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Review article

Catalytic Isomerization of Light Alkanes: Thermodynamic, Kinetic, and Technological Aspects

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ABSTRACT

The gradual tightening of environmental standards, combined with growing global demand for environmentally friendly fuels, has significantly increased the importance of advanced technologies in oil refining. In this context, the catalytic isomerization of light alkanes (C_4–C_6 fraction) is one of the most strategic processes for improving gasoline quality without increasing the concentration of aromatic hydrocarbons or adding hazardous additives. From a chemical standpoint, this process promotes the structural rearrangement of linear paraffins into corresponding branched isomers, which possess a higher octane numbers. This results in a significant improvement in the fuel's combustion characteristics, while reducing the formation of environmentally harmful emissions.

This review systematically examines the fundamental principles underlying the isomerization of alkanes. Particular attention is given to the reaction mechanism, which proceeds via carbocationic intermediates at acidic catalytic sites, reflecting the well-established mechanism of acid-catalyzed hydrocarbon transformations. Furthermore, the thermodynamic constraints governing the equilibrium distribution of isomers, as well as the kinetic factors influencingreaction rate, product selectivity, and overall process efficiency, are critically analyzed. Special emphasis is placed on bifunctional catalytic systems combining metal and acid functions, enabling the simultaneous hydrogenation–dehydrogenation and skeletal isomerization steps. The role of competing side reactions, notably hydrocracking and aromatization, is also addressed due to their influence on product yield and catalyst stability.

Beyond theoretical considerations, this review examines the complexities inherent in real industrial systems. In practice, the attainment of thermodynamic equilibrium is often limited by kinetic constraints, resistance to mass transfer within particles and between phases, as well as by the gradual deactivation of the catalyst due to coke formation or poisoning. These factors require a more detailed understanding of process behavior under industrial operating condition.

Keywords: *catalytic isomerization; light alkanes; hydroisomerization; bifunctional catalysts; carbocation mechanism; thermodynamic equilibrium; reaction kinetics; zeolite catalysts; catalyst deactivation; octane number enhancement.*

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Научный обзор

Каталитическая изомеризация лёгких алканов: термодинамические, кинетические и технологические аспекты

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АННОТАЦИЯ

Постепенное ужесточение экологических норм в сочетании с растущим мировым спросом на экологически чистые виды топлива значительно повысило значимость передовых технологий в нефтепереработке. В этом контексте каталитическая изомеризация лёгких алканов (фракция C_4–C_6) является одним из наиболее стратегически важных процессов, позволяющих улучшить качество бензина без увеличения концентрации ароматических углеводородов или добавления опасных присадок. С химической точки зрения этот процесс способствует структурной перегруппировке линейных парафинов в соответствующие разветвленные изомеры, обладающие более высоким октановым числом. Это приводит к значительному улучшению характеристик сгорания топлива при одновременном снижении образования вредных для окружающей среды выбросов.

В данном обзоре рассматриваются фундаментальные принципы, лежащие в основе изомеризации алканов. Особое внимание уделяется механизму реакции, протекающему через карбокатионные промежуточные соединения на кислотных каталитических центрах, что отражает классическую схему кислотно-катализируемых превращений углеводородов. Кроме того, анализируются термодинамические ограничения, определяющие равновесное распределение изомеров, а также кинетические параметры, определяющие скорость реакции, селективность продукта и общую эффективность процесса. Особое внимание уделяется бифункциональным каталитическим системам, которые сочетают металлические и кислотные функциональные группы, что позволяет одновременно осуществлять этапы гидрирования-дегидрирования и изомеризации основной цепи. Также рассматривается роль конкурирующих побочных реакций, в частности гидрокрекинга и ароматизации, ввиду их влияния на выход продукта и стабильность катализатора.

Помимо теоретических соображений, в данном обзоре рассматриваются сложности, присущие реальным промышленным системам. На практике достижение термодинамического равновесия часто ограничивается кинетическими ограничениями, сопротивлением массопереносу внутри частиц и между фазами, а также постепенной дезактивацией катализатора из-за образования кокса или отравления. Эти факторы требуют более детального понимания поведения процесса в промышленных условиях эксплуатации.

Ключевые слова: *каталитическая изомеризация, лёгкие алканы, гидроизомеризация, бифункциональные катализаторы, карбокатионный механизм, термодинамическое равновесие, кинетика реакции, цеолитные катализаторы, дезактивация катализатора, повышение октанового числа.*

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Жеңіл алкандарының каталитикалық изомеризациясы: термодинамикалық, кинетикалық және технологиялық аспектілер

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АҢДАТПА

Экологиялық нормалардың біртіндеп күшеюі экологиялық таза отынға деген әлемдік сұраныстың артуымен бірге мұнайды қайта өңдеудегі озық технологиялардың маңыздылығын едәуір арттырды. Бұл тұрғыда жеңіл алкандардың каталитикалық изомерленуі (C_4–C_6 фракциясы) хош иісті көмірсутектердің концентрациясын арттырмай немесе қауіпті қоспаларды қоспай-ақ бензин сапасын жақсартудың ең стратегиялық маңызды процестерінің бірі болып табылады. Химиялық тұрғыдан алғанда, бұл процесс сызықтық парафиндердің құрылымдық қайта түзілуіне ықпал етіп, оларды октан саны жоғары сәйкес тармақталған изомерлерге айналдырады. Бұл қоршаған ортаға зиянды шығарындылардың түзілуін азайта отырып, жанармайдың жану өнімділігінің айтарлықтай жақсаруына әкеледі.

