A COMSOL-based Model for Simulation of Methane-Hydrate Dissociation by the Injection of Superheated Carbon Dioxide

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Introduction: Immense amounts of methane are stored as gas-hydrate deposits in deep layers of oceanic sediments. This has raised considerable interest to develop strategies for producing natural gas from marine hydrates. One potential production strategy is the injection of supercritical CO_2 into methane hydrate-bearing sand layers to release the CH_4 as a gas and sequester the CO_2 as hydrate (Fig. 1). The method is environmentally attractive and may reduce potential hazards of slope instabilities.

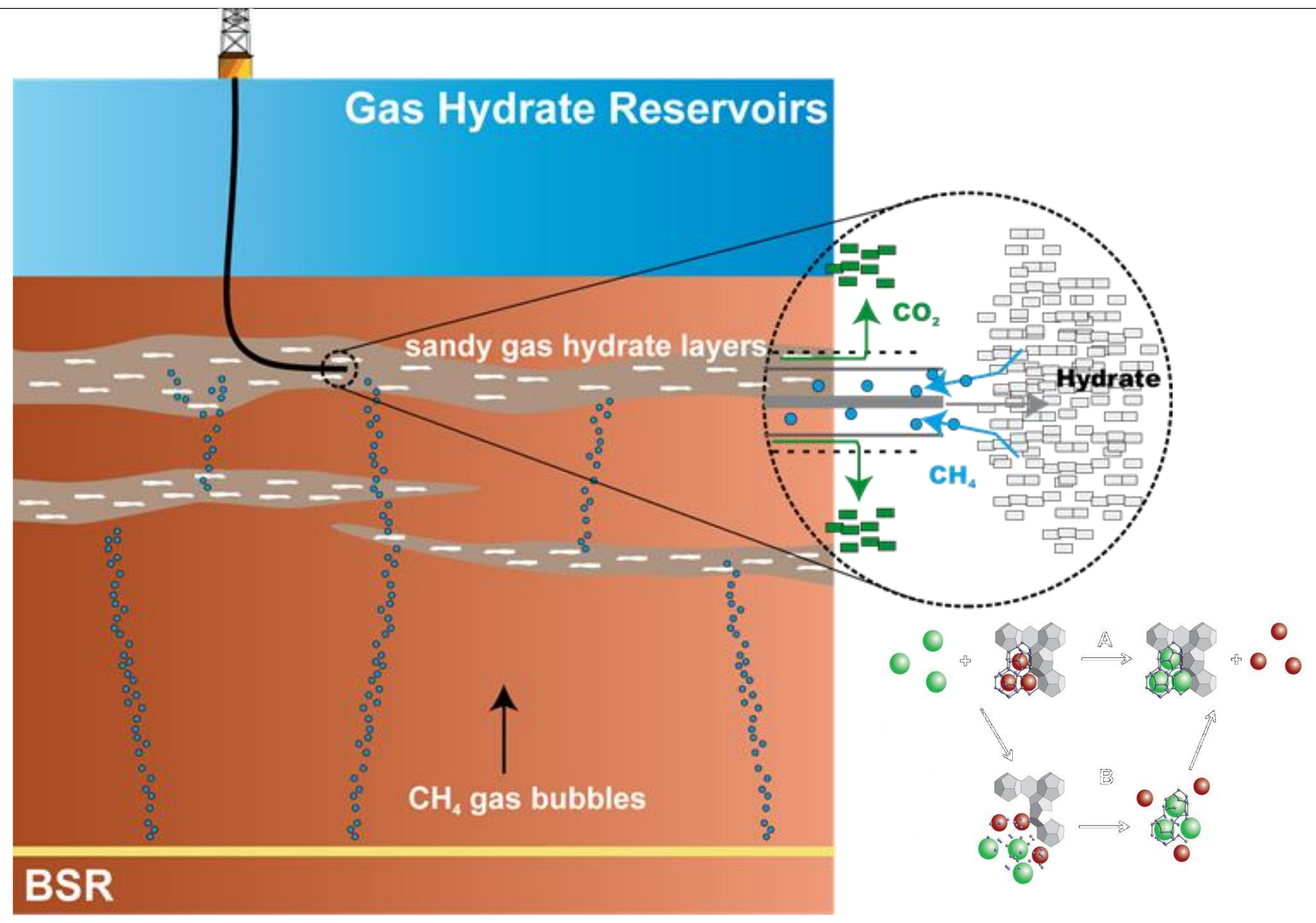

Figure 1. schematic view of Methane-hydrate exploitation by injection of CO_2

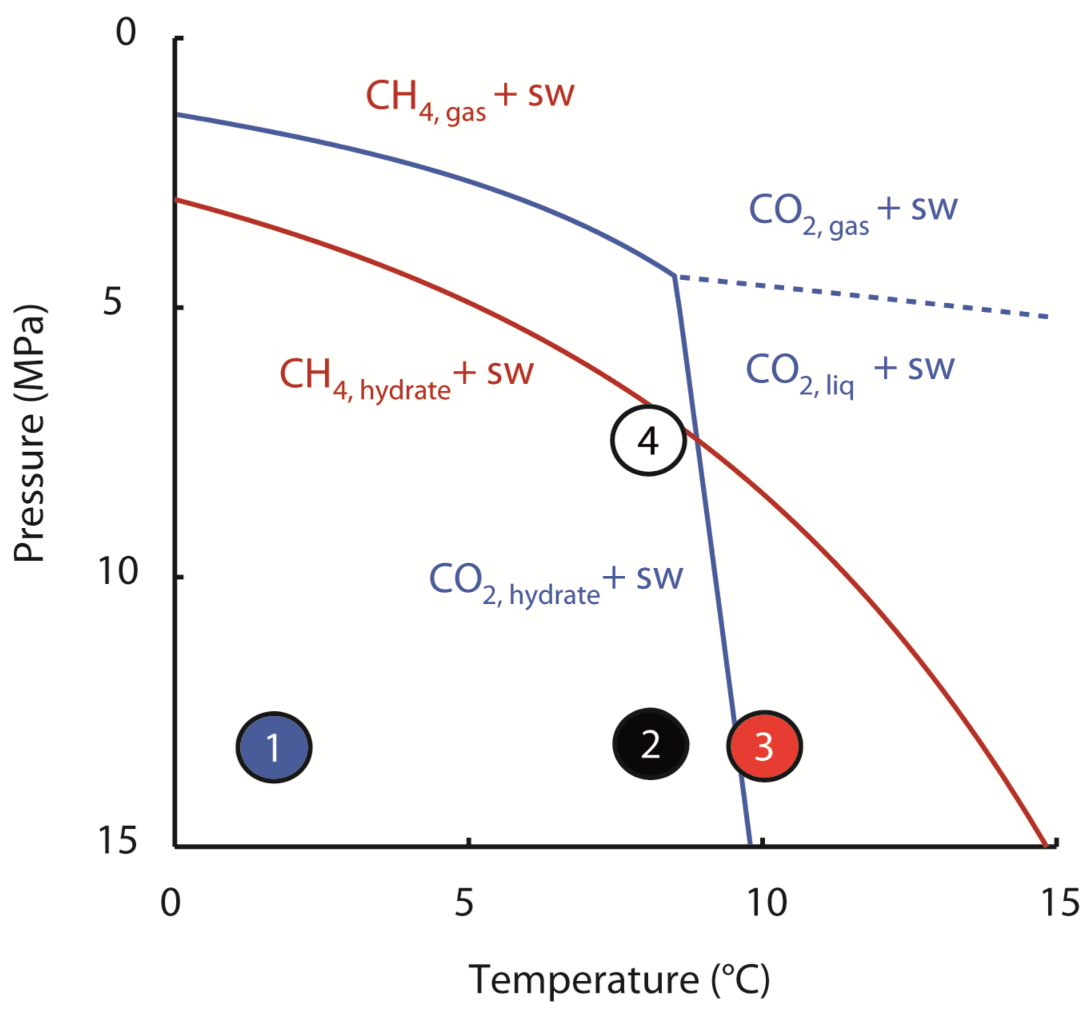

Figure 2. p/T conditions in the experiments (Deusner et al, 2011)

Experimental Setups: We used COMSOL Multiphysics® to model the lab-scale experiments in which hot (supercritical) carbon dioxide was injected 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 (Fig. 2) .

