MOLECULAR DYNAMICS SIMULATION ON THE ADSORPTION BEHAVIOUR OF IBUPROFEN ONTO POLYETHYLENE MICROPLASTIC

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By

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ABSTRACT

Microplastics and pharmaceuticals have long been identified as water pollutants. The combination of the MPs' size and physicochemical properties results in particle dispersion and distribution. In addition, microplastics have been proven to transport pollutants including pharmaceutical compounds. If the pharmaceutical pollutants, specifically ibuprofen (IB), can be absorbed by the polyethylene microplastics (PE MP), the combined pollutants might create unknown effects. A lot of studies have been conducted on the effect of interaction between pharmaceuticals and microplastics which includes stunted growth and major health problems for humans, plants and animals. Therefore, this project was conducted to investigate the interaction of IB and PE MP. The first objective of this project was to validate the adsorption parameters of IB onto PE microplastics empirically. The second objective was to simulate the adsorptive molecular properties of IB onto PE MP. In this study, characterization and batch adsorption experiments of IB and PE MP were conducted to investigate the effect of different parameters such as contact time, pH, IB concentration, PE MP concentration and temperature on the adsorption process. In addition, molecular dynamics (MD) simulation was also conducted to study the adsorption of IB onto PE MP at the molecular level. It was found that the adsorption of IB onto PE MP reached a state of a plateau at 32 h. The kinetics model showed a good regression, (R^2=0.9856) by Elovich models, followed by Pseudo-Second Order (R^2=0.9824), Intraparticle Diffusion (R^2=0.9331) and Pseudo-First Order (R^2=0.8946). For the effect of pH, the results showed that as the pH was increased, both PE MP adsorption capacity and IB removal decreased. For the effect of PE MP concentration, as more PE MP was administered into the system, the IB removal was increased accompanied by a decrease in PE MP adsorption capacity. The effect of IB concentration, on the other hand, showed an increase in the PE MP adsorption capacity and a decrease in IB removal as the IB concentration was increased. The isotherms model showed a good regression, (R^2=0.9671) by Temkin models, followed by Dubinin-Raduskevich (R^2=0.9194), Freundlich (R^2=0.9177) and Langmuir (R^2=0.9173). The models showed that the adsorption of IB onto the PE MP was more likely by chemical adsorption and can be either a single or multiple-layer adsorption process. The MD result was extracted and showed a stable result as the energy and temperature deviations obtained were within 10 %. It was also found that the non-bond interactions have largely occurred in the adsorption of IB onto PE. Finally, by comparing the result of the effect of contact time with the simulation, it was found that the patterns exhibited were similar.