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Molecular dynamics simulation of temperature-dependent atrazine aqueous solution

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ABSTRACT

The molecular dynamic simulations have been performed to investigate the atrazine aqueous solution at different temperature. Molecular structure, transport characteristics, hydrogen bonds dynamics and vibration power spectra were obtained by using the OPLS and TIP4P models. Simulation results show that the atrazine molecules do not have a significant effect in water and the tiny solubility of atrazine due to the molecular surface area and structure. As the temperature increases, the water's tetrahedral structure and the hydrated shells are weakened. The hydrogen bonding lifetimes of atrazine-water and water-water show a decrease with temperature. The self-diffusion coefficient of water increase linearly and the self-diffusion coefficient of atrazine shows an nonlinear increment. The vibration power spectrum of atrazine was calculated and compared with the existing infrared spectra.

1. Introduction

Atrazine (2-chloro-4-ethylamino-6-isopropylamino-s-triazine) is one of the most common herbicidal ingredients. Because of the widespread use of herbicides which contains atrazine components, atrazine has a lot of residue in the natural environment [1], which has a great negative impact on biological diversity and human health [2–4].

Liquid-liquid extraction (LLE) is a conventional pesticide pretreatment technology [5]. However, it has a lot of problems, such as incomplete phase separation, low recovery, and the need for large amounts of organic solvents. Although they have been circumvented by using Solid Phase Extraction (SPE) [6,7], but the SPE require a large number of samples and reactant. Gas chromatography (GC) [8–10] is also used to analyze and isolate complex multi-component mixtures. Similar to the former, GC also has many deficiencies, for instance, sample extraction is slow, we need to combine other methods to accurately analyze (GC–MS [11]) and other defects. The research of atrazine kinetics is focused on its photodegradation and adsorption behavior of soil surfaces [12–15] or seek the method to remove the atrazine contained in the solution [16]. According to the author, there are few molecular dynamics studies on atrazine. Therefore, it is necessary to further understand the microscopic mechanism of the mixture of atrazine and water under temperature changes.

Atrazine has a stimulating effect on the human body and it is easily decomposed at high temperatures. It is very inconvenient to analyze atrazine by experimental methods. Molecular dynamics simulations (MD) have a great advantage in the analysis of toxicants. Simultaneously. Molecular dynamics is a powerful tool for studying the interaction between particles under microscopic conditions and can comprehend the structural and kinetic characteristics of molecules [17]. In this paper, the radial distribution function, the diffusion coefficient and the hydrogen bonding lifetimes have been obtained to explore the microscopic mechanisms of atrazine aqueous solution at different temperatures. Vibration power spectrum was also calculated to compared with the infrared spectrum.

2. Simulation details

The simulation was performed using the GROMACS 4.5.5 [18] simulation software package with the optimized potentials for liquid simulations (OPLS) force field and the TIP4P water model. 5 atrazine molecules and 4063 water molecules were added to the simulated box. The whole simulations of atrazine solution were performed under the 7 different temperatures: 298 K, 308 K, 318 K, 328 K, 338 K, 348 K and 358 K, and set the pressure to 0.1 MPa. Before the system was relaxed, we use the steepest descent method for minimizing energy. Termination gradient of 5000/kJ mol^{-1} nm^{-1} was used. Using the Nose'-Hoover thermostat [19] to keep the temperature. The Ewald method [20,21] to calculate long distance static electricity within the relative tolerance range. A cut-off distance of 10 Å was used to real-space Ewald interactions. Van der Waals interacts with the same value. The LINCS algorithm [22] was applied to constrain bonds lengths of hydrogen atoms. Leap-frog algorithm [23] was accompanied by a timestep of 1 fs (Fig. 1).