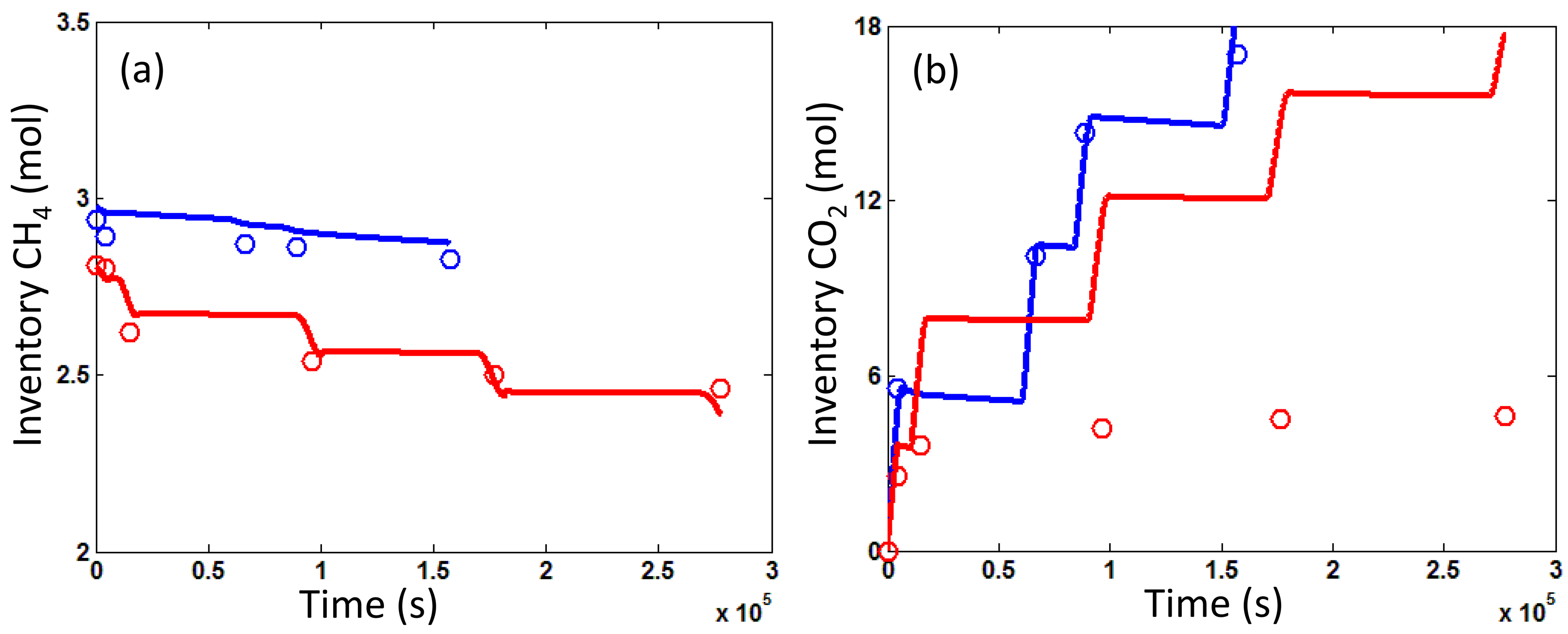

Figure 3. (a) Total Methane and (b) total CO_2 in the system from experiment 1 (blue) and experiment 3 (red) are shown by points. The CSTR-based modeling results are illustrated by the lines.

Use of COMSOL Multiphysics®: The first 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 production rate of methane from gas-hydrate. The model is used to estimate the effective dissociation rate of gas-hydrate by fitting the simulation results to the experimental data (Figs. 3). In addition to the solution of mass transport and energy balance, the model considers the following reactions between the substances:

Hydrate dissolution/formation (under/oversaturation at stable p/T conditions):

- **CH_4-hydrate ←→ $CH_{4,aq}$ + H_2O**
- **CO_2-hydrate ←→ $CO_{2,aq}$ + H_2O**

Gas dissolution / exsolution (under/oversaturation)

- **$CO_{2,aq}$ ←→ $CO_{2,gas}$**
- **$CH_{4,aq}$ ←→ $CH_{4,gas}$**

Hydrate dissociation (if not stable at p/T conditions):

- **CH_4-hydrate → $CH_{4,aq}$ + H_2O**
- **CO_2-hydrate → $CO_{2,aq}$+ H_2O**

Simulation results indicate that with a marginal offset the model was able to simulate some of the experimental scenarios (Fig. 3a). 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 the CSTR setup (Fig. 3b). To obtain a complete reservoir model at field-scales, a two-phase fluid flow model was developed (Fig. 4) and was merged to the CSTR model.