Бұл шолуда алкандардың изомерленуінің негізгі принциптері қарастырылады. Қышқыл каталитикалық орталықтардағы карбокациялық аралық қосылыстар арқылы жүретін реакция механизміне ерекше назар аударылады, бұл көмірсутектердің қышқыл-катализденетін түрленулерінің классикалық схемасын көрсетеді. Сонымен қатар, изомерлердің тепе-теңдік таралуын анықтайтын термодинамикалық шектеулер, сондай-ақ реакция жылдамдығын, өнімнің селективтілігін және процестің жалпы тиімділігін анықтайтын кинетикалық параметрлер талданады. Металл және қышқылдық функционалды топтарды біріктіретін қос функционалды каталитикалық жүйелерге ерекше назар аударылады, бұл гидрлеу-дегидрлеу және негізгі тізбекті изомерлеу қадамдарын бір уақытта жүзеге асыруға мүмкіндік береді. Сондай-ақ өнім шығымына және катализатордың тұрақтылығына әсер ететін бәсекелес жанама реакциялардың, атап айтқанда гидрокрекинг пен ароматтану процестерінің рөлі қарастырылады. Іс жүзінде термодинамикалық тепе-теңдікке қол жеткізу көбінесе кинетикалық шектеулермен, бөлшектердің ішінде және фазалар арасында масса алмасуға төзімділікпен, сондай-ақ кокс түзілуіне немесе улануға байланысты катализатордың біртіндеп дезактивациясымен шектеледі. Бұл факторлар өндірістік пайдалану жағдайында процестің әрекетін егжей тегжейлі түсінуді талап етеді.

Негізгі сөздер: *каталитикалық изомеризация, жеңіл алкандар, гидроизомеризация, бифункционалды катализаторлар, карбокация механизмі, термодинамикалық тепе-теңдік, реакция кинетикасы, цеолит катализаторлары, катализаторды залалсыздандыру, октан санын көбейту.*

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Introduction

Over the past few decades, the global oil refining industry has undergone profound changes, driven by increasingly stringent environmental regulations and growing demand for high-quality, high-performance fuels. One of the primary missions of modern refineries is to produce high-octane gasoline while minimizing the concentration of environmentally harmful components, particularly aromatic hydrocarbons, sulfur compounds, and leaded additives [1].

In this context, the catalytic isomerization of light paraffins has become a process of crucial technological importance. This process converts low-octane normal alkanes into their branched structural isomers, which exhibit better anti-knock properties and thus help improve engine performance and fuel efficiency. Unlike catalytic reforming, isomerization does not lead to the intensive formation of benzene or other toxic aromatic compounds, making it a more environmentally friendly method for improving gasoline quality [2].

Light naphtha fractions, particularly those containing C_4–C_6 hydrocarbons, are the optimal feedstock for isomerization processes. These fractions are abundant in crude oil and can be effectively upgraded through intramolecular rearrangement without altering their general molecular formula. Consequently, isomerization plays a key role in increasing the yield of high-octane components intended for blending in modern refining concepts [3].

From a fundamental perspective, the isomerization of alkanes constitutes a complex catalytic system, determined by the interaction between thermodynamic constraints, reaction kinetics, and catalyst functionality. The reaction mechanism generally involves carbocationic intermediates formed at active acid sites and comprises a sequence of elementary steps, including hydride shifts, skeletal rearrangements, and reversible hydrogenation-dehydrogenation reactions. At the same time, competing side reactions such as hydrocracking and aromatization may occur, which impairs selectivity and complicates process optimization [4].

Another important factor is the discrepancy between theoretical and practical process values. Although thermodynamic analysis determines the upper limit of the isomer yield that can be achieved, actual industrial results are often limited by kinetic constraints, diffusion and mass transfer resistances, as well as catalyst deactivation phenomena due to coke deposits or poisoning. To achieve optimal operating conditions, it is therefore necessary to carefully and systematically harmonize the reaction parameters, catalyst design, and reactor configuration [5].

In recent years, both in scientific research and in industrial practice, there has been an increasing use of advanced mathematical modeling and simulation methods to gain a deeper understanding of isomerization systems. These tools facilitate the prediction of equilibrium compositions, the elucidation of reaction pathways, and the accurate modeling of industrial plant performance under various operating conditions.

For this reason, this review aims to provide a comprehensive analysis of the thermodynamic, kinetic, and catalytic properties of light alkane isomerization, as well as a critical evaluation of modern technological approaches and the key challenges associated with their large-scale industrial implementation [6].

Consequently, studies devoted to the systematic optimization of industrial isomerization plants remain relatively rare in the available scientific literature. This is primarily due to the difficulty of developing rigorous kinetic models, which are a fundamental component of any reliable optimization scheme for isomerization reactors. Creating such models requires a detailed consideration of extensive reaction networks, as well as the inclusion of catalytic and transport phenomena, which significantly complicates their practical implementation [7].

