



## Numerical Study of Formation Mechanisms of CO<sub>2</sub> Hydrate

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Recently, methane gas extraction from gas hydrate deposits has been widely discussed and studied. There is an advance production strategy by using CO<sub>2</sub> injection. There are several attractive features of this novel technique. Injecting CO<sub>2</sub> into a gas hydrate deposit causes the replacement between CO<sub>2</sub> molecules and CH<sub>4</sub> molecules inside the hydrate crystal structure. The reaction leads to the CO<sub>2</sub> hydrate formation and CH<sub>4</sub> gas release. The free CH<sub>4</sub> gas can be produced by depressurization process. Because of the formation of CO<sub>2</sub> hydrate, we also benefit from the CO<sub>2</sub> sequestration. However, the mechanisms of CO<sub>2</sub> hydrate formation play essential roles in this operation. Numerical simulation can be a convenient tool to study gas hydrate production. Therefore, it is crucial to establish a reliable module of CO<sub>2</sub> hydrate reaction. The propose of this study is to determine the thermal dynamic parameters of CO<sub>2</sub> hydrate reaction, for a simulation use, depending on a laboratory experiment data.

In this study, a numerical model used for CMG-STARs reservoir simulator is set up according to a laboratory experiment of CO<sub>2</sub> hydrate formation. The experiment was done by a research team from National Taiwan University of Science and Technology (NTUST). The numerical grids are designed to imitate the real equipment that had been used in the experiment. To observe the influence of different parameters which are affective to the reaction, there are series of sensitive analyses of flow properties, hydrate reaction parameters, and thermal properties. Afterward, a CO<sub>2</sub> hydrate reaction module is built according to the history matching of the temperature and pressure data from an experimental CO<sub>2</sub> hydrate formation research. Then, the hydrate saturation result is verified by an analytical solution.

The major findings in this study are: (1) A CO<sub>2</sub> hydrate reaction module is established according to the experimental CO<sub>2</sub> hydrate formation data. (2) The reaction parameters in the module such as activation energy and reaction equilibrium constant are the key elements of the CO<sub>2</sub> hydrate phase behaviors. The phase changes process inside the porous media controls the molecular exchange with CH<sub>4</sub> hydrate. (3) The thermal properties of the porous media can influence the amount of formation and dissociation of CO<sub>2</sub> hydrate. (4) Both results of experiment and simulation work show similar reaction that CO<sub>2</sub> hydrate formation begins at the interface between water and gas. This indicates that this study successfully establishes a CO<sub>2</sub> hydrate module which is capable of simulating the actual CO<sub>2</sub> hydrate reactions of laboratory experiment.