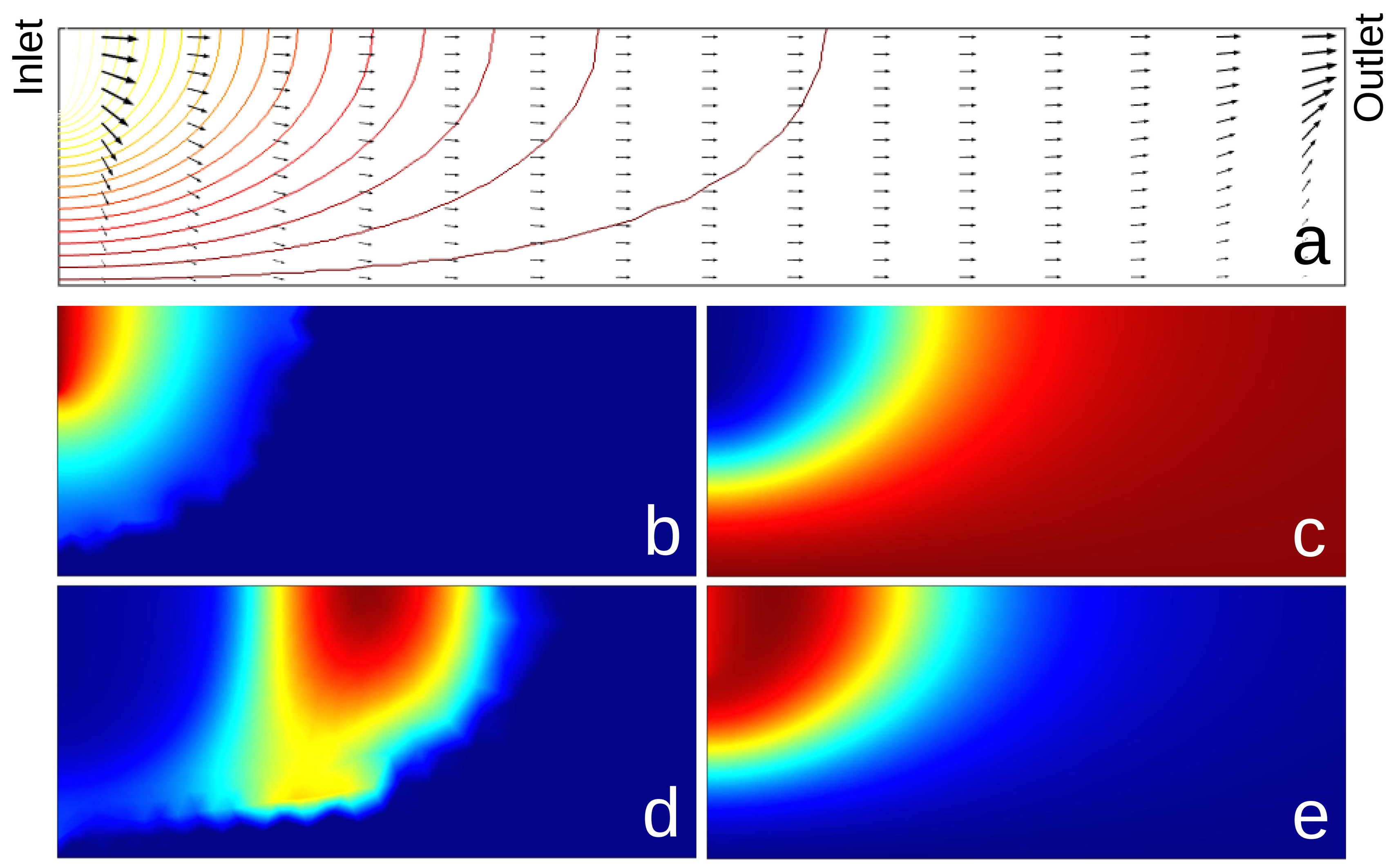

Figure 4. Modeling results of a 2D section of the cylindrical vessel: (a) Isothermal contours; (b) Injected CO_2 to the vessel; (c) Hydrate concentration; (d) released methane and (e) Hydrate dissociation rate. Note that except (a), the other plots illustrate only left half of the vessel. CO2 is injected from top-left inlet and outlet is located at top-right.

References:

C. Deusner , N. Bigalke, E. Kossel and M. Haeckel, Methane Production from Gas Hydrate Deposits through Injection of Supercritical CO_2, Energies 2012, 5, 2112-2140.

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