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## Assessment of colloidal gas aphrons stability for soil remediation: experiments and molecular dynamics simulations

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Colloidal gas aphrons (CGAs) are layered microbubbles with sizes between 10 and 100  $\mu\text{m}$  and a gas fraction of 40-70% [1]. CGAs can enhance contaminant removal from soil and aquifers due to their low environmental impact, high surface area, versatility, and stability as an alternative to surfactant solutions and conventional foams. Hence, it can physically remove organic contaminants and heavy metals and deliver chemical additives, microorganisms, and oxygen to polluted zones [2].

Prior studies have investigated CGAs' stability and the effect of surfactant-polymer concentrations, salinity, and the impact of stirring rate and time were previously studied at the bubble scale [3], [4]. However, a complete understanding of CGAs' stability and the effect of various physicochemical processes on stability at the interface, specifically at the molecular level with and without contaminants, still needs to be made clear. In addition, understanding the relationship between the interaction of molecules and bubbles requires further elucidation.

This study aims to address the knowledge gap by performing experimental research on the stability of CGAs at a bubble scale and the impact of various surfactant-polymer concentrations. Additionally, to numerically investigate the interactions between CGA components at the atomic level via molecular dynamics (MD) simulations.

The experimental process involves generating CGAs using a base fluid designed by a specific concentration of xanthan gum (XG) polymer in demineralized water by mixing with a digital overhead stirrer at 8000 RPM for 20 minutes [5]. Then, a concentration of sodium dodecyl sulfate (SDS), a surfactant, was added to the base fluid and mixed at the same rotation speed for two minutes to generate CGAs. We performed CGAs with various concentrations for the surfactant (1–10 CMC) and polymer (1000–10,000 ppm). CGAs' bubble size variation was investigated using a Zeiss digital microscope with a charge-coupled device (CCD) camera [6]. The images were analyzed using "ImageJ" software to determine bubble size distribution as a function of time. MD simulations are conducted based on similar surfactants, polymer segments, and water fractions using the GROMACS software.

As a result, the concentration of polymer and surfactant are the main factors affecting the stability of CGAs. At polymer concentrations starting from 6000 ppm, optimal stability and a decrease in bubble size are observed. As the polymer concentration increases, the effect of surfactant concentration on the size distribution of CGA bubbles decreases. As polymer concentration increases, smaller bubbles result from decreased air penetration caused by increased base fluid viscosity. Moreover, MD simulations revealed the intermolecular interactions among polymer segments, surfactants, and water molecules and the detailed interfacial structure. This study concluded that selecting the optimal concentrations of the polymer and surfactant is necessary based on the results of bubble stability testing and MD simulations.

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### References

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