

Critical Analysis of Clathrate Hydrate Formation, Growth and Dissociation Models

N.A. Shostak 

Kuban State University, 149 Stavropol'skaya str., Krasnodar, 350040, Russia

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Corresponding author: [N.A. Shostak](mailto:N.A.Shostak@kubsu.ru)

Abstract. The study presents a comprehensive analysis of the existing physical and mathematical models describing the formation, growth, and dissociation of clathrate hydrates—complex condensed systems exhibiting hierarchical phase transitions across multiple spatial and temporal scales. The review systematizes thermodynamic, kinetic, molecular-dynamic, and hybrid approaches, emphasizing their theoretical foundations, applicability, and limitations. It is shown that despite decades of progress, existing models remain fragmented across scales and mechanisms. The absence of a unified description capable of linking molecular parameters, interparticle potentials, and macroscopic kinetic and thermobaric properties limits the predictability of hydrate behavior under both natural and technological conditions. The analysis is based on the comparative assessment of governing equations, physical assumptions, and scalability criteria of different model classes. The work substantiates the necessity of developing an integrative physical–mathematical framework combining equilibrium thermodynamics, transport phenomena, and non-equilibrium kinetics to adequately describe hydrate systems across formation and dissociation cycles.

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View Table of Contents: <https://reviewsamt.com/issues>

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