Literature review

A number of previous studies have approached this problem from various methodological perspectives. The influence of metal-acid balance in Ni/SAPO-11 catalysts for n-hexane hydroisomerization was also considered by Lyu, et al. [8]. For example, Besl, et al., presented a brief assessment of the optimization of the Penex isomerization process at a German refinery, thereby offering one of the first practical insights into process improvement on an industrial scale. However, their work was primarily focused on applied aspects and did not include a detailed mechanistic interpretation of the underlying reaction pathways [9].

In contrast, simplified kinetic model that accounts only for the main reaction pathways, namely isomerization and cracking. This model was applied to optimize the process using a liquid aluminum chloride ($AlCl_3$)-based catalytic system and demonstrated that reduced-order kinetic models can still serve as effective tools in process development and optimization [9].

Akhari, et al., investigated the effect of feed composition, specifically the presence of methylcyclopentane, on isomerization yield using process simulation in HYSYS[1]. In addition, they conducted experimental studies on the effect of hydrogen partial pressure on the activity of Pt-mordenite zeolite-based catalysts and on the conversion of n-paraffins. Based on these results, kinetic equations were proposed for the conversion of C_5 and C_6 hydrocarbons [10].

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[1] Aspen HYSYS (or simply HYSYS) is a chemical process simulator currently developed by AspenTech used to mathematically model chemical processes, from unit operations to full chemical plants and refineries.

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Further experimental work by Brito, et al., focused on Pt-Ni / mordenite catalysts with various metal ratios. Their results showed that the composition of the metal phase has a significant effect on catalytic activity and selectivity. In addition, a kinetic model was developed to describe the catalyst's behavior during deactivation, which is crucial for assessing the catalyst's long-term stability [11].

Koncsag, et al., developed a kinetic model of C_5–C_6 isomerization on Pt / zeolite H catalysts under conditions typical of industrial production, which improved the reliability of process modeling when applied at the refinery scale [12].

Surla, et al., proposed an event-driven approach to kinetic modeling to describe C_5–C_6 isomerization on chlorinated aluminum oxide-based catalysts. This methodology provides a more detailed mechanistic description of the elementary reaction steps and allows for a deeper understanding of complex networks of catalytic reactions [13].

Most recently, Chekantsev, et al., proposed a comprehensive kinetic model applicable to the three main classes of isomerization catalysts. Their reaction network includes 36 elementary steps, providing a highly detailed view of the system. The study showed that, although the overall reaction rates are comparable for different types of catalysts, there are significant differences at the level of individual isomerization pathways. It is important to note that the model agrees well with experimental data for all the catalytic systems studied, which confirmed its validity and reliability [14].

Materials and methods

This review article is based on an analysis of recent scientific literature on the isomerization of light paraffinic hydrocarbons and the development of industrial hydroisomerization catalysts. The theoretical basis of the study was determined using peer-reviewed publications indexed in major scientific databases, including Scopus, Web of Science, ScienceDirect, MDPI[2], ACS Publications[3], and Chemical Society Reviews, with a focus on articles published between 2019 and 2025. Other sources were studies of industrial isomerization technologies and the thermodynamic foundations of catalytic processes.

The bibliography was selected and prepared using a number of key terms such as hydroisomerization, isomerization of light naphtha, bifunctional catalysts, Pt / Cl-Al_2O_3, zeolites, SAPO-11, sulfated zirconium oxide, equilibrium constant, thermodynamics, metal acid equilibrium, hydrocracking, catalyst deactivation, formation, coke isomerization, paraffin isomerization, branched isomers, catalytic acid, and hydrogenation–dehydration function.

The collected data was processed using comparative, thermodynamic, and content analysis approaches. The studies were evaluated in terms of how temperature, acid content in the catalyst, metal-acid site ratio, pore structure, and carrier type affect the activity, selectivity, and stability of hydroisomerization catalysts. Particular attention was paid to how the reaction temperature affects the thermodynamic equilibrium, the equilibrium constant (Keq), the distribution of the product between different isomers, and the degree of side reactions such as hydrocracking and coke formation. In addition, the literature on the modification of catalysts with metals such as Pt, Ni, and Pd was reviewed, as well as comparisons of catalytic systems based on chlorinated aluminum oxide, zeolite, SAPO-11, and sulfated zirconium oxide. Important performance indicators were taken into account, including n-alkane conversion, selectivity to isoparaffins, operating temperature ranges, resistance to sulfur-containing and water-containing impurities, and catalyst deactivation rates associated with coke separation.

In general, the information collected was summarized to clarify the relationship between thermodynamic constraints and catalytic behavior in various systems, determine optimal conditions for modern hydroisomerization processes, and evaluate the industrial potential of modern bifunctional catalysts to improve the octane number of light petroleum fractions.

Results

A review of the literature shows that the catalytic isomerization of light alkanes is affected not by a single factor, but by the complex effect of catalyst acidity, metal function, reaction temperature and pore structure. In most studies, bifunctional catalysts are considered the most effective systems for isomerizing C–C alkanes. This is because metal centers are responsible for hydrogenation-dehydrogenation reactions, while acid centers contribute to the formation and rearrangement of intermediate carbenium ions.

