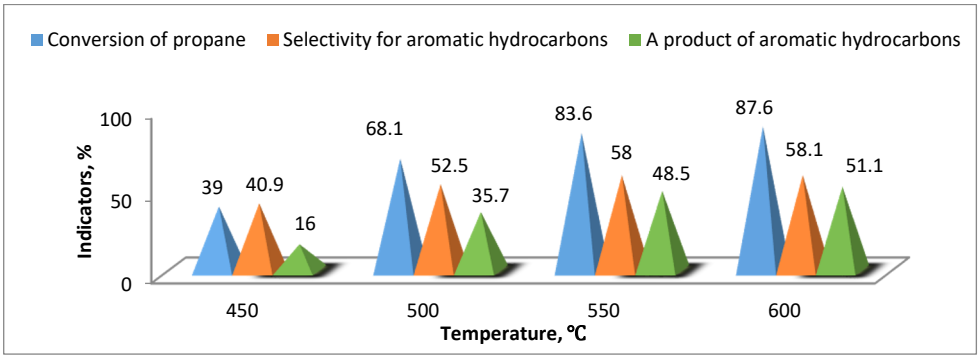


Fig. 9. Temperature dependence of the main process parameters for catalyst 5%Zr-2%Zn-7%Mo/MPS (soaking)

At a constant volumetric rate of V = 500 h^{-1}, the temperature for the catalytic dehydroaromatization of propane was varied between 450°C and 500°C. Key process metrics are summarized in Table 7. Figure 10 illustrates the effect of temperature on conversion, yield, and aromatic selectivity in the catalytic dehydroaromatization of propane. At 450°C, the yield of aromatic hydrocarbons with the 5%Zr-2%Zn-7%Mo/MPS catalyst was 17.8%. As the temperature increased, the yield improved, reaching 52.4% at 600°C. Initially, the conversion of propane at 450°C was 42.4%, but it rose to 95.8% at 600°C, which is slightly higher than observed in previous experiments.

Table 7. Key performance of propane aromatization process on 5% Zr-7%Mo/MPS catalyst prepared by solid phase modification method

T, °C	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	42.4	9.8	10.6	1.0	2.6	23.8	17.8
500	73.7	16.5	16.4	1.4	0.7	34.8	39.0
550	85.2	20.4	18.0	1.5	0.0	39.6	45.5
600	95.8	22.4	19.7	2.0	0.0	42.7	52.4
T, °C	KC_3H_8	Product selectivity, %					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArU
450	41.2	23.6	25.8	2.4	6.4	58.0	42.2
500	73.7	22.4	22.4	1.7	1.0	47.4	52.8
550	85.2	23.7	21.4	1.7	0.0	46.6	53.4
600	94.2	22.4	20.9	2.2	0.0	45.4	54.6

The temperature dependence of propane catalytic aromatization showed a further increase in methane yield. As the temperature rose from 450°C to 600°C, the methane yield increased from 9.8% to 22.4%. Additionally, the proportion of benzene in the aromatic hydrocarbon mixture formed during the catalytic aromatization of propane with the 5%Zr-2%Zn-7%Mo/MPS catalyst saw a notable increase compared to the previous experiment.

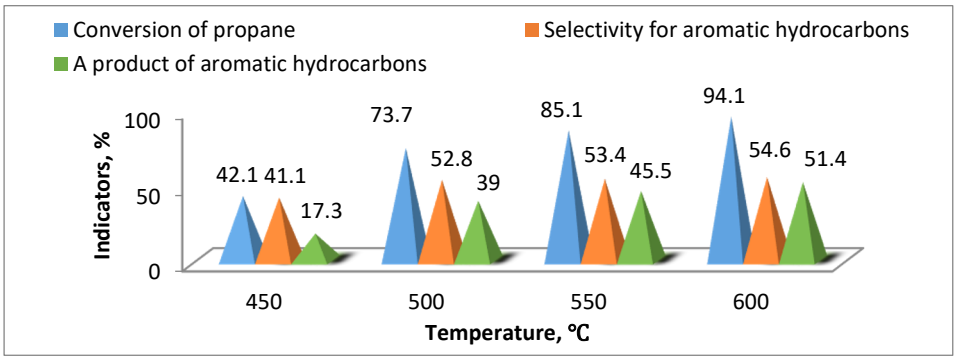


Fig. 10. Temperature dependence of the main process parameters for catalyst 5%Zr-2%Zn-7%Mo/MP (solid phase modification)

