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Surface Tension and Bulk Density of Ammonium Nitrate Solutions: A Molecular Dynamics Study

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Abstract : Ammonium nitrate (NH_4NO_3, AN) is commonly used as the main component of AN emulsion and fuel oil (ANFO) explosives, that use extensively in civilian and mining operations for underground development and tunneling applications. The emulsion formulation and wettability of AN prills, which affect the physical stability and detonation of ANFO, highly depend on the surface tension, density, viscosity of the used liquid. Therefore, for engineering applications of this material, the determination of density and surface tension of concentrated aqueous solutions of AN is essential. The molecular dynamics (MD) simulation method have been used to investigate the density and the surface tension of high concentrated ammonium nitrate solutions; up to its solubility limit in water. Non-polarisable models for water and ions have carried out the simulations, and the electronic continuum correction model (ECC) uses a scaling of the charges of the ions to apply the polarisation implicitly into the non-polarisable model. The results of calculated density and the surface tension of the solutions have been compared to available experimental values. Our MD simulations show that the non-polarisable model with full-charge ions overestimates the experimental results while the reduce-charge model for the ions fits very well with the experimental data. Ions in the solutions show repulsion from the interface using the non-polarisable force fields. However, when charges of the ions in the original model are scaled in line with the scaling factor of the ECC model, the ions create a double ionic layer near the interface by the migration of anions toward the interface while cations stay in the bulk of the solutions. Similar ions orientations near the interface were observed when polarisable models were used in simulations. In conclusion, applying the ECC model to the non-polarisable force field yields the density and surface tension of the AN solutions with high accuracy in comparison to the experimental measurements.

Keywords : ammonium nitrate, electronic continuum correction, non-polarisable force field, surface tension
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