Comparison of different catalytic systems showed that chlorinated alumina-based catalysts have very high activity at relatively low temperatures, usually in the range of 120–180°C Zeolite-based catalysts, such as Pt/mordenite and Pt/HBEA, generally require higher operating temperatures, but are more stable, more resistant to contamination, and have a longer service life. Molecular sieves of SAPO-11 and other silicoalumophosphates are also important, since their porous structure allows form selectivity and promotes the formation of monoramidal isomers.

The literature also confirms that temperature plays a dual role in the isomerization process. At lower temperatures, the formation of branched isomers is thermodynamically favorable, but the reaction rate is still limited because the formation of active

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[2] MDPI (Multidisciplinary Digital Publishing Institute) is a publisher of peer-reviewed, open access journals since its establishment in 1996.

[3] ACS (The American Chemical Society) is a scientific society based in the United States that supports scientific inquiry in the field of chemistry.

intermediates is slow. At higher temperatures, the reaction is faster, but selectivity may decrease due to stronger hydrocracking, aromatization and coke formation. For this reason, the optimal temperature range should be selected according to the type of catalyst and the required balance between the conversion, selectivity and stability of the catalyst.

Coke formation has also been identified as a major cause of catalyst decontamination. In some cases, a small amount of coke can have a positive effect, since it blocks non-selective external acid centers and increases selectivity. However, excessive coke build-up blocks micropores, reduces the number of available active sites, and hinders the diffusion of reagents and products. Hierarchical catalysts with additional mesoporous channels have better diffusion properties and slower deactivation than conventional microporous catalysts.

Fundamentals of Alkane Isomerization

Alkane isomerization is a fundamental class of transformations in hydrocarbon chemistry, which involves the rearrangement of the carbon skeleton while maintaining the molecular formula. In the context of petroleum refining, this process predominantly refers to the conversion of linear (conventional) alkanes into their branched counterparts. Despite its apparent structural simplicity, this transformation is determined by the complex interaction of molecular structure, energy factors and catalytic effects. Conventional alkanes have a relatively low chemical reactivity, which can be explained by the presence of strong σ bonds (C-C and C-H) and the absence of functional groups or π-systems. In terms of molecular orbitals, their highest occupied molecular orbitals are characterized by low energy levels, while the lowest unoccupied molecular orbitals remain energetically inaccessible under mild conditions. This electronic configuration explains its inherent inertia, which requires the use of highly active catalytic systems capable of generating reactive intermediates to initiate the isomerization process [15].

The thermodynamic driving force of alkane isomerization is due to the difference in the stability of the linear and branched isomers. Branched alkanes tend to be thermodynamically more stable due to the combined effect of hyperconjugation and the electron-donating inductive effect of the alkyl substituents. This higher stability is directly related to a higher compression ignition resistance, which leads to a higher octane number and better fuel efficiency. From a constructive point of view, the degree of branching plays a decisive role in determining the quality of fuel. Single-stranded isomers, such as methylpentanes, generally have a moderate octane number, while more branched structures, including dimethylbutanes, have significantly higher anti-knock properties. Therefore, industrial isomerization processes are designed not only to facilitate the conversion of n-alkanes, but also to selectively promote the formation of highly branched isomers [16].

Isomerization is particularly relevant for light hydrocarbons in the C_4–C_6 range, which make up a significant part of the light naphtha fluxes. Due to their relatively simple molecular structure, these compounds undergo efficient structural adaptation under catalytic conditions, which makes them an ideal raw material for increasing the octane number. In addition, light alkanes, in contrast to heavier hydrocarbons, are able to approach thermodynamic equilibrium under correspondingly optimized process conditions. An additional feature of alkane isomerization is its reversible nature. The reaction takes place in a thermodynamic equilibrium state, the final distribution of the isomers being determined mainly by temperature and, to a lesser extent, by pressure. As a result, the composition of the product is determined not only by kinetic factors, but also by equilibrium constraints [17]. In industry, isomerization is usually integrated with other refining processes such as hydrogen treatment and fractionation to improve the overall efficiency of the process. Before isomerization, the raw materials are usually subjected to purification steps to remove catalytic chemical agents, including sulfur- and nitrogen-containing compounds, as well as moisture, which can negatively affect the catalytic activity and stability. Therefore, alkane isomerization is a key to improving modern petroleum refining by combining the basic principles of physical chemistry with advanced technological processes that enable cleaner fuels with a higher octane number [18].

Mechanism of Catalytic Isomerization

The catalytic isomerization of alkanes is a mechanically complex multiphase process that occurs due to the formation of highly reactive intermediates and involves the synergistic contribution of acid-catalyzed and metal-catalyzed transformations. The reaction mechanism is most often interpreted within the framework of carbocation chemistry (carbene ion chemistry), which provides a consistent theoretical basis for describing not only the desired skeletal rearrangements, but also the formation of undesirable by-products [19].

In industrial conditions, alkane isomerization is usually carried out in bifunctional catalytic systems containing both metallic and acidic active centers. These functions perform complementary and interdependent functions across the entire reaction network. In particular, the metal component promotes reversible hydrogenation-dehydrogenation steps, which allow the formation of reactive olefin or carbocation precursors, while acidic centers contribute to structural restructuring through the formation and transformation of carbocation intermediates. Effective cooperation between these two types of active centers is a critical factor for the catalytic activity, selectivity, and overall efficiency of the process [20].

