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The Surfactant Adsorption in Solid-Liquid Interface

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Abstract: ***Surfactants is known as "industrial MSG", because of low content of surfactants to produce a great impact on the product performance, sometimes even play a decisive role. At present, there are many kinds of surface active agents, and the application field is expanding. It is the chemical additives required in many industrial sectors.the amount is small, the effect is large. Often play an unexpected effect. As one of the important methods of scientific research, computer molecular simulation study is not a substitute for experimental and theoretical studies. It can simulate the static structure of the molecules, but also can simulate the dynamic behavior of the molecules, such as: the adsorption behavior of molecules on the surface and molecular diffusion, etc. Computer molecular simulation in the view of statistical mechanics, the development of Monte-Carlo (MC) method and molecular dynamics method (MD)***

Keywords: Surfactant Molecular simulation Solid/quid interface

1. Simple Introduction of Surfactant

1.1 Characteristics and Properties of Surfactants

There are at least two parts of surface active agents. One part can be dissolved in a specific liquid (lyophilic part), the other of which cannot be dissolved. (lyophobic part). Hydrophilic portion called the head, the hydrophobic part is called the tail. Due to its special molecular structure. It not only has function of preventing the oil-water become mutual exclusion ,but also can be adsorbed on the interface to have a unique interface activity, and in very low concentrations, can significantly change the interfacial material properties. In addition, surface active agent could significantly reduced the surface tension of the liquid.In the wet process, it has dissolved, wetting, penetration, diffusion and emulsification, leveling, cleaning effect. [1] The nature of gas - liquid, liquid - liquid and solid - liquid interface can be changed because of surfactants,so that it has the function of bubbling, defoaming, demulsification of emulsion, dispersion, agglomeration, wetting, waterproof. [2] In addition, the derived properties of the surface active agents are: soft, antistatic, bactericidal and anti - corrosion.

1.2 Types of Surfactants

There are many kinds of surface active agents, commonly divided into: anionic surfactants, cationic surfactants, nonionic surfactants, nonionic surfactants.

1) **Anionic Surfactant**
   Anionic surfactant is composed of a hydrophobic group of hydrocarbon and a or two hydrophilic group . Anion is the carrier of the nature of the surfactants. In molecule,the hydrophilic group which is attached to the hydrophobic group is an anion. It is often used in cleaning formulations.
2) **Cationic Surfactant**
   The cationic surfactant contains a hydrophobic hydrocarbon and one or more hydrophilic groups, and the cationic is a carrier of the nature of the surfactant.In molecule,the hydrophilic group which is attached to the hydrophobic group is a cation.
3) **Zwitterionic Surfactants**
   Amphoteric surfactants are simultaneously having properties of both ions. Its hydrophilic group containing both yin, yang two types of ons, after molecules are dissolved in the water and ionized. The nature of anions is showed in alkaline media, properties of the cations in the acidic medium, and the nature of the anion and cation in the appropriate medium. At present, the majority of the production of varieties is the type of carboxyl group.
4) **Non-Ionic Surfactants**
   Nonionic surfactant is a kind of important surfactant that the ionization does not occur after the molecular is dissolved in water, and the ion isn't showed as surface activity. The lipophilic group of this kind of surfactant molecules is often composed by the hydrocarbon chain that contain 8 ~ 18 carbon atoms(either aliphatic or aromatic).hydrophilic group often is hydroxyl or polyoxyethylene.

2. Model and Method

2.1 Monte Carlo (MC) Method

MC method, also known as stochastic simulation method [(3,4)]Through sampled each random variable, then substituted it into the data model to determine function values.The basic idea:to solve a specific problem, build a probabilistic model or random process, making parameters equal to the solution of the problem : when the question itself is a random problems, MC model can be built by the actual situation of the physical laws of probability, then by observing the model or process or taking a sample test to calculate the statistical characteristics of the demand parameters,finally the approximate value is obtained.

Using the MC method to carry out molecular simulation calculations by the following steps [(5)]:

(1) Using a random number generator to generate a random molecular configuration, and to calculate its energy U(r^N).

(2) To make no rules change of coordinate of particles in this molecular configuration, then produce a new molecular structure.Calculating the energy of the new molecular configuration.

(3) Comparing of energy change of the new molecular configuration and the molecular configuration before change, and determine whether or not to accept the configuration.

$$P_{acc}(o \to n) = \min\{1, \exp[-\beta[U(r'^N) - U(r^N)]]\}.$$

If the energy of new molecular configuration is lower than the original molecular configuration, the new configuration is accepted, and the configuration is used to do the next iteration.If the energy of new molecular configuration is higher than the original molecular configuration , the calculation the Boltzmann constant, while producing a random number. If the random number is greater than the calculated Boltzmann factor, then give up this configuration, recalculated. If this random number is less than the calculated Boltzmann factor, accept the configuration and use this configuration do repeat write one iteration.

(4) Such an iterative calculation is done until the energy of the molecular configuration is lower than the given one.

2.2MD (Molecular Dynamics) method

MD method is to determine the interaction potential between atoms through experimental results or empirical model with small computation,.it can solve the problem of large scale but portability is poor. Her advantages of system motion is physically correct basis, high precision, can simultaneously obtain the system dynamic and thermodynamic data, and can be widely applicable to systems and various characteristics of the study. the advantages is that the system has the correct physical basis for the motion, high precision, the system dynamic and thermodynamic data can be obtained simultaneously, and its widely applicable to various systems and characteristics of study.

3. Surfactant Adsorption at the Solid-Liquid Interface

To study the aggregation morphology of surface active agents on the surface of solid (hydrophobic) by Lattice MC method. The simulation results under different interaction parameters in addition to the observed experimental reported hemispherical micelles and outer monolayer structure also found four other aggregate morphology: non-stable micelles, mixed micelles hemisphere half cylindrical, wormlike micelles and perforated semi-cylindrical shape monolayer. And the surface adsorption is stronger, the surface active agent in the surface of the surface of the formation of low curvature of the aggregation morphology. In contrast, the stronger the attraction between surfactant head groups and water, the surfactant tend to form a high curvature surface topography aggregation. In addition, the hydrophobicity of the surfactant tail group is more strong, the surfactant is more inclined to adsorb on the surface, and gathered together. The smaller the proportion of the head and tail of the surfactant, the more stronger of hydrophobic of the surfactant, the more inclined to adsorb on the surface, and gather together. The effects of the adsorption and reaction of surfactant head groups and water not only affect the aggregation morphology of the surface active agents but also affect the surface adsorption capacity. Surface adsorption energy is stronger and the adsorption capacity is higher.

To research aggregation morphology of surfactant that limited in crack hole by using lattice MC method, change the distance between the two surfaces and the surface active concentration. The results found that there are three different surfactant aggregates morphology. Except the common single-layer and double-layer structure, also found a new structure -- bridge structure.

4. Conclusion

In the research of solid liquid adsorption, the study of adsorption of surfactants is the most, because the surface active agent has the characteristics of directional adsorption at the interface, which significantly changes the physical and chemical properties of the interface. Also we can put the broken characteristics applied to emulsifier and aggregate, to improve the performance of emulsified asphalt. Although there are many studies on the surfactants the research that applied in the asphalt direction is still relatively small.It has the value of further research.

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