ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

Application Progress of Carbon Dioxide in Chemical Industry by Molecular Simulation Technology

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Abstract: *CO_2 has attracted much attention due to its unique physical and chemical properties. Supercritical CO_2 has been widely used because of its mild conditions, non-toxicity and wide sources. In the field of material chemistry, molecular simulation technology, as a new scientific research method, plays an important role in the basic theory and application of CO_2. This paper reviews the progress of molecular simulation technology in the field of CO_2 research in recent years, including physical properties, supercritical point properties, transcritical point characteristics, diffusion, adsorption separation, extraction and other mass transfer properties, as well as interface properties. Compared with the traditional method, the computer simulation method has obvious advantages.*

Keywords: *CO_2; supercritical; molecular simulation; chemical industry; research progress*

1. Carbon dioxide

In general, as pressure and temperature change, substances can assume three states: solid, liquid and gas. Each substance has its own specific critical temperature and critical pressure, and the critical parameters are the physical parameters of the substance. When the temperature exceeds the critical temperature and the pressure exceeds the critical pressure, the fluid is in a supercritical state. Supercritical fluids have the physical and chemical properties of substances in liquid and gaseous states, flow well and diffuse easily, and are widely used in industries [1, 2]. Slight changes in temperature and pressure can cause large fluctuations in the density and viscosity of supercritical fluids, thus affecting their dissolution and mass transfer capabilities. Temperature and pressure are easily adjustable during experimental studies, which is why supercritical fluids have been widely used in many fields such as energy, medicine, environmental protection, printing and dyeing, fragrances, cleaning and food in recent years, and have become a hot spot and frontier of research at home and abroad.

CO_2 is a gas at room temperature and pressure. The gas density is small and easy to remove, and it is used in different fields without residue, which is relatively green and environmentally friendly. Compared to other substances, supercritical CO_2 is widely used because of its lower critical temperature and pressure and milder conditions. In addition, CO_2 is non-flammable, non-toxic, widely available and inexpensive, so the potential for commercial applications of supercritical CO_2 fluids is growing. Supercritical CO_2 is environmentally friendly. Its density, solubility and heat transfer coefficient are close to the liquid, while the viscosity and diffusion coefficient are close to the gas, and the lower critical temperature and critical pressure, making it easy to reach the supercritical state for application. Supercritical CO_2 is well established in the fields of material preparation, degradation, textiles, extraction, fire extinguishing and cleaning and drying [3, 4]. As a cleaning agent, supercritical CO_2 can penetrate well into the crevices of objects due to its excellent properties; it is a non-polar gas and has a good solubilisation effect on non-polar organic pollutants, which can be enhanced by the addition of entraining agents. After cleaning, the supercritical carbon dioxide can be recycled for secondary use or directly discharged into the atmosphere without causing new pollution and without residue; no drying is required after cleaning, the cleaning time is short, and the whole process is easy to operate and manage [5, 6]. This work focuses on a more comprehensive classification and overview of the molecular simulation research applications of CO_2 and clarifies the important role played by molecular research techniques of CO_2 in the chemical industry.

ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

2. Molecular simulation technology

Molecular simulation technology is a new computer science and technology. It is based on the basic theory of Newtonian mechanics and quantum mechanics. Firstly, the real experiment is simulated by electronic computer, and then the atomic structure information of various compounds obtained in the experiment is injected into the software by using the developed application software, so as to construct the initial model of chemical reaction experiment and clarify the microscopic structure of compounds. Through this molecular simulation method, it can not only simulate the structure of the compound itself, but also simulate the dynamic changes of the compound during the chemical reaction process [7-10], which is a powerful supplement between conventional chemical experimental techniques and theoretical research methods. In addition, due to the rapid development of computer technology and the further correction of computational theory in the application of simulation calculation, computer chemical simulation technology has been improved day by day, and its advantages are increasingly apparent. The molecular simulation techniques currently used mainly include three categories: molecular mechanics simulation, molecular dynamics calculation, and Monte Carlo calculation. By using the computer's graphical interface, people can directly study the behavior of chemical processes from a microscopic perspective, especially for special cases that are more difficult to achieve in conventional experiments, such as supercritical, deep undercooling, and biological nanomaterials. Its advantages will be more obvious. At present, molecular dynamics simulation technology has been applied in various fields such as chemistry, life science, medicine and material science [11]. This paper will focus on the specific application of molecular simulation technology in the fields of carbon dioxide physical properties, mass transfer process and interface behavior.