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Formation of Reactive Intermediates

The initial stage of the isomerization mechanism involves the activation of a relatively inert alkane molecule, which is an important kinetic barrier in the overall process. In bifunctional catalytic systems, this stage usually begins with the active metal centers, where the alkane is dehydrogenated to form alkenes or intermediates bound to the surface. The formation of this unsaturated intermediate is important because it significantly increases the reactivity of the molecule and ensures its subsequent participation in acid-catalyzed transformations [21].

After the formation of the alkaline intermediate, it moves to the acidic active center, where it is protonated, resulting in the formation of a carbenium ion. This positively charged intermediate plays a central role in the isomerization mechanism because it provides the electronic and structural flexibility needed to rearrange carbon-carbon bonds. In systems characterized by an exceptionally high acid content, such as superacid media, an alternative activation pathway may be used.

In such cases, carbocations can be formed directly by separating the hydride from the alkane, avoiding the intermediate stage of alkene formation. Regardless of the specific pathway, the formation of carbenium ions is a critical mechanical step, since it provides a subsequent restructuring of the skeleton, which leads to the formation of branched isomers [22].

Skeletal Rearrangement

Once generated, the carbenium ion undergoes a sequence of structural rearrangements through a series of elementary transformations. The most significant among these are 1,2-hydride shifts and alkyl shifts, involving the migration of methyl or larger alkyl groups along the carbon framework. These intramolecular rearrangements result in the progressive stabilization of the carbocation, generally following the well-established stability order: primary < secondary < tertiary [23].

From a mechanistic standpoint, two principal types of rearrangements are typically distinguished. Type A rearrangements involve relatively straightforward hydride or alkyl shifts and proceed at comparatively high rates due to their lower activation barriers. In contrast, Type B rearrangements are associated with the formation of more highly branched structures and often proceed via non-classical intermediates, such as protonated cyclopropane-like species. These pathways are usually more complex but are essential for generating isomers with superior structural branching.

The intrinsic tendency of carbocation intermediates to evolve toward more thermodynamically stable configurations serves as the primary driving force for skeletal rearrangement. As a result, the reaction network ultimately favors the formation of highly branched isomers, which are both energetically preferred and technologically desirable due to their enhanced fuel properties [24].

Chain Propagation and Product Formation

After rearrangement, the carbocation undergoes a hydride transfer from another alkane molecule. This step produces the final branched alkane and simultaneously generates a new carbocation, allowing the reaction to proceed as a chain process.

In bifunctional catalysts, the final step involves hydrogenation of the intermediate species on metal sites, ensuring the formation of stable saturated hydrocarbons and preventing excessive accumulation of olefins [25].

Side Reactions

Following skeletal rearrangement, the carbenium ion undergoes a hydride transfer reaction with a neighboring alkane molecule. This step results in the formation of the final branched alkane product while simultaneously generating a new carbocation species, thereby sustaining the reaction through a chain-type propagation mechanism.

In bifunctional catalytic systems, the final step involves hydrogenation of intermediate species on metal sites, ensuring the formation of stable saturated hydrocarbons and preventing excessive accumulation of olefinic compounds, which could otherwise lead to catalyst deactivation [26].

Role of Catalyst Structure

The mechanism of alkane isomerization is strongly governed by the physicochemical properties of the catalyst, which determine both activity and selectivity of the process. In particular, the most influential parameters include: (i) the strength and density of acid sites responsible for carbocation formation and rearrangement, (ii) the dispersion and intrinsic activity of metallic sites involved in hydrogenation–dehydrogenation steps, and (iii) the pore architecture of the catalyst, which imposes diffusion constraints and shape-selective effects on reactant and intermediate species.

Industrial isomerization of light alkanes is usually carried out using bifunctional catalysts containing both metallic and acid-active centers. The overall performance of these catalyst systems depends on several important factors, including the acidity of the catalyst, the distribution of metal components, the structure of the auxiliary material, the resistance of the catalyst to attenuation, and the selected operating conditions. The most used catalysts in modern purification practice include chlorinated alumina catalysts, zeolite-based systems, and silicoaluminophosphate molecular sieves, particularly SAPO-11, each of which has its own advantages and limitations specific to industrial use [27]. The main industrial catalytic systems used for the isomerization of light alkanes and their comparative characteristics are given in Tab. 1 [25–29].