Aromatization in zirconium aluminosilicates

The temperature for the catalytic dehydroaromatization of propane was varied between 500°C and 650°C at a constant volumetric rate (V = 500 h^{-1}) using a zirconium aluminosilicate catalyst. Key process indicators are summarized in Table 8. Figure 11 illustrates how conversion, yield, and aromatic selectivity are affected by temperature during the catalytic dehydroaromatization of propane. At 450°C, the yield of aromatic hydrocarbons with the 5%Zr-2%Zn-7%Mo/MPS catalyst was 12.5%.

Table 8. The main parameters of the process of aromatization of propane in zirconium aluminosilicates

T, °C	KC_3H_8	Product yield,%					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	26.8	4.9	6.8	0.6	1.8	14.0	12.5
500	44.4	8.0	8.7	1.0	0.4	18.4	26.0
550	76.4	13.7	15.4	1.7	0.4	30.9	45.5
600	89.6	14.4	18.4	2.9	0.0	35.0	54.4
T, °C	KC_3H_8	Product selectivity, %					
		CH_4	ΣC_2	C_3H_8	ΣC_4	ΣC_1-C_4	ArH
450	25.5	19.4	26.0	2.4	7.2	54.8	45.4
500	44.4	18.4	19.8	2.4	0.9	41.4	58.8
550	76.4	18.0	20.0	2.4	0.4	40.4	59.6
600	88.4	17.9	19.5	2.4	0.0	39.7	60.4

As the temperature increased, the yield of aromatic hydrocarbons in the catalytic aromatization of propane with the 5%Zr-2%Zn-7%Mo/MPS catalyst rose to 54.4% at 600°C. The conversion rate of propane in the catalytic dehydroaromatization process improved significantly from 26.8% to 89.6% as the temperature was raised from 450°C to 600°C. The production of gaseous products from propane aromatization is notably affected by the reaction temperature. Specifically, the yield of methane increased from 4.9% to 14.4%, while the yield of C2 hydrocarbons grew from 6.8% to 18.4% with the temperature rise from 450°C to 600°C.

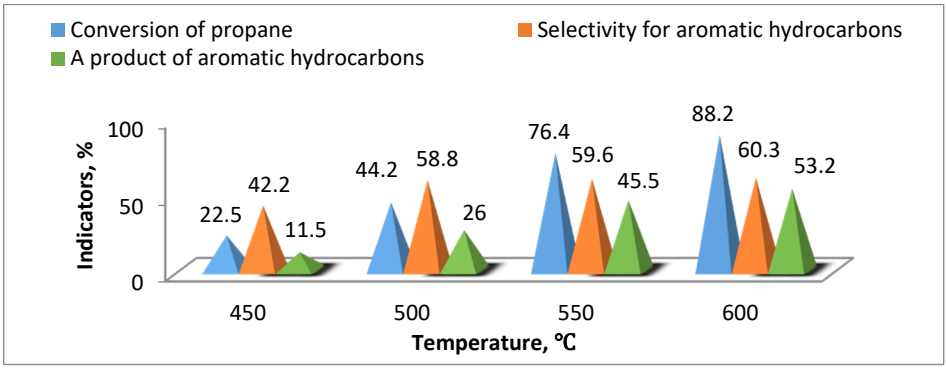


Fig. 11. Temperature dependence of the main process parameters for zirconium aluminosilicate catalyst

4 Conclusions

This study investigated the temperature-dependent behavior of propane catalytic dehydroaromatization, focusing on conversion rates, productivity, and aromatic hydrocarbon selectivity. Two different catalysts were evaluated: the 2%Zr-2%Zn-7%Mo/MPS and the 5%Zr-2%Zn-7%Mo/MPS.