The molecular mechanics simulation method is called MM for short. It is based on the basic theory of molecular force field in classical mechanics. In the operation, the movement direction of atoms is not considered, and only the stretching, rotation and bond angle change of chemical bonds are considered. Meantime, a large number of experimental parameters are introduced in the operation process, thus shortening the operation process and operation time. MM can find the stable structure with the lowest potential energy in the force field, and obtain the most stable geometric optimization structure, and then perform dynamic modeling or Monte Carlo simulation.

The molecular dynamics simulation method, abbreviated as MD, is based on the study of the structural scale of atoms and molecules. It is designed based on Newton's law of mechanics, and all the substances in its structure have certain motion orbits. In the study of dynamics, it is necessary to select the appropriate original structure, and then select the appropriate initial conditions, such as particle coordinates, number and boundary conditions. Subsequently, the experimental computer will automatically adjust the kinetic energy of the entire system according to the method used until the thermal equilibrium state is reached, and store the operating curves of all particles in the system for further study. MD is a good experimental method, which can simulate the interaction between two phases from the microscopic aspect, which is also impossible to achieve by real experimental methods.

Monte Carlo technology, also known as MC, is a technology based on thermodynamics. It simulates the simple movement and rotation of particles in a specific system environment. According to the established molecular potential energy function, the internal energy is added. Through the Metropolis sampling technique, the structure of all microscopic particles in a system can be obtained, and then gradually approaches the most stable Boltzmann state. At present, this method has been applied to various fields of polymer science, which has greatly promoted the development of theoretical basis [8].

3. Application of molecular simulation in CO_2 research

3.1. Physical studies

3.1.1. Geological storage

The storage technology of carbon dioxide in geological structure has high maturity and high emission reduction efficiency, which is the most efficient technology in carbon dioxide emission reduction. Carbon dioxide is put into and developed into a new original oil and gas reservoir, which can permanently seal CO_2 in the geological structure, thus effectively reducing greenhouse gas emissions. Dissolving carbon dioxide in crude oil can improve the physical properties of crude oil, so that the volume of crude oil increases rapidly, thus effectively increasing the recovery of crude oil. At the same time, the accurate calculation of the volume expansion coefficient of carbon dioxide-crude oil has also

ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

become an important basis for effectively realizing carbon dioxide storage and oil displacement. Although there are many research data on the expansion coefficient of carbon dioxide and crude oil, in view of the complex chemical composition of raw materials, different physical properties, and lack of regular morphological identification, and with the change of contact time and characteristics of crude oil-carbon dioxide system, the adaptability is also very poor. Therefore, the current determination method of expansion coefficient of CO_2-crude oil system still has shortcomings, and further scientific research methods are urgently needed. However, the researchers [12] have studied the volume expansion coefficient and solubility coefficient of CO_2. They simulated petroleum cracking reaction system through a large number of values of volume expansion coefficient in CO_2 and organic system obtained from long-term research, and clarified the principle of volume expansion from the perspective of molecular structure and molecular mechanics.

Through molecular simulation, the researchers clarified the volume expansion changes of CO_2 and alkane systems and the effects of temperature [13], pressure and molecular configuration on volume expansion changes and microscopic mechanisms. The microscopic process of volume expansion between carbon dioxide and alkane systems shows that it is precisely because of the increase of the average distance between alkane molecules and their mutual stretching between molecules that more and more CO_2 is dissolved into alkane molecules, so the interaction between carbon dioxide and alkane molecules has become an important reason for the expansion of the system. The volume change of carbon dioxide in acetate system under different CO_2 mole fractions was studied by MD experiment, and the solubility and diffusion coefficient of carbon dioxide in heavy crude oil system were studied by molecular dynamics theory [14-15].

3.1.2. Physical properties of supercritical CO_2

CO_2 has been widely used due to its good working properties. In addition to its advantages in the normal state, it has been studied more extensively in recent years for its applications as its extraction capacity far exceeds that of organic solvents at supercritical conditions. As the study of supercritical fluids generally requires high temperature and pressure, experimental studies require high equipment conditions and are not easy to observe, whereas computer simulation methods are not limited by harsh experimental conditions and can obtain data on fluid transfer and microstructural information under supercritical conditions.

