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DATA-DRIVEN INSIGHTS INTO PARTIAL MOLAR VOLUMES AND WATER-IN-OIL DROPLET COALESCENCE

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ABSTRACT

In recent years, data mining techniques have become indispensable for extracting valuable information from complex molecular simulations of colloidal and interfacial systems. This work utilizes these techniques to probe partial molar volumes (PMVs) and explore water-in-oil droplet coalescence using molecular dynamics (MD) simulations.

Examining PMVs provides important insights into structural analyses and molecular interactions in multi-component systems. However, traditional ways of calculating PMVs are time consuming and involve complex procedures. To overcome this challenge, a novel PMV calculation method was developed in our work by employing linear regression. This method uses systematic data sampling from standard MD trajectories, where compositions remain unchanged throughout the simulation. It achieved deviations as low as 1.18% compared to experimental data. Validation on two systems showed an average deviations of 6.19 cm^3/mol for mesitylene and 7.80 cm^3/mol for isopropanol. The method was then applied to investigate systems involving asphaltene, organic solvents, and chemical inhibitors, with violanthrone-79 (VO-79) used as a proxy for asphaltene. It was found that adding chemical inhibitors to systems containing VO-79 and solvents led to a decrease in the PMV value, suggesting a reduced Hildebrand solubility parameter and enhanced solubility with increasing amounts of chemical inhibitors.

In addition to PMVs, disentangling behaviors of different substances in multi-component systems allow us to capture the effects of solution environments. For instance, extracting the growing path of water-in-oil droplets can help us understand the effects of solvents and solutes on water emulsion stabilities. In our work, an in-house tool was developed to enable automated tracking of droplet coalescences in triple-component systems consisting of proxy asphaltene, organic solvent, and water. This tool extracts and quantifies water molecular behaviors from the high-dimensional space of simulation trajectories. It was found that the growth of water droplets is dominated by the largest droplet acting as the nucleus site. A nonmonotonic trend in the stacking of VO-79 molecules with increasing droplet size was observed, driven by the competing effects of aggregation and adsorption.

The above findings highlight the utility of data mining techniques in analyzing complex molecular systems. The methods developed can be applied to various systems in the food, cosmetic, and petroleum industries, enriching our understanding of molecular interactions and collective behaviors in colloidal and interfacial systems.