Influence of N_2 micro-nanobubbles (MNBs) on the nucleation behavior of CO_2 hydrate as revealed by molecular dynamics simulation

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Small bubbles called micro-nano bubbles (MNBs) are closely associated with the nucleation and formation of gas hydrates. MNBs can be generated artificially or naturally when initial gas hydrates are dissociated. MNBs are known to facilitate the faster hydrate nucleation, even when the components of MNBs are incompatible with the guest types of the gas hydrates. Nevertheless, the precise nature and exact role of MNBs have been rarely reported due to the extremely small size of MNBs and the complexity of hydrate nucleation mechanism. In this study, molecular dynamics (MD) simulations were used to investigate how MNBs affect the hydrate nucleation and formation, especially when there was a mismatch in the gas components between gas hydrates and MNBs, e.g) CO_2 vs N_2. We observed that N_2 bubbles could facilitate CO_2 hydrate formation by (1) inducing heterogeneous distributions of CO_2 in solution, (2) providing additional nucleation sites, and (3) earlier formation of small (5^{12}) cages due to extra N_2 molecules in solution. Our study will contribute to a better understanding of MNB effect on the hydrate nucleation mechanism and the further hydrate formation.