The energy, radial distribution functions and self-diffusion coefficients of supercritical CO_2 and co-solvent systems have been investigated at different pressures and compositions of matter [16]: the density rise and fall of the system was present, but not at high pressures. The co-solvent aggregation was described in terms of radial distribution function and coordination number, which inhibited the diffusion of co-solvent molecules and resulted in a small self-diffusion coefficient. In addition, a group of researchers [17] used MD simulations to study the diffusion coefficients of organic matter in supercritical CO_2, laying the kinetic foundation, and also detailing the simulation work related to the solubility and diffusion coefficients of organic matter in supercritical CO_2 in recent years.

3.1.3. Physical properties of transcritical CO_2

Molecular dynamics method can be used to analyze the microstructure characteristics of carbon dioxide system across the critical point. Using the radial distribution function, it can be found that the structural difference before and after the critical point is very small, which is mainly caused by the strengthening effect of the interaction between the molecular structure and the nearest neighbor, while the change of the near molecular structure is mainly caused by the change of the number of paired molecules [18]. In the quasi-critical region system, the interaction distance between the products near the critical point increases rapidly.

Using the molecular dynamics simulation method, the distortion correction characteristics of CO_2 physical properties near the critical point can be explained from a microscopic perspective [19]. The simulation results of molecular dynamics show that the COMPASS force field has relatively high accuracy when it is far away from the critical point, and the accuracy is relatively low when it is near the critical point, but it can still reflect the density distortion problem. In different simulation spaces, the density fluctuation properties of the system are different. Near the critical point, the density fluctuation value is large, and before and after the critical point, the density fluctuation value is asymmetric.

Yao [20] used MD to calculate the viscosity and thermal conductivity at the critical point of CO_2, and analyzed the error of the simulation results, and proposed the error compensation measures. The closer to the critical point, the greater the average relative deviation of viscosity and thermal conductivity of

ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

CO_2. In order to compensate for the average relative deviation of viscosity and thermal conductivity of near-critical CO_2, the number of CO_2 molecules in the simulation can be further increased, or the viscosity and thermal conductivity of near-critical CO_2 can be simulated from a mesoscopic perspective.

3.2. Study of mass transfer properties

Mass transfer is a mass transfer problem caused by the imbalance of material content in the system. In the chemical industry, the mass transfer process between gas-solid, liquid-liquid and solid-liquid systems is usually applied. In recent years, with the progress of computer hardware technology and the rapid development of simulation software, the study of mass transfer process through simulation technology has also attracted the attention of many researchers. The most involved is the dynamic simulation of chemical reactions such as adsorption, diffusion, extraction and absorption. In the two-phase mass transfer reaction, diffusion plays a great influence. Many researchers have used molecular dynamics simulation technology to carry out in-depth research.

3.2.1. Absorption

According to the fact that the total amount of flue gas in the factory is relatively large, the partial pressure of carbon dioxide is relatively small, and the general organic amine absorbent is insufficient, the liquid of tetramethylammonium lysine was successfully prepared by using the advantages of relatively low pressure, stable physical and chemical properties and controllable structure of ionic liquid vapor, and its aqueous solution was used to adsorb CO_2 [21]. The adsorption characteristics, reaction mechanism and kinetics were studied. The results show that the absorption effect of polyamino high-performance liquid aqueous solution is significantly higher than that of monofunctional amine liquid. Because the functional group amines at each site of the anion cannot participate in the CO_2 reaction together, and cannot participate in the later hydrolysis reaction together. After studying the reaction mechanism by molecular simulation technology, researchers believe that the electronegativity of N may interfere with the binding process of functional group amines with CO_2.

3.2.2. Extraction

The extraction method has been applied in industrial production because of its important function in the field of separation and purification, but the in-depth study of its microstructure and extraction principle is relatively backward. There are many difficulties in the experiment of extraction reaction by conventional test methods, but the computer simulation technology can solve all the problem factors in the experimental method. Therefore, in recent years, the use of MD simulation technology to solve the extraction problem has always been the focus of our domestic experts. Similar to the conventional fluid simulation technology, the selection of potential energy parameters is a technical problem.