Table 1. Comparative analysis of the major industrial catalysts used for light alkane isomerization [25–29]

Catalyst system	Typical operating temperature, °C	Activity	Selectivity to branched isomers	Sulfur / water resistance	Coke formation tendency	Main advantages	Main limitations
Pt / Cl-Al$_2$O$_3$	120–180°C	Very high	Very high	Very low	Moderate	High octane enhancement at low temperature	Sensitive to moisture and sulfur compounds
Pt / Zeolite (mordenite, HBEA)	220–280°C	High	High	Good	Lower than chlorinated catalysts	Higher thermal stability and longer catalyst life	Requires higher operating temperature
Pt / SAPO-11	250–320°C	Moderate	High for mono-branched isomers	Good	Low	Excellent shape selectivity and stability	Lower overall conversion
Pt-Ni / Mordenite	220–300°C	High	High	Moderate	Moderate	Improved metal dispersion and hydrogenation ability	More complex catalyst preparation
Sulfated zirconia-based catalysts	150–220°C	Very high	Moderate	Low	High	Strong acidity and high low-temperature activity	Rapid deactivation due to coking

The isomerization of light naphtha is an important purification process for improving the quality of gasoline by increasing the octane number. This is achieved by converting straight-chain paraffins into their valuable branched isomers. For this purpose, different catalyst systems are used in industry, which behave differently depending on the balance of activity, selectivity and stability. One of the most active types of catalysts is PT / Cl-Al$_2$O$_3$, which operates at relatively low temperatures (120–180°C). It has a high activity and high selectivity to branched products, which means that it is very efficient in processing raw materials under mild conditions. But its main disadvantage is the sensitivity to impurities such as sulfur and water. Even small amounts of these impurities can quickly disable the catalyst, which makes it difficult to work in less purified energy systems [26–27].

On the other hand, Pt / zeolite-based catalysts (for example, mordenite, ZSM-5 (Zeolite Socony Mobil-5, an MFI-type zeolite) and β-zeolite) operate at high temperatures (220–280°C). Although they are somewhat inactive at low temperatures, they are much more stable and resistant to contamination. This makes them convenient for industrial use, especially in real refinery conditions, where perfect purification of raw materials is not always possible. Catalysts based on SAPO-11 generally operate at 250–320°C. and are known for their high form selectivity. Due to their one-dimensional porous structure, they contribute to the formation of single-branched isomers [28].

However, their total conversion is lower compared to zeolite-based catalysts, which limits their use in large-scale industrial applications that require high performance. Pt-Ni / mordenite-based catalysts have improved performance by increasing the dispersion of metals and improving hydrogenation-dehydrogenation processes, which helps to improve the efficiency of isomerization. The downside is that they are more difficult to cook and tend to be more expensive. Another important class of catalysts are sulfonated zirconium-based catalysts, which can have a very high acidity and high activity at low temperatures (150–220°C) [29].

However, they quickly fail due to long-term intensive coking and low temperature resistance. In general, isomerization does not have a single “ideal” catalyst. Systems based on chlorinated alumina offer very low temperature properties but are very sensitive. Zeolite-based catalysts are an industrially balanced and reliable solution. SAPO-11 materials have high selectivity, but low conversion rate, and sulfonated zirconium systems have high activity, but are unstable over time. As a result, the choice of catalyst always involves an interaction between activity, selectivity, resistance to poisoning and long service life under the conditions of use [27–28].

Isomerization Catalysts and Coke Formation

The isomerization of n-alkanes in bifunctional Pt / H-beta catalysts is strongly influenced by several key factors, including catalytic acid, pore structure, reaction temperature, hydrogen pressure and coke formation during the reaction. The high catalytic activityof Pt / H-beta systems is mainly due to the synergistic interaction between the platinum centers, which promote hydrogenation-dehydrogenation reactions, and the Brønsted acid centers, which are responsible for the formation of carbocations and the structural rearrangement of hydrocarbon molecules.

For the isomerization of n-pentane, the most favorable catalytic performance is generally observed at temperatures between 250°C and 300°C. In this temperature range, a balance between conversion and selectivity with respect to isopentane can be achieved. At lower temperatures, the reaction rate decreases, since the formation of reactive carbocation intermediates is kinetically restricted. On the contrary, temperatures above 300°C favor secondary hydrocracking reactions and accelerate the formation of coke, which has a negative effect on the stability of the catalyst. Under optimal conditions, the selectivity with respect to the branched C_5 isomers can exceed 80%, while the formation of crack products remains relatively limited.

The formation of coke plays a complex role in the functioning of the catalyst. Thermogravimetric analysis shows that the coke content gradually increases over time, reaching about 3–7 wt.-% can reach.% depends on the intensity of the reaction and the composition of the raw material. A small amount of coke can partially block the non-selective external acid centers, which improves the selectivity of the form and promotes the formation of monoramidal isomers. However, the continuous accumulation of coke eventually blocks the microporous channels and reduces the activity of the catalyst.

Temperature-programmable oxidation and UV-Raman spectroscopy show that carbon deposits are gradually converted from low-condensed hydrocarbon forms to more condensed aromatics and graphite structures during long-term operation. These highly condensed coke particles significantly reduce the availability of active centers and limit the diffusion of hydrocarbon molecules within the zeolite structure.

Stronger diffusion restrictions are observed in the isomerization of heavier hydrocarbons such as n-hexadecane. At temperatures close to 300°C and hydrogen pressures up to 50 bar, the Pt / h beta catalysts are gradually deactivated due to the intensive coke deposition within the microporous structure. Under such conditions, the hydrocracking reactions become more dominant, while the selectivity to the branched C_{16} isomers decreases with increasing reaction time. The introduction of mesoporosity by desalination significantly improves the performance of the catalyst. Hierarchical pt / H-beta catalysts containing additional mesoporous channels allow better molecular diffusion and less coke accumulation compared to conventional microporous zeolites. As a result, these catalysts exhibit a higher sealing activity, a better selectivity with respect to branched hydrocarbons and lower decontamination rates in long-term operation.

