



SIMULATION OF CHEMICAL REACTIONS AND THE ROLE OF ARTIFICIAL INTELLIGENCE

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Abstract: *Deep understanding of the nature of chemical reactions, determination of their kinetic characteristics, and prediction of interatomic changes at each stage of the process is considered one of the most complex areas of modern chemistry. In traditional laboratory conditions, such studies require significant time and resources and often involve the use of hazardous substances. Therefore, simulating chemical reactions in a virtual environment has become an integral part of contemporary science. Using simulation technologies, intermolecular interactions, energy changes, stability of intermediate complexes, and the properties of products formed in reactions can be rapidly evaluated using mathematical models. In recent years, the development of artificial intelligence (AI) has taken this process to a new level. AI algorithms can independently learn from various chemical databases, classify reactions, propose new reaction pathways, evaluate the stability of molecular structures, and generate optimal synthesis strategies. In particular, deep learning and generative models provide the ability to identify the most favorable conditions for synthesizing complex organic compounds, optimize catalyst activity, and predict the properties of pharmaceutical substances in advance. Additionally, AI-based simulation platforms improve efficiency by processing experimental results in real time, deriving generalized conclusions, and planning new experiments. This work elaborates on the scientific and practical significance of AI tools in chemical simulations. The study analyzes the strengths and weaknesses of AI models, ways to improve computational accuracy, new approaches to visualizing intermolecular changes, and the prospects of applying these tools in*

chemical industry, ecology, and pharmaceuticals. The results demonstrate that AI in chemical process prediction is emerging not only as an auxiliary tool but also as a generator of new scientific ideas.[2,4,5,7,8]

Key words: chemical reaction simulation, artificial intelligence (AI), molecular modeling, deep learning algorithms, reaction mechanism prediction, quantum chemical calculations, generative models, catalyst optimization, intermolecular interactions, pharmaceutical synthesis, computational chemistry, virtual experiments.

Аннотация: Глубокое понимание природы химических реакций, определение их кинетических характеристик и прогнозирование межатомных изменений на каждом этапе процесса считается одной из наиболее сложных областей современной химии. В традиционных лабораторных условиях такие исследования требуют значительных временных и материальных затрат и нередко связаны с использованием опасных веществ. В связи с этим моделирование химических реакций в виртуальной среде стало неотъемлемой частью современной науки. С использованием технологий моделирования межмолекулярные взаимодействия, изменения энергии, устойчивость промежуточных комплексов и свойства продуктов, образующихся в реакциях, могут быть оперативно оценены с помощью математических моделей.

В последние годы развитие искусственного интеллекта (ИИ) вывело данный процесс на новый уровень. Алгоритмы ИИ способны самостоятельно обучаться на основе различных химических баз данных, классифицировать реакции, предлагать новые реакционные пути, оценивать устойчивость молекулярных структур и формировать оптимальные стратегии синтеза. В частности, методы глубокого обучения и генеративные модели позволяют определять наиболее благоприятные условия для синтеза сложных органических соединений, оптимизировать активность катализаторов и заранее прогнозировать свойства фармацевтических веществ. Кроме того,

платформы моделирования на основе ИИ повышают эффективность исследований за счёт обработки экспериментальных результатов в реальном времени, получения обобщённых выводов и планирования новых экспериментов. В данной работе подробно рассматриваются научная и практическая значимость инструментов ИИ в химическом моделировании. Анализируются сильные и слабые стороны моделей ИИ, пути повышения вычислительной точности, новые подходы к визуализации межмолекулярных изменений, а также перспективы применения данных инструментов в химической промышленности, экологии и фармацевтике. Полученные результаты показывают, что ИИ в прогнозировании химических процессов формируется не только как вспомогательный инструмент, но и как генератор новых научных идей. [2,4,5,7,8]

Ключевые слова: *моделирование химических реакций, искусственный интеллект (ИИ), молекулярное моделирование, алгоритмы глубокого обучения, прогнозирование механизмов реакций, квантово-химические расчёты, генеративные модели, оптимизация катализаторов, межмолекулярные взаимодействия, фармацевтический синтез, вычислительная химия, виртуальные эксперименты.*

Objectives and Tasks The main goal of this research is to study chemical reaction simulation technologies in depth, analyze their theoretical and practical foundations, and scientifically substantiate the role of AI algorithms in this process. Given the increasing need for rapid, accurate, and safe experiments, modeling chemical processes in a virtual environment and using AI is of growing scientific and practical importance. The study aims to explain how these technologies work, how they complement or replace traditional laboratory experiments, and their strengths and weaknesses in real applications. Specifically, the research addresses: Theoretical foundations and modern models of chemical reaction simulation. Evaluation of AI algorithms, including deep learning, generative models, and

optimization systems, in predicting chemical processes. Comparison of simulation results with real experiments.