The results of supercritical CO_2 extraction of light components of heavy oil showed that [22], the four components of heavy oil were unevenly distributed in the polymer of heavy oil, and the association force with asphaltene was high. Due to the strong interaction between asphaltene and rock surface, supercritical CO_2 was difficult to migrate from asphaltene. However, due to the weak interaction between aromatic hydrocarbons, saturated hydrocarbons and rock surface, supercritical CO_2 was easy to migrate from aromatic hydrocarbons and saturated hydrocarbons, and the diffusion coefficient was large. The application of molecular dynamics to study the newly discovered microscopic kinetic mechanism was of great significance to understand the light composition of heavy oil extracted from supercritical CO_2.

3.2.3. Diffusion and adsorption

An in-depth study of the decomposition of aromatic compounds in supercritical CO_2 was carried out by Liu [23] through molecular dynamics simulations. The problem of diffusion coefficients was systematically studied using the Einstein technique, and the mass transfer mechanism of solids extracted from supercritical fluids was first explored by means of molecular dynamics simulations. In contrast, Shi [24] systematically investigated the ways to predict the self-diffusion coefficient of supercritical CO_2 and the infinitely dilute self-diffusion coefficient of polar and non-polar dilute solvents in supercritical CO_2 based on experimental results and molecular dynamics simulations.

The diffusion of CO_2 and O_2 molecules in a PLA/PVDF blend was systematically investigated by using molecular dynamics modelling [25]; the free volume fraction and the diffusion coefficient of CO_2 in the blend system were systematically measured, and the interaction between the free volume fraction and the diffusion coefficient was discussed. The experimental results showed that the diffusion

ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

coefficient was the smallest; the smaller the kinetic radius of the small molecules in the blends, the larger the diffusion coefficient; in different blends, the variation of the free volume fraction was the same as the diffusion coefficient, which was consistent with the free volume theory.

The results of the GCMC and MD studies investigated the adsorption, diffusion and decomposition of CO_2, CH_4 and N_2 in MER-type zeolites [26]. The results showed that the adsorption rate and heat of adsorption of the three substances in zeolites are mainly determined by the molecular structure of the zeolite, the ions outside the skeleton and the properties of the adsorbent. The expansion of gaseous substances in the three-dimensional channels of zeolites is anisotropic. The interaction between zeolite and gas also has an important influence on the diffusion performance of gaseous substances, with the ions outside the zeolite skeleton being an important factor in the diffusion performance.

3.3. Studies on interfacial properties

Molecular dynamics simulation can be used to study the behavior of phase interface. Molecular dynamics simulation can be used to calculate the motion state of gas-solid, liquid-liquid, gas-solid, liquid-solid and other surface materials. It is a powerful method to explore surface problems at the molecular level by using the graphical interface of the computer to directly see the molecular hierarchy of the surface.

Chai [27] used a molecular dynamics approach to study the orientation behavior and kinetic properties of the water-supercritical flow carbon dioxide interface. A distinct two-phase was formed between water and carbon dioxide, with carbon dioxide in a small amount of dissolved state in the aqueous phase, while water had almost no water molecules present in the carbon dioxide phase. Due to the anisotropic nature of the interfacial system environment, the self-diffusion properties of both water and carbon dioxide were clearly anisotropic. The diffusion in the direction perpendicular to the interface was much smaller than the diffusion in the direction parallel to the interface. The variation of the diffusion coefficient was explained from the perspective of the water coordination number.

Using molecular dynamics simulations, Li [28] investigated the interaction between montmorillonite and different concentrations of CO_2 fluids, and calculated the distribution of CO_2 between montmorillonite layers, diffusion properties and free energy changes. The density distribution and free energy curves show that dissolved CO_2 is preferentially distributed between the montmorillonite layers. The diffusion activity of CO_2 between the montmorillonite layers is reduced compared to that in the pores of the montmorillonite particles. The diffusivity of CO_2 in the inter-particle pores is positively correlated with its concentration, whereas the diffusivity of CO_2 between montmorillonite layers is not significantly affected by concentration.

Hu [29] explored the morphological characteristics and dynamic properties of gold nanoparticles and solvent substances at different supercritical CO_2 densities. The results showed that the gold nanoparticles had a great absorption effect on the supercritical CO_2 solution components, which surrounded the supercritical CO_2 molecules tightly around its surface and produced two very obvious solvent surfaces. As the solvent density increased, the degree of solventization of nanoparticles in supercritical CO_2 decreased. The transfer properties of the interfacial CO_2 molecules were investigated by analysing the mean square displacement and residence time distribution of supercritical CO_2 molecules in different regions of the solid-liquid interface.