For the 2%Zr-2%Zn-7%Mo/MPS catalyst, the yield of aromatic hydrocarbons at a reaction temperature of 450°C was measured at 13.8%. As the reaction temperature was increased to 600°C, the yield of aromatic hydrocarbons showed a significant improvement, reaching 55.4%. At the lower temperature of 450°C, the propane conversion rate was relatively modest at 30.4%. However, with rising temperature, there was a substantial enhancement in conversion efficiency, culminating in a high conversion rate of 94.0% at 600°C.

Similarly, for the 5%Zr-2%Zn-7%Mo/MPS catalyst, the yield of aromatic hydrocarbons at 450°C was observed to be 17.8%. Upon increasing the temperature to 600°C, the yield increased to 52.4%. These results indicate that both catalysts exhibit improved aromatic hydrocarbon yields with higher reaction temperatures, although the specific yields and conversion rates differ between the two catalysts. The findings underscore the influence of temperature on the efficiency of propane dehydroaromatization, suggesting that optimizing reaction conditions can significantly enhance the overall performance of catalytic processes.

References

1. Bhan A.; Delgass W.N., Catal. Rev. **50,** 19–151 (2008)
2. Zhang P.; Tan L.; Yang G.; Tsubaki NChem. Sci. **8,** 7941–7946 (2017)
3. Guisnet M.; Gnep N.S.; Alario F., Appl. Catal.A Gen. **89**, 1–30 (1992)
4. Al-Yassir, N.; Akhtar, M.N.; Al-Khattaf, S. Physicochemical properties and catalytic performance of galloaluminosilicate in aromatization of lower alkanes: A comparative study with Ga/HZSM-5. J. Porous Mater. **19**, 943–960 (2012)
5. Su X.; Wang G.; Bai X.; Wu W.; Xiao L.; Fang Y.; Zhang J., Chem. Eng. J. **293**, 365–375 (2016)
6. Choudhary V.R.; Sivadinarayana C.; Kinage A.K.; Devadas P.; Guisnet M., Appl. Catal. A Gen. **136**, 125–142 (1996)

7. Montes A.; Giannetto G., Appl. Catal. A Gen. **197**, 31–39 (2000)
8. Rodrigues V.O.; Faro Júnior A.C., Appl. Catal. A Gen. **435**, 68–77 (2012)
9. Choudhary V.R.; Kinage A.K.; Sivadinarayana C.; Devadas P.; Sansare S.D.; Guisnet M., J. Catal. **158**, 34–50 (1996)
10. Han J.; Jiang G.; Han S.; et al. Catalysts **6,** 13 (2016)
11. Al-Yassir N.; Akhtar M.N.; Ogunronbi K.; Al-Khattaf S., J. Mol. Catal. A Chem. **360**, 1–15 (2012)
12. Guisnet M.; Gnep N.S.; Aittaleb D.; Doyemet Y.J., Appl. Catal. A Gen. **87**, 455–270 (1992)
13. Biscardi J.A.; Iglesia E., J. Phys. Chem. **102**, 9284–9289 (1998)
14. Meriaudeau P.; Naccache C., J. Catal. **157**, 283–288 (1995)
15. 31.Fajzullaev, N.I., Fajzullaev, O.O. //Khimicheskaya Promyshlennost' **(4),** 204–207 (2004)
16. Muradov, K.M., Fajzullaev, N.I. //Khimicheskaya Promyshlennost' **(6),** 3–7 (2003)
17. Aslanov, S.C., Buxorov, A.Q., Fayzullayev, N.I.// International Journal of Engineering Trends and Technology **69(4),** 67–75 (2021)
18. Bukhorov A.Q., Aslanov S.C., Fayzullaev N.I. //AIP Conference Proceedings **2432**. 1. 050010 (2022)
19. Bukhorov A. Q., Aslanov S. C., Fayzullaev N. I. //AIP Conference Proceedings **2432**. 1. 050011 (2022)
20. Bukhorov A. Q., Aslanov S. C., Fayzullaev N. I. //AIP Conference Proceedings **2432**. 1. 050012 (2022)