

# A COMSOL Multiphysics®-based Model for Simulation of Methane-Hydrate Dissociation By Injection of Superheated Carbon Dioxide

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## Abstract

### Introduction

Carbon dioxide exchange with methane in the clathrate structure has been shown to be beneficial for the production of natural gas from hydrate-bearing sediments in many lab-scale experiments and in a recent field test below Arctic permafrost. The method is environmentally attractive due to the potential formation of CO<sub>2</sub>-hydrate in the reservoir, leading to the sequestration of carbon dioxide in deep layers of oceanic sediments. The natural gas obtained by this method features as an emission-free fossil fuel to replace conventional coal resources for power generation.

### Use of COMSOL Multiphysics®

In the present study, we used COMSOL Multiphysics® to model the lab-scale experiments of hot carbon dioxide injection into a pressure vessel containing a mixture of methane-hydrate and quartz sand. The experiments were performed at different temperatures and pressures to examine various rates of methane hydrate dissociation at such conditions. In this respect, the model aimed to estimate the effective dissociation rate of gas-hydrate by matching the simulation results with the results from the experiments. In addition to the solution of mass and energy balance, the model assumes the following reactions between the substances:

CH<sub>4</sub>-hydrate  $\rightleftharpoons$  CH<sub>4</sub>(aqueous) + H<sub>2</sub>O (at p-T conditions where hydrate is stable)

CO<sub>2</sub>(aqueous) + H<sub>2</sub>O  $\rightleftharpoons$  CO<sub>2</sub>-hydrate (at p-T conditions where hydrate is stable)

CO<sub>2</sub>(aqueous)  $\rightleftharpoons$  CO<sub>2</sub>(gas)

CH<sub>4</sub>(aqueous)  $\rightleftharpoons$  CH<sub>4</sub>(gas)

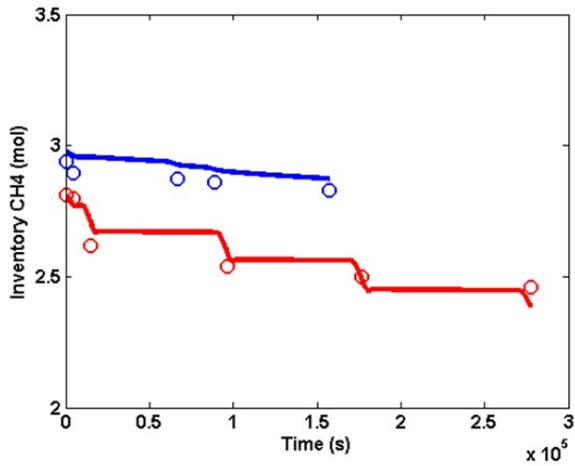
CH<sub>4</sub>-hydrate  $\Rightarrow$  CH<sub>4</sub>(aqueous) + H<sub>2</sub>O (at p-T conditions where hydrate is dissociating)

CO<sub>2</sub>-hydrate  $\Rightarrow$  CO<sub>2</sub>(aqueous) + H<sub>2</sub>O (at p-T conditions where hydrate is dissociating)

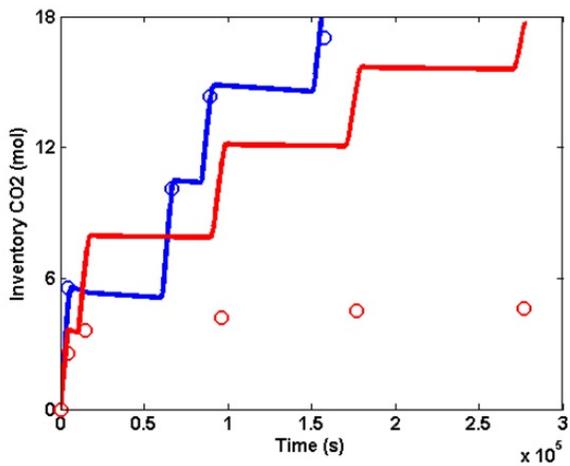
The model considers the experimental pressure vessel as a continuous-stirred tank reactor (CSTR) where transport limitation effects are assumed to be included into the effective reaction rates. Simulation results indicate that with a marginal offset the model was able to simulate different experimental scenarios (Fig. 1). The discrepancies between some of the modeling results and those from the experiments were related to the transport limitation effects that were not possible to tackle with current setup (Fig. 2). To achieve a complete reservoir model at field-

scales, a two-phase fluid flow model was developed (Fig. 3) and will be merged to the current CSTR model.

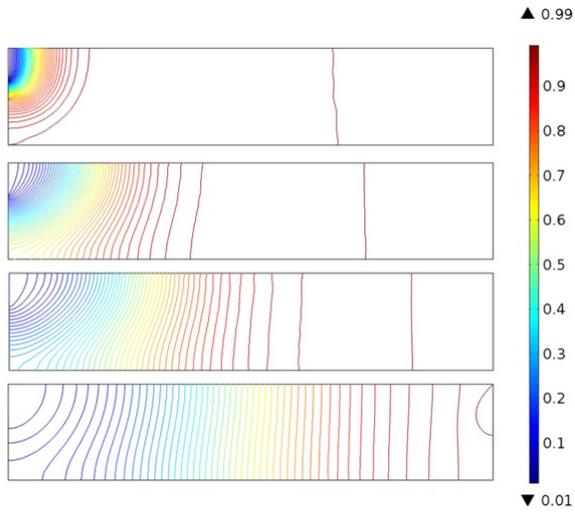
## Figures used in the abstract



**Figure 1:** Total Methane in the system for experiment 1 (2°C / 13 Mpa) and experiment 3 (10°C / 13 MPa) shown by points. Modeling results are sketched by a line.



**Figure 2:** Total CO2 in the system for experiment 1 (2°C / 13 Mpa) and experiment 3 (10°C / 13 MPa) shown by points. Modeling results are sketched by a line.



**Figure 3:** Saturation of water phase in the system replaced by continuous injection of CO<sub>2</sub>. CO<sub>2</sub> injected from top-left and water discharges from top-right of the medium.