4. Summary and outlook

Molecular simulation technology is a new scientific research method widely used. Researchers at home and abroad have done a lot of research work by using computer molecular simulation technology. This paper briefly summarizes the application of molecular simulation of CO_2 in chemical industry, including geological storage, supercritical and transcritical properties exploration, absorption, adsorption, interface research and other fields. These basic research results provide research ideas and theoretical guidance for the subsequent application of molecular simulation technology to the utilization and performance optimization of CO_2.

In different fields, supercritical CO_2 plays a unique advantage. CO_2 is non-toxic and harmless, which is in line with the concept of green sustainable development. Introducing unique supercritical CO_2 fluid into all walks of life has become a research hotspot. As an emerging technology, supercritical CO_2 still faces many technical, environmental and economic challenges. Supercritical CO_2 requires high pressure, and there are many uncertainties in the reaction process. The investment capital of the

ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

equipment in the early stage is large, and it is difficult to large-scale industrialization; in the process of use, CO_2 leakage may occur, causing problems such as damage to the ecological environment. In the context of "double carbon", the development of new energy sources and the reduction of CO_2 emissions are one of the effective ways to reduce the CO_2 content in the atmosphere. At the same time, we should also realize that most of the CO_2 emissions are inevitable. Based on this, many scholars consider converting CO_2 into available energy or material, which may be a new challenge and breakthrough.

Molecular simulation technology has been widely used in the basic theory and application research of CO_2. These research results have strong guiding significance for the experimental study of CO_2 application. With the rapid development of computer hardware and software technology, the continuous updating of experimental characterization methods and the continuous improvement of simulation methods, molecular simulation technology will greatly promote the research and application level of researchers on carbon dioxide.

Acknowledgements

Funding Projects: Scientific Research Project of Taishan University (2022HX396).

References

[1] Zhan S. P., Ding S. Q., Wang W. J., et al. Progress in the Preparation of Biodegradable Polymer/drug Nanoparticles by Supercritical Fluid Technology[J]. Journal of Chemical Engineering, 2020, 71(3): 923 - 935.

[2] Liu Y. B., Xiong M. Q., Zhang J. F. et al. Research Progress of Supercritical CO_2 in Chemical Industry[J]. Energy Saving Technology, 2022, 4(5):403-408.

[3] Zhao S, Wang C, Bai B, et al. Study on the PolystyrenePlastic Degradation in Supercritical Water /CO_2 Mixed Environment and Carbon Fixation of Polystyrene Plastic in CO_2 Environment[J]. Journal of Hazardous Materials, 2021(421):126763.

[4] Vecchia FD, Santos V, Schütz M, et al. Wellbore Integrityin a Saline Aquifer: Experimental Steel-cement Interface Degradation under Supercritical CO_2 Conditions Representative of Brazil's Parana Basin[J]. International Journal of Greenhouse Gas Control, 2020(98) 103077.

[5] Huang L. J., Kang H., Cheng S., et al. Application of Supercritical CO2 Cleaning Technology in CMOS Image Sensors[J]. Micro- and Nanoelectronics, 2017, 54 (4): 273-278, 290.

[6] Pérez M, Ramil M, Cela R, et al. Supercritical Fluid Chromatography-mass Spectrometric Determination of Chiral Fungicides in Viticulture-related Samples[J]. Journal of Chromatography A, 2021(1644): 46212426-32.

[7] Li G. Q, Qiu J, Liu D. L., et al. Advances in Molecular Simulation of Montmorillonite [J] Mineral Comprehensive Utilization 2019, 8(4):26-32.

[8] Li Y. G., Liu J. C., Molecular Simulation and Chemical Engineering [J]. Modern Chemical Industry, 2001, 21(7):10-13.

[9] Francoeur. Introduction to Molecular Simulation[M]. Beijing: World Book Publishing Company, 2010.

[10] Frenkel Smit. Molecular Simulation from Algorithms to Applications [M]. Beijing: Chemical Industry Press, 2002.

[11] Wu F. D., Zheng H. D., Liu J. X. Advances in the Application of Molecular Dynamics Simulation in Chemical Industry [J]. Journal of Chongqing University of Technology (Natural Sciences). 2013, 27(10) 59-65.