The importance of the Brønsted external acid centers was further confirmed by selective poisoning experiments with 2,6-di-tert-butylpyridine. The blocking of the external acid centers suppresses the secondary cracking reactions and improves the selectivity of the impregnation, which indicates that the reactions occurring within the closed zeolite channels are more favorable for selective skeletal rearrangement. The pre-coking treatment with n-pentane and toluene as coke precursors also influences the catalytic properties. In particular, coke derived from toluene forms more condensed aromatic deposits which suppress the cracking reactions and stabilize the selectivity with respect to the desired branched products. However, the excess of pre-coke eventually leads to a strong clogging of the pores and a significant decontamination of the catalyst [16, 29].

Equilibrium Limitations in Real Systems

In the catalytic isomerization of light alkanes, thermodynamic equilibrium plays a fundamental role in determining the theoretical upper yield limit of the branched isomer. However, in real industrial systems, the observed product distribution often differs significantly from the equilibrium composition due to a combination of kinetic constraints, transport phenomena, and catalytic constraints. Therefore, thermodynamic equilibrium should be considered as an idealized reference state, and not as a condition achievable during operation [23].

From a thermodynamic point of view, the isomerization of n-alkanes into iso-alkanes is a reversible and moderately exothermic process. At relatively low temperatures, the equilibrium position shifts towards the formation of highly branched isomers, which exhibit greater thermodynamic stability as a result of increased molecular compactness and lower Gibbs free energy. On the contrary, with increasing temperature, the equilibrium composition gradually shifts towards less branched or even linear species, which is consistent with the Le Chatelier principle. This internal thermodynamic behavior determines the optimal temperature regime for industrial operation.

The relationship between reaction temperature and isomerization conversion is illustrated in Fig. 1 [16]. As can be seen, at lower temperatures the process is predominantly limited by reaction kinetics, whereas at higher temperatures thermodynamic equilibrium becomes the main limiting factor. The optimal operating temperature corresponds to the maximum achievable actual conversion under industrial conditions. As shown in Fig. 2, at lower temperatures the process is predominantly limited by reaction kinetics, whereas at higher temperatures thermodynamic equilibrium becomes the main limiting factor [23].

Despite the favorable equilibrium position at low temperatures, industrial operation in such conditions is impossible due to serious kinetic limitations. Sufficient activation energy is required for the formation of carbenium ion intermediates, and at low temperatures, the rate of their formation is significantly reduced. As a result, the system may remain far from equilibrium, even when thermodynamic conditions favor the formation of branched isomers. This discrepancy between the thermodynamic driving force and kinetic availability is a key limitation in practical isomerization reactors [13–14].

The limitations of mass transfer are another critical factor contributing to the deviation from equilibrium. In heterogeneous catalytic systems, especially those based on zeolite or microporous materials, the rate of diffusion of reagents and products within the particles can become decisive. The pronounced difference in diffusion rates between linear and branched isomers can lead to the appearance of internal concentration gradients inside the catalyst particles [6, 15].

Consequently, the observed distribution of products reflects patterns of reaction kinetics and transfer resistance rather than true thermodynamic equilibrium. Deactivation of the catalyst further exacerbates deviations from equilibrium in industrial systems.

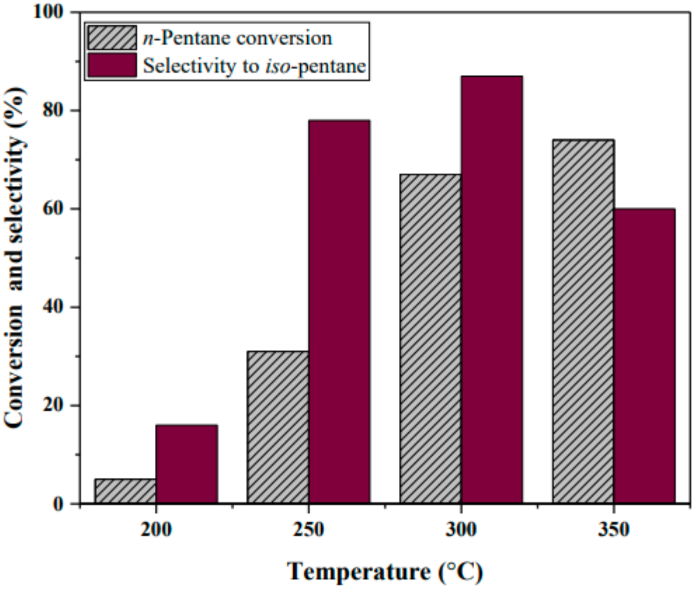

Figure 1. Conversion of n-pentane and selectivity to iso-pentane of the catalytic isomerisation of n-pentane over 0.5 g Pt / H-Beta catalyst at WHSV of 1.5 h-1, H_2 / pentane mole ratio of 3.12, and at 200, 250, 300, and 350°C reaction temperatures [16]

