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# Molecular Engineering of Natural Gas Hydrate Anti-Agglomerants: Decoupling Free Energy-Entropy Synergy Mechanisms through Integrated Experimental and Simulation Approaches

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***Annotation.*** *The molecular design of hydrate anti-agglomerants (AAs) requires fundamental breakthroughs in interfacial thermodynamic/kinetic regulation mechanisms. This study pioneers a dual experimental-simulation platform combining rocking cell measurements with steered molecular dynamics to unravel free energy-entropy coupling effects governing hydrate aggregation. Results demonstrate that high-performance AA establishes 3D spatial barriers through entropy-driven chain conformation dynamics while maintaining thermodynamic non-spontaneity. Surface density optimization amplifies energy barriers 20-fold via molecular packing transitions, achieving critical barrier positioning at Z=2.76 nm. These findings establish molecular interface engineering principles for next-generation AAs combining rigid anchoring motifs with entropy-elastic chain architectures.*

***Keywords:*** *hydrate flow assurance, anti-agglomeration mechanism, molecular interface engineering, free energy landscape, conformation entropy.*

Anti-agglomerants (AAs) have been recognized as an effective method for gas hydrate risk management in oil and gas pipelines [1]. The development of AAs is undergoing a paradigm shift from empirical screening to molecular engineering design,necessitating fundamental understanding of their action mechanisms at thermodynamic/kinetic levels and discovery of precise virtual evaluation criteria. The transition from empirical AA screening to molecular design paradigms demands quantitative understanding of interfacial energy-entropy compensation mechanisms [2]. Current evaluation systems predominantly rely on macroscopic performance indices [3], lacking molecular-level resolution of aggregation pathways.

In this study, thermodynamic quantification via high-pressure rocking apparatus measuring torque reduction and induction time under 80 bar/4°C. Free energy profiling using umbrella sampling with 330 ns simulations. Conformation entropy analysis through principal component analysis of AA monolayer fluctuations. Experimental data revealed performance hierarchy of AAs, correlating with molecular interfacial occupancy. Potential of mean force (PMF) analysis identified two critical barriers. High-density CDA monolayers exhibited compressed chain persistence length, generating dynamic steric shields through entropic spring effects. This multi-scale methodology provides a roadmap for designing entropy-enhanced AAs.

## References

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