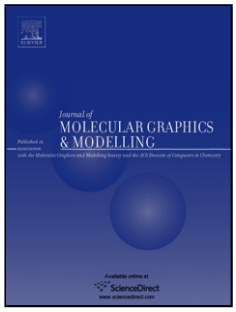

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A molecular dynamic study on the dissociation mechanism of SI methane hydrate in inorganic salt aqueous solutions

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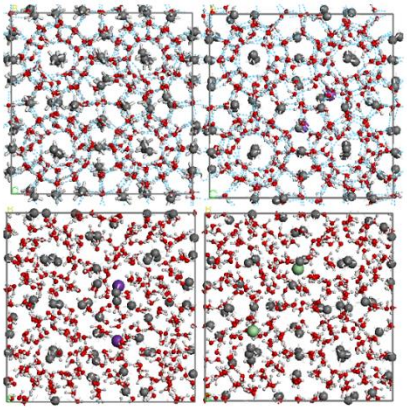
Graphical abstract



Highlights

- A liquid film generates during hydrate dissociation, and delays the dissociation.
- The hydrate dissociation rate increases with increasing concentrations of KCl and $CaCl_2$, but not obviously with NaCl.
- The liquid film is most compact in NaCl solutions, followed by $CaCl_2$, and the least compact in KCl solutions.
- The decomposing ability of the ions follows the sequence of Ca^{2+}>$2K^+$>$2Cl^-$>$2Na^+$. The coexistence of cations and anions weakens their decomposing effect on hydrate.

Abstract: Gas hydrate is not only a potential energy resource, but also almost the biggest challenge in oil/gas flow assurance. Inorganic salts such as NaCl, KCl and $CaCl_2$ are widely used as the thermodynamic inhibitor to reduce the risk caused by hydrate formation. However, the inhibition mechanism is still unclear. Therefore, molecular dynamic (MD) simulation was performed to study the dissociation of structure I (SI) methane hydrate in existence of inorganic salt aqueous solution on a micro-scale. The simulation results showed that, the dissociation became stagnant due to the presence of liquid film formed by the decomposed water molecules, and more inorganic ions could shorten the stagnation-time. The diffusion coefficients of ions and water molecules were the largest in KCl system. The structures of ion/H_2O and H_2O/ H_2O were the most compact in hydrate/NaCl system. The ionic ability to decompose hydrate cells followed the sequence of: Ca^{2+} >$2K^+$ >$2Cl^-$ >$2Na^+$.