

Application of potential function in molecular dynamics simulation of natural gas hydrate

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Abstract:- In the study of natural gas hydrate, it is particularly important to determine the accuracy of the potential function used in the study of the nature of the gas hydrate. The potential function is not only required to reflect the true nature of the material to be studied, and it is also required to have a relatively simple mathematical expression. Through the comparative study of different properties using a potential function that interaction between the molecules in the reaction of natural gas hydrate in the study of natural gas hydrate stability, simple point charge (simple point charge SPC^[1] potential function and the Lennard Jones potential LJ^[2] function can very well. In addition, TIP4P^[3] potential function model and OPLS^[4] function model also can be better applied to the study of natural gas hydrate stability. Among them, the interaction potential between the water and the water molecules is the TIP4P potential model, the object and the subject, and the OPLS potential energy model is used between the object and the guest molecule.

Key words:- natural gas hydrate, potential energy function, molecular dynamics

I. Introduction

Gas hydrate^[5] is a non stoichiometric cage compound formed by water and gas molecules under low temperature and high pressure. The study of gas hydrate was first to solve the problem of blockage in natural gas pipeline transportation^[6]. With the natural gas hydrate is a lot of proven, as the future of clean, efficient alternative energy, gas hydrate research is paid attention to day by day, at present study of natural gas hydrate is mainly using simulation method of molecular dynamics.

Simulation of molecular dynamics (MD) is to microscopic simulation of macroscopic properties of a computer simulation method, has been widely used in the study of natural gas hydrate^[7-12]. Molecular dynamics is defined on a consists of N particles (atoms or molecules) system, the first step is to determine the interaction potential between atoms (molecules) and analysis the interaction between atoms (molecules), to determine the initial conditions and boundary conditions, and by Newton's equations of motion do numerical integration, in order to get the trajectories of particles, and the of corresponding statistical analysis to obtain physical information^[13].

The standard LJ potential function is widely used because of its simple form. In molecular dynamics simulation of methane hydrate stability is applied to the interaction between the guest molecules, and main water molecules between the interaction potential is used classic SPC potential model, the PSC model assumptions between the oxygen atoms exist LJ role^[14]. In simulating the stability of methane hydrate, the TIP4P potential energy model is also used to describe the interaction between the water molecules, and the guest molecules, and the POLS potential energy model is used between the guest molecules and the host molecules.

The main purpose of this work is to study the potential function of methane hydrate, and the simulation results

of different potential functions are obtained, and the form of the potential function of methane hydrate is obtained.

II. The potential function based on Lennard-Jones is used to describe the interaction potential between the guest molecules.

Dong Hai Mei, et al in the structural stability of the natural gas hydrate is studied, using molecular dynamics simulation method, water molecules as the non spherical molecules, two non polar guest molecules are considered for spherical molecules, which the interactions between the guest molecules potential by LJ potential energy model. Its mathematical expression is:

$$U(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] \quad (1)$$

In the formula, R is the interatomic distance; and epsilon sigma potential parameters, varied for different types of atoms. The minimum potential energy point, the size of the potential energy curve reflects the depth. In the LJ potential function, the R-12 term is repulsive, and the R-6 term is attractive. When the R is large, the LJ potential energy tends to zero, which indicates that there is no indirect effect on each other when the atoms are far away from each other. Figure 1 the role of LJ potential energy function describing the interaction between methane and methane. Figure 2 The curve of the role of the LJ potential energy function describing the interaction between octane and octane. Figure 3. The effect of the potential energy function describing the interaction between methane and the octane number of the LJ. From the above three groups of simulation of the potential function of curve can be seen, the lowest point of the potential energy between methane and methane in the =0.42nm, cyclooctane and cyclooctane between the lowest point of potential energy in the =0.90nm, while the lowest point of the potential energy between the guest molecules of methane and cyclooctane is located in 0.64nm. by comparing, we found that, the maximum distance between the guest molecules cyclooctane and cyclooctane between the lowest point of potential energy, it is concluded that the molecular value larger guest molecules between the minimum potential energy between the values of the distance is greater. In the following three pieces of simulation, we see not hard, between methane and cyclooctane potential well depth is greater than the other two guest molecules between the depth of the potential well, it is not difficult to find that different kinds of guest molecules between the depth of the potential well will be even greater.

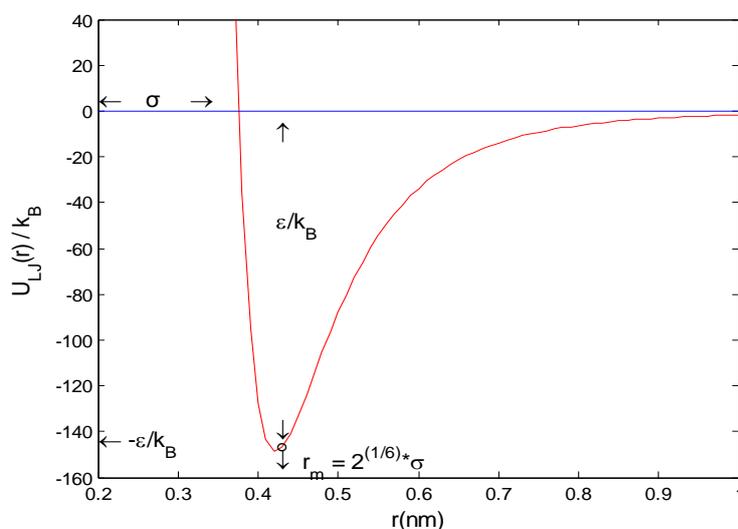


Fig1 shows the role of LJ potential energy function describing the interaction between methane and methane.