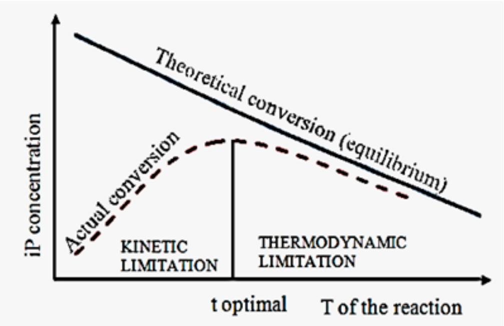

Figure 2. Effect of reaction temperature on actual and theoretical conversion in light alkane isomerization [23]

Over time, the active centers may gradually become blocked due to the deposition of coke, highly adsorbed reaction intermediates, or impurities in the raw materials. This leads to a decrease in the number of available acid and metal centers, thereby reducing the overall catalytic activity and changing the balance between isomerization and competing side reactions. In addition, spatially uneven deactivation along the catalyst layer can cause axial fluctuations in activity, which further deviates the system from the equilibrium state. The presence of parallel side reactions, including cracking, hydrogenolysis, and aromatization, also plays an important role in limiting the achievement of equilibrium. These reactions compete directly with the isomerization process for the presence of reagents and intermediates and, as a rule, intensify at elevated temperatures and longer holding times. Under such conditions, the system can approach a steady state that differs significantly from the thermodynamically equilibrium composition [16, 24].

The partial pressure of hydrogen indirectly affects the approach to equilibrium, although it does not directly participate in the stoichiometry of isomerization. Hydrogen plays a crucial role in stabilizing the metal sections responsible for the stages of hydrogenation and dehydrogenation, and in suppressing the formation of coke. Insufficient availability of hydrogen can contribute to the accumulation of olefins, thereby accelerating secondary reactions and increasing the deviation from equilibrium conditions. Finally, the hydrodynamics of the reactor and factors related to the design introduce additional imperfections [10, 12].

In fixed-bed reactors, phenomena such as channel formation, axial dispersion, and radial temperature gradients can lead to local deviations from optimal operating conditions. These spatial inhomogeneities lead to the fact that sections of the catalyst layer operate in suboptimal modes, thereby preventing the achievement of general equilibrium in the system. In general, equilibrium constraints in alkane isomerization systems arise from a complex interaction of thermodynamic constraints, finite reaction kinetics, mass transfer resistances, catalyst deactivation, and competing reaction pathways. A comprehensive understanding of these deviations is necessary to develop accurate reactor models and optimize industrial processes aimed at maximizing the yield of high-octane branched isomers [10, 13–14].

Discussion

The catalytic isomerization of light alkanes (C_4–C_6) remains one of the most technologically significant processes in modern oil refining, playing a central role in the production of components for mixing high-octane gasoline. This process makes it possible to convert linear paraffinic hydrocarbons into their branched isomers, which have significantly improved anti-knock properties, while minimizing the formation of highly toxic aromatic compounds commonly associated with alternative enrichment methods such as catalytic reforming. This review shows that the process of alkane isomerization is regulated by a complex and interdependent combination of thermodynamic, kinetic, and catalytic factors. From a thermodynamic point of view, branched isomers are preferable to use at lower temperatures due to their higher internal stability and lower Gibbs free energy. On the contrary, an increase in temperature shifts the equilibrium composition towards less branched structures and at the same time increases the likelihood of undesirable secondary reactions.

However, the practical implementation is significantly limited by the kinetics of the reaction, since sufficient activation energy is required for the formation of intermediate compounds of carbenium ions and subsequent structural rearrangements, which limits the possibility of carrying out a low-temperature process. The mechanistic analysis highlights the critical importance of bifunctional catalytic systems in which metallic regions contribute to the hydrogenation-dehydrogenation stages, while acidic regions contribute to the restructuring of the skeleton with the help of intermediate carbenium ions. The synergistic interaction between these two types of active centers determines both the catalytic activity and the selectivity of the product. However, the effectiveness of the catalyst is constantly affected by competing side reactions, including hydrocracking, aromatization and coking, which contribute to a decrease in selectivity and gradual deactivation of the catalyst.

Conclusion

The key conclusion of this study is that real industrial systems rarely achieve true thermodynamic equilibrium. Significant deviations occur as a result of internal kinetic constraints, resistance to intra- and interparticle mass transfer in porous catalysts, imperfect reactor hydrodynamics, and gradual deactivation of the catalyst. Together, these factors determine the actual distribution of the product and, therefore, must be carefully considered when designing the reactor, expanding production and optimizing the technological process. In general, the efficient operation of isomerization plants requires an integrated approach combining thermodynamic analysis, detailed kinetic modeling, and advanced catalyst development technologies. Recent developments in the field of catalytic materials, reactor configurations, and computer modeling techniques have significantly improved the productivity and selectivity of the process.

However, further research is still needed to achieve a more complete understanding of reaction systems at the molecular level and to develop catalysts with increased stability, activity, and selectivity in industrial environments. In conclusion, it should be noted that alkane isomerization is a mature but constantly evolving field of oil refining, in which continuous progress is mainly due to global demand for environmentally friendly fuels, increased energy efficiency and more environmentally friendly refining technologies.

ADDITIONAL INFORMATION

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