Box-Size Numerical Modelling of Hydrogen Migration and Trapping: Testing bio-chemical sinks

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We introduced the usage of a box-size numerical model of miscible multiphase flow, with explicit advection and diffusion in both the liquid and gas phases, to model the migration and trapping of hydrogen in sedimentary basins in a previous communication (LINK - https://igiltd.com/news/modelling-hydrogen-migration-and-trapping-phase-1). Here, we demonstrate the usage of the box model to test the consumption-preservation of hydrogen in underground conditions of pressure and temperature that might be favorable –or not– for the development of microbial communities.

Microbial consumption of H_2 ("hydrogenotrophy") is the dominant process under anoxic subsurface conditions and is likely to be enhanced in H_2 reservoir formations (e.g. Thaysen et al., 2021). In porous media, microbes are embedded in a biofilms that cover minerals/sediment grains (Figure 1). Migrating from porewater, H_2 travels diffusively within the biofilm, and a variety of bacteria and archaea microbes are involved in its consumption, with the three most significant metabolic processes being: 1) hydrogenotrophic methanogenesis ($CO_2 + 4\ H_2 \rightarrow CH_4 + 4\ H_2O$); 2) sulphate reduction ($SO_4^{2-} + 5\ H_2 \rightarrow H_2S + 4\ H_2O$); and 3) acetogenesis ($CO_2 + 2H_2 \rightarrow CH_3COOH$) (e.g., Derya et al., 2015). Unless H_2 is sufficiently abundant, they compete for the H_2 substrate and the microbes able to live at the lowest H_2 concentration thresholds outcompete the other groups. Here we report on initial tests of multiphase H_2 migration with the consideration of microbial consumption of dissolved H_2, where the kinetic reaction of hydrogenotrophic methanogenesis is applied in a simplified form to the bulk representative element volume, without explicit consideration of the dynamics of (and within) the biofilm layer.

To simulate microbial growth, we follow the general assumption that growth rates are reasonably well reproduced by Monod kinetics (e.g., Thaysen et al., 2021):

$$\mu = \mu max \frac{[H2]}{Ks[H2]},$$

where μ is the specific growth rate, μ_{max} the maximum specific growth rate, [H2] the $H_{2(aq)}$ concentration, and Ks the half-saturation constant. The above equation implies that for this exercise we ignore the concentration of CO_2, assuming it is always available, and non-limiting in the reaction.

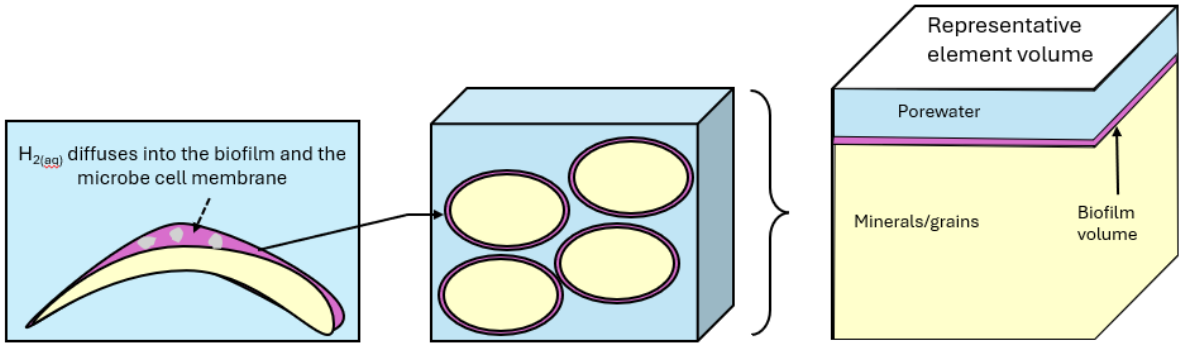

Figure 1. *Illustration of the coupled pore-scale model for methanogenic microbial activity in underground hydrogen storage (after Ebigbo, et al., 2013).*

The microbial biomass at any given time is represented by an exponential relationship controlled by the growth rate:

$$X(t) = X(0)e^{\mu t},$$

where X(t) is the biomass at a given time (t), X(0) the initial biomass and μ the specific growth rate.

The rate of substrate depletion (microbial sink) is thus given by the general formula:

$$\frac{d[H2]}{dt} = -\mu X(t)$$

In the models we assume coupling between the rate of H_2 consumption and microbial growth, depending on the concentration of dissolved H_2, and include a dependence of microbial growth on temperature. The models are initiated with a low concentration of microbial biomass in the system.

We test the microbial sinks in our high resolution advection-diffusion fluid flow box model (Fig. 2a) for two surface P-T conditions: (1) at 100 m depth with a temperature at top of the model of 20°C (Fig. 2b); and (2) at 1000 m depth with a top temperature of 46°C (Fig. 2c). The models run for approximately 10 yr, after which they reach an approximate steady state, as a result of the high generation rates and the simple reservoir-seal parametrization in this model setup. The relatively high H_2 input rates would represent, for example, an active serpentinization front or stimulated H_2 generation in the neighbourhood of the domain, providing the input boundary conditions.

At near surface conditions (low pressure), the solubility of the gas in the water is low, the saturation of the gas phase is high, and the models predict the development of trapped gas layer controlled by the retarding capability of the lower permeability layers (Fig. 2b). Due to the low H_2 saturation in the liquid phase, the predicted microbial sink is also very small. The low

temperatures in this model are also not optimal for a rapid microbial growth. In contrast, at higher pressure conditions, the models predict significantly higher H_2 dissolution, with only a small fraction of the H_2 in the gas phase, and significant microbial consumption.

