Clean Water: Analysis of Interfacial Tension Anionic Surfactant Effects on Evaporative Rate, Molecular Similarity Analysis, and Oil Spill Modeling

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Increasing pollution in large water bodies poses a significant threat to the availability of safe drinking water. As pollutants (surfactants) decrease interfacial tension, when a contaminant is introduced to a body of water, the surface tension is almost immediately compromised. This research analyzes the interfacial tension of polluted systems through three different angles: 1) Surface tension and evaporation rate: This experimentation section investigated the relationship between changes in the surfactant concentration in pacific ocean saltwater (POSW) and its surface tension (and associated evaporation rate). Results reveal that both surface tension and evaporation rates decrease as surfactant concentration increases until reaching the critical micelle concentration (CMC) point. The findings highlight the complexity of surfactant effects on water dynamics and suggest potential downstream implications for the hydrological cycle. 2) Oil spill diffusion model: Using cellular automata, an oil spill derived from the National Oceanic Atmospheric Administration (NOAA) was modeled by creating a mutate and search algorithm that picks a random rule, randomly mutating several times until it closely matches the 2D NOAA oil spill. 3) Molecular similarity analysis: Using QSAR analysis, molecular similarity and boiling point constant value were correlated. As the molecular structural similarity of a surfactant increases, the range of boiling point constant value decreases, and the range of the interfacial tension of each compound also decreases.