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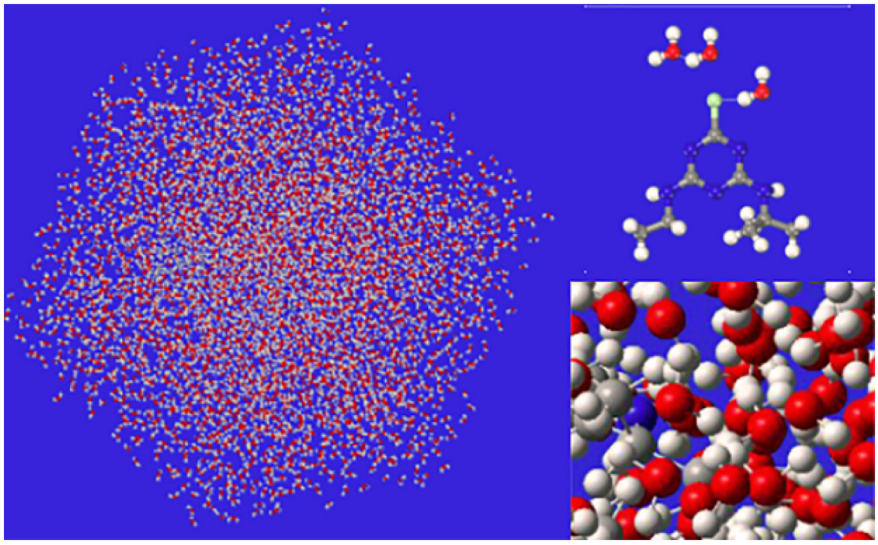

Fig. 1. Molecular structure of atrazine and snapshot of the simulation box.

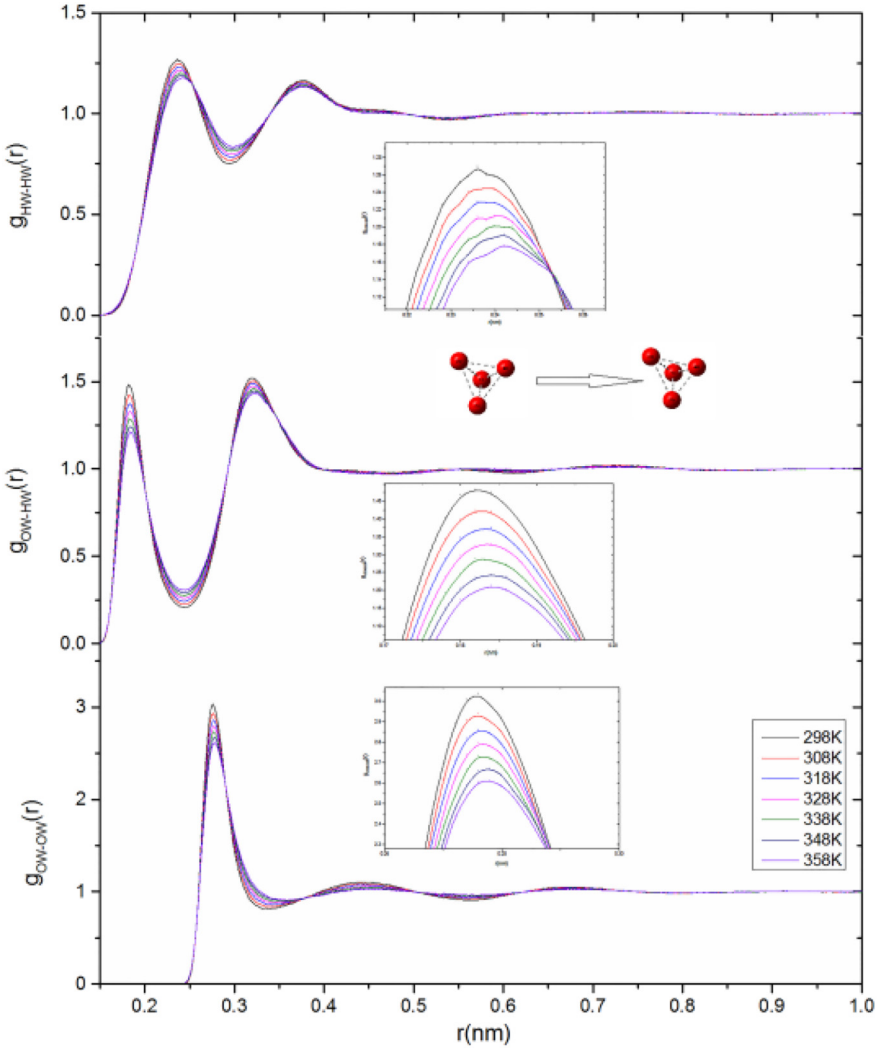

Fig. 2. Radial distribution functions of atrazine solution as a function of temperature. The difference is: $H_w - H_w{\cdot}H_w - O_w{\cdot}O_w - O_w$. The inset images are the first peaks of the functions.