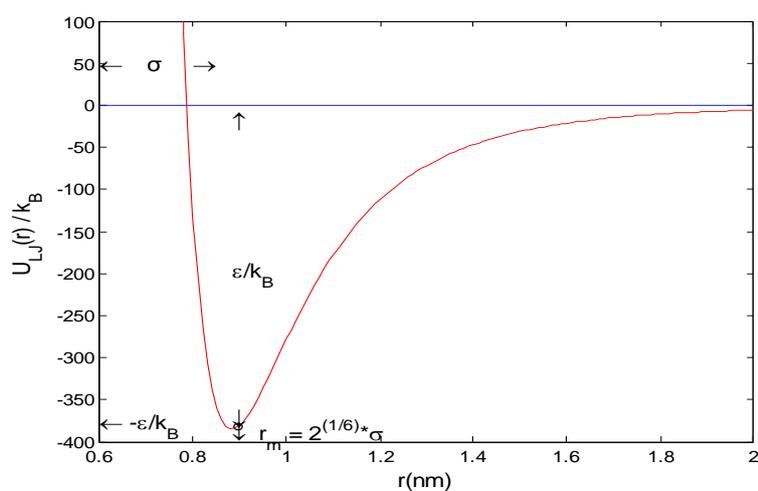


Fig 2 shows the curve of the role of the LJ potential energy function describing the interaction between octane and octane.

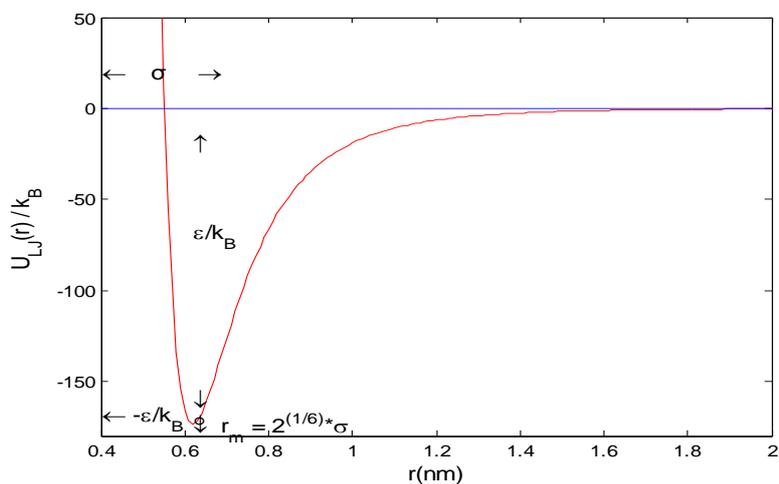


Fig 3 shows the LJ potential function to describe the effect curve between the guest molecules of methane and octane ring.

Table 1 potential parameters of LJ potential function

Type of interaction	ϵ/k_B	$\sigma \times 10/nm$
Water-water	78.2	3.1656
Methane-methane	148.6	3.7580
Cyclooctane - Cyclooctane	384.3	7.8650
Water-methane	108.8	3.4618
Water-cyclooctane	173.4	5.5153
Methane-cyclooctane	239.0	5.8115

III. Potential model SPC is used to simulate the water molecules.

The interaction potential of water molecules is a classical simple point charge (points charge Simple) SPC potential energy function. The point charge in the PSC model is better consistent with the position of the cluster. The selection of the charge should be based on the minor modification of the energy E, and the final choice depends on the minimum cut off radius. Figure 4 for the SPC potential function model chart. In the model constructed in the graph, scientists are looking for a linear three point charge model..

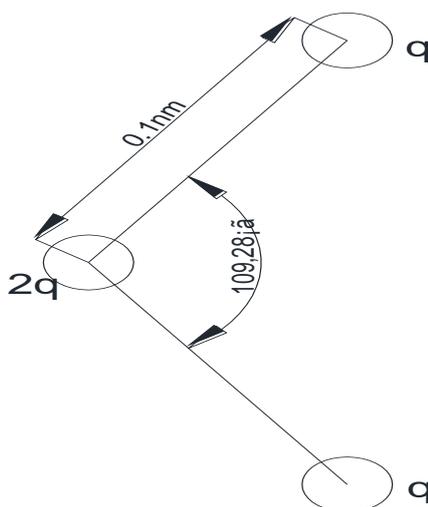


Fig. 4 model of SPC potential function

In e later study, the SPC potential function of the Mei East China Sea is further studied, and the O-H bond length of the water molecule is controlled by 0.09570nm. The H-O-H bond angles for 104.52o in process simulation, three coordinate directions using periodic boundary conditions and recent imaging method, the initial position of the molecular [16-17] are determined according to the diffraction experiment results, the orientation of the water molecules are randomly assigned. The SPC model divides the interaction between water molecules into an LJ phase and a long-range electrostatic interaction:

$$u (r_{ij}) = \sum_{i=1}^3 \sum_{j=1}^3 \frac{q_i q_j}{r_{ij}} + \frac{B}{r_{ij}^{12}} - \frac{C}{r_{ij}^{16}} \quad (2)$$

Among them, for the SPC potential model, only the oxygen atom of water molecule and the LJ interaction between the two nonpolar guest molecules exist. For the molecular parameters of the interaction, the classical Lorentz-Berthelot mixing rule is adopted.

IV. Conclusion

Abrief Introduction of the application of molecular dynamics simulation and theoretical knowledge of natural gashydrate. Elaborated in recent years for the study of methane hydrate in the wider application of LJ potential model and SPC potential model research obtained in molecular dynamics simulation, the LJ potential function can very good application in the description of the interactions between the guest molecules, and in the description of the interaction between the main water molecules, apparently SPC function model can be used better.

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