[12] Xie L. F. Progress in the Study of Volume Expansion Coefficient of CO2-petroleum Hydrocarbon Substances [J]. Light Industry Science and Technology. 2018, 34(9):38-40.

[13] Bing L, Shi J, Sun B, et al. Molecular Dynamics Simulation on Volume Swelling of CO2-alkane System[J]. Fuel, 2015, 143:194-201.

[14] Aida T, Aizawa T, Kanakubo M, et al. Analysis of Volume Expansion Mechanism of CO2-acetate Systems at 40°C [J]. Journal of Supercritical Fluids, 2010, 55(1):56-61.

[15] Kavousi A, Torabi F, Chan C W, et al. Experimental Measurement and Parametric Study of CO2, Solubility and Molecular Diffusivity in Heavy Crude Oil Systems[J]. Fluid Phase Equilibria, 2014, 371(12): 57-66.

[16] Liu J. H., Lou Y. M., Zhou X. P., et al. Molecular Dynamics Simulation of Supercritical Carbon Dioxide with Co-solvent Methano [J]. Journal of Southwest Normal University: Natural Science

ISSN 2616-5880 Vol. 4, Issue 4: 7-13, DOI: 10.25236/AJMC.2023.040402

Edition, 2009, 34(6): 28-33.
[17] Higashi H, Iwai Y, Arai Y. Solubilities and Diffusion Coefficients of High Boiling Compounds in Supercritical Carbon Dioxide [J]. Chem Eng Sci, 2001, 56(10): 3027-3044.
[18] Tang J., Huang Y. P., Wang J. F., Molecular Dynamics Simulation of the Microstructural Characteristics of Carbon Dioxide Systems at Transcritical times [J]. Nuclear Dynamics Engineering, 2021, 42(4):14-20.
[19] J. Tang, Y. P. Huang, J. F. Wang, Molecular Dynamics Study of the Physical Distortion Properties of CO_2 near the Critical poin [J]. t Nuclear Dynamics 2021, 42(4):73-79.
[20] Yao B. X., Liu F. Molecular Dynamics Simulation of CO2 Viscosity and Thermal Conductivity at the Critical Point [J]. Cryogenic/Refrigeration Technology, 2021, 49(9):77-81.
[21] Sun C., Liu F., Shen L. Mechanism and Kinetics of Carbon Dioxide Absorption by [N1111] [Lys] Aqueous Solutions [J]. Journal of Chemical Engineering in Universities No. 2020, 34(5):1135-1142.
[22] Li H. Y. Molecular Dynamics Simulation of Supercritical Carbon Dioxide Extraction of Deep Thick Oil Components [J]. Science Technology and Engineering, 2021, 21(29):12543-12550.
[23] Liu Y. Molecular Dynamics Simulation of the Diffusion Properties of Supercritical Fluids and Extraction of Active Ingredients in Deer Antler [D]. Tianjin: Tianjin University, 2006.
[24] Shi J. Experimental Study and Molecular Dynamics Simulation of the Diffusion Coefficient of Supercritical CO_2 System [D]. Tianjin: Tianjin University, 2006.
[25] Li S. Y., Sun L., Cai H. F. Molecular Dynamics Simulation of Diffusion Behavior of CO_2 and O_2 in PLA/Poly (vinylidene fluoride) blends[J]. China Plastics, 2021, 35(10):51-55.
[26] Shi Q. Molecular Dynamics Simulation of Diffusion and Separation of $CO_2/CH_4/N_2$ in MER-type Zeolite [J]. Journal of Fuel Chemistry [J] 2021, 49(10):1531-1539.
[27] Chai J. C., Yang X. N. Molecular Dynamics Simulation of Water-supercritical Carbon Dioxide Interface [J]. Journal of Yangzhou University (Natural Science Edition) 2008, 11(2):34-39.
[28] Li Q., Lu X. C., Zhang L. H. Molecular Simulation of the Interaction between Montmorillonite and Carbon Dioxide Fluids[C]. Joint Annual Meeting of Chinese Geosciences, 2020:3368.
[29] Hu Y., Yang X. N. Molecular Simulation of Interfacial Properties of Gold Nanoparticles in $scCO_2$ Solvent [J]. Journal of Chemical Engineering, 2011, 62(2):295-300.