Identification of new reaction pathways, optimal conditions, and effective catalysts using AI. Practical applications of AI-based reaction modeling in chemistry, ecology, pharmaceuticals, and industry.[2,3,5]

Relevance: This study demonstrates that simulation and AI integration represent one of the most promising areas of modern science. Simulation tools allow faster, safer, and more convenient analysis of intermolecular processes compared to real experiments. Observing complex reaction mechanisms, energy profiles, and particle interactions without multi-step calculations significantly increases research efficiency. This advances chemistry not only academically but also in applied fields such as industry, pharmaceuticals, and ecology. AI algorithms handle large datasets, predict reactions, generate new molecular structures, and identify optimal conditions faster and more accurately than humans. This provides opportunities in drug synthesis, catalyst optimization, environmentally friendly technologies, and new material development. AI also fundamentally changes the methodology of studying chemical reactions: many scientific projects are first tested virtually before practical implementation, reducing errors, improving efficiency, and saving resources. In pharmaceuticals, AI predicts new molecule efficacy, safety, and synthesis pathways. In summary, combining simulation and AI is a key factor shaping the future of chemistry. These technologies enable faster, more accurate research while supporting ecological safety, economic efficiency, and innovation. AI introduces not only convenience but also new scientific ideas and solutions, playing a decisive role in understanding, controlling, and creating new chemical processes and materials. Overall, chemical reaction simulation and AI application have become integral to scientific and technological progress. Further AI development is expected to enhance efficiency, generate new scientific achievements, and optimize modern industrial processes, providing significant practical benefits for science and society.[1,7]

Main Part: Chemical reactions are inherently linked to human life; they occur not only in laboratory settings but also in every home, street, nature, and even within the human body. Every day, humans breathe this is a chemical reaction; food is digested another complex chemical process; a phone battery charges again, chemical transformations occur. Understanding chemical reactions deeply is crucial for human progress. However, real experiments are not simple: chemicals can be expensive, reactions can be hazardous, and achieving results may require considerable time. In such cases, simulating chemical reactions, i.e., representing them virtually on a computer, has become an essential tool. The development of simulation methods has gained new momentum with the advent of technology, particularly artificial intelligence. Previously, envisioning reactions required complex mathematical theories or multi-step laboratory experiments. Today, computers perform these tasks quickly, safely, and accurately. AI can analyze large amounts of data and generate new knowledge and conclusions. In chemistry, the data volume is enormous: millions of reactions, hundreds of thousands of compounds, energy values changing under various conditions, different types of catalysts and their effects. Humans cannot process this, but AI can. So, what does simulating chemical reactions mean? It involves representing intermolecular interactions through mathematical models, algorithms, and virtual computations. For example, how two substances bond, at which stage energy increases or decreases, which step is the slowest, and what products are formed all can be predicted through simulation.[3,5,7] This allows scientists to “observe” reactions on a computer before going to the laboratory. Such an approach saves time, reduces material usage, and most importantly, ensures safety. In real life, a small error can cause significant problems. For instance, a substance mixed under incorrect conditions may explode or release harmful gases. Simulation methods anticipate such risks and help ensure safe laboratory operations. Consequently, many scientific centers worldwide first simulate chemical experiments before implementing them in practice. Now, regarding AI’s role: ordinary computer programs calculate reactions based on

predefined formulas. AI, however, learns independently, compares reactions, identifies similarities, and can even propose new reaction pathways. This is particularly valuable in pharmaceuticals. Creating a new drug typically takes 10–15 years, as each molecule's effect, side effects, stability, and behavior in the body must be studied individually. AI can analyze thousands of molecules in minutes and identify which will yield the best results, saving significant time, cost, and labor. A practical analogy: imagine creating a new recipe in the kitchen. Testing every ingredient combination to find the best taste takes time. If you had an assistant who remembered millions of recipes and could suggest the optimal combination, the process would be easier. AI serves this “intelligent assistant” role in chemistry. AI algorithms used in chemical simulation take various forms. Neural networks interpret complex reaction mechanisms, while generative models “invent” entirely new molecules.[4,6,8] Optimization algorithms determine which conditions allow reactions to proceed fastest or which catalysts yield the best results. Catalysts are crucial in chemistry; they act like advisors, accelerating reactions. Choosing the wrong catalyst may halt or slow the reaction. AI helps avoid such errors. The chemical industry also extensively uses AI. For example, in plastic production, the optimal quantities of substances, temperatures, and pressures are pre-evaluated through simulations, reducing production costs and improving quality. AI also contributes to environmental protection. Chemical waste from factories can harm air or water; AI can analyze harmful compounds and suggest chemical processes to neutralize them. Processes at the molecular level cannot be visualized by humans due to their tiny scale and speed. Simulation, however, makes these processes visible, as if under a microscope. How two molecules approach each other, which atoms bond, where energy increases or decreases all can be shown visually. This approach helps students, young researchers, and beginners understand chemistry easily. Another practical example: we use phones daily but cannot see how electrons move inside them; simulation makes the invisible visible. Another advantage of AI models in chemistry is adaptability. New data can be incorporated, and AI updates

itself, similar to how a human improves upon previous experiments. AI learns, compares, draws conclusions, and refines its predictions. Creating energy-efficient reactions is also a key modern requirement. Reducing energy consumption benefits both economics and ecology. AI calculates reaction energy profiles and identifies paths that require minimal energy. Efficiency increases without human error, and environmental impact decreases. Combined, simulation and AI make the future of chemistry faster, more precise, and user-friendly. Research is no longer limited to laboratory benches; virtual environments accelerate progress. Students gain visual, understandable, and practical examples, while scientific centers perform complex experiments with minimal risk and maximum accuracy.

Conclusion Simulating chemical reactions and integrating AI into this process is one of the fastest-growing directions in modern science. These technologies allow not only the improvement of existing processes but also the creation of entirely new compounds and reactions. Just as chemical processes are omnipresent in life, technologies that help understand and control them will gain increasing importance in the future.[1,2]

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