Modelling microbially enhanced coal-bed methane production: From batch experiments to a numerical model

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Key words: coal-bed methane, reactive transport, and microbiology

Introduction

Microbially enhanced coal-bed methane (MECBM) production is an innovative idea to stimulate biogenic coal-bed methane (CBM) production by providing nutrients to the native microbial community. However, little is known about the effects of microbes and nutrients on the CBM production in the subsurface. Through additional substrate for bacteria in the subsurface, a stimulation of bacteria and archaea happens, which leads to an increased methane production, see Figure 1. Experimental studies, performed at Montana State University (MSU), provide the basis for modeling MECBM production with two-phase multi-component transport processes using the numerical simulator DuMu$^{\mathrm{X}}$ [1]. Coal beds in the Powder River Basin (PRB), located in Montana

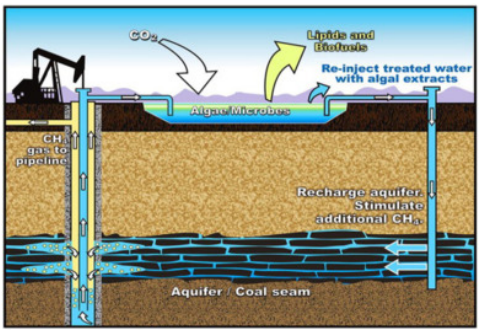

Figure 1: Schematic of MECBM production from coal. Water is pumped from the coal-bed to release the stored methane. [2] have shown that the CBM water can be used to cultivate algae and that adding algae cells or algal residues after lipid extraction can stimulate methane production from coal. Figure from [2].

and Wyoming, show methane production of primarily biogenic origin [3]. Methane production in such coal beds seems to be a continuous process and potentially the production rate as well as the volume of microbially produced methane can be increased [4]. Numerical modeling has proven to be a valuable and efficient tool to test hypotheses developed from experimental studies and to design new experimental setups.

Experimental studies

Multiple experimental studies have been performed at MSU regarding the stimulation of coal-to-methane conversion, the microbial community of coal-beds, as well as the effect of different types and concentrations of the added amendment [2, 5, 6]. These studies show, that amendments are able to stimulate coal-dependent methane production [2]. Additionally, the different microbial communities in coal-beds might have an influence on the methane production, while coal treatments for enhancing coal bioavailability can also have an effect [5]. The latest studies by Davis et al. show, that organic amendments increase the biogenic conversion of coal-to-methane. However the increase is not proportional to the amendment concentrations [6]. Therefore, adding small amounts of amendments increases the rate of biogenic methane production while also increasing the amount of totally produced methane to some extent. Davis et al. show that for an amendment concentration of 0.1 g/L, the amended coal systems produce more methane than the sum of methane production for the isolated "coal only" and "amendment only" systems. This suggest that there is an enhancement of the coal-to-methane conversion. The batch studies performed by Davis et al. provide the basis for the calibration of the reaction kinetics. Column experiments, including flow and transport, are currently conducted and evaluated and will provide more input for the numerical model.

Model concept, mathematical and numerical model

The first step in building the numerical model is the identification of the relevant processes, that can be described mathematically and parameterized accordingly. Therefore, the experimental evidence from the team at MSU and from literature is evaluated and a simplified conceptual model is set up. It consists of coal and biomass as solids, water and gas as fluids, amendment as substrate as well as hydrogen, carbon dioxide, acetate and methyl groups as intermediate products that are all dissolved in the fluids. The biomass is divided into two groups. One group consists of two types of bacteria converting amendment and/or coal to intermediates and the other group of three types of archaea using these intermediates to produce methane and carbon dioxide.

The numerical model is implemented in the numerical simulator DuMu$^{\mathrm{X}}$ [1]. All reactive and mass-transfer processes are accounted for by the mass balance equations for the components in Equation 1:

$$\sum_{\alpha}\left[\frac{\partial}{\partial t}\left(\phi\rho_{\mathrm{mol},\alpha}x_{\alpha}^{\kappa}S_{\alpha}\right)+\nabla\cdot\left(\rho_{\mathrm{mol},\alpha}x_{\alpha}^{\kappa}\mathbf{v}_{\alpha}\right)-\nabla\cdot\left(\rho_{\mathrm{mol},\alpha}\mathbf{D}_{\mathrm{pm},\alpha}^{\kappa}\nabla x_{\alpha}^{\kappa}\right)\right]=q^{\kappa},\ \alpha\in\{\mathrm{n};\mathrm{w}\}. \tag{1}$$

Here, t is time, ϕ porosity, $\rho_{\mathrm{mol},\alpha}$, S_{α}, and $\mathbf{v}_{\alpha}$ the molar density, saturation and the velocity of phase α respectively, x_{α}^{κ} the mole fraction of component κ and $\mathbf{D}_{\mathrm{pm},\alpha}$ is the dispersion tensor in phase α. q^{κ} is the source term of component κ due to biogeochemical reactions. The mass balances for the solid phases, namely "cc" as the for biomass convertible fraction of coal, two types of bacteria (ab, cb) and three types archaea (aa, ha, ma), consist only of a storage and source term as shown in Equation 2:

$$\frac{\partial}{\partial t}\left(\phi_{\varphi}\rho_{\varphi}\right)=q^{\varphi},\varphi\in\{\mathrm{cc};\mathrm{ab};\mathrm{cb};\mathrm{aa};\mathrm{ha};\mathrm{ma}\}. \tag{2}$$

Here, ϕ_{φ}, ρ_{φ} and q^{φ} are the volume fraction, mass density and source term due to biogeochemical reactions of the solid phase φ respectively. Microbial growth rates are implemented using Monod Kinetics, while the decay rate is considered to be a first order approximation. Component source and sink terms are calculated using biomass and component-dependent yield reaction terms for each microbial conversion. The calibrated model is then extended to column studies involving flow and reactive transport.

Calibration and Results

The first calibration is performed using methane production data from the batch experiments performed at MSU [6]. The results from two batch setups are used for calibration, while all other setups serve as validation. The amendment-dependent parameters are calibrated from a setup with glass beads, formation water and three amendment injections over time. Then the coal-dependent parameters are calibrated from a setup with just coal and formation water. These parameters are used to simulate all other variations with different coal, glass beads and amendment injection scenarios. The simulation of the column studies is set up according to the experimental column studies using the reaction kinetics and assumptions from the batch fits. Ad- and desorption are included in the model, and show to be ineffective due to the high water content and low pressure in the batch systems.

Results The batch simulation results show very good agreement with the experimental batch results. The general assumptions, the reaction kinetics and the considered microbiological pathways are validated. The simulation of the column studies behave as expected and show good agreement with the first experimental column setups. Biomass distribution, amendment consumption, intermediates, methane production and transport of all components are simulated successfully. Experimental data obtained with ^{13}C labeled substrate are expected to provide further insight into the reaction kinetics. These results show, that the numerical model is capable of capturing the relevant processes for MECBM. Reactive transport can be modeled and the model can be used to test hypotheses that are not easily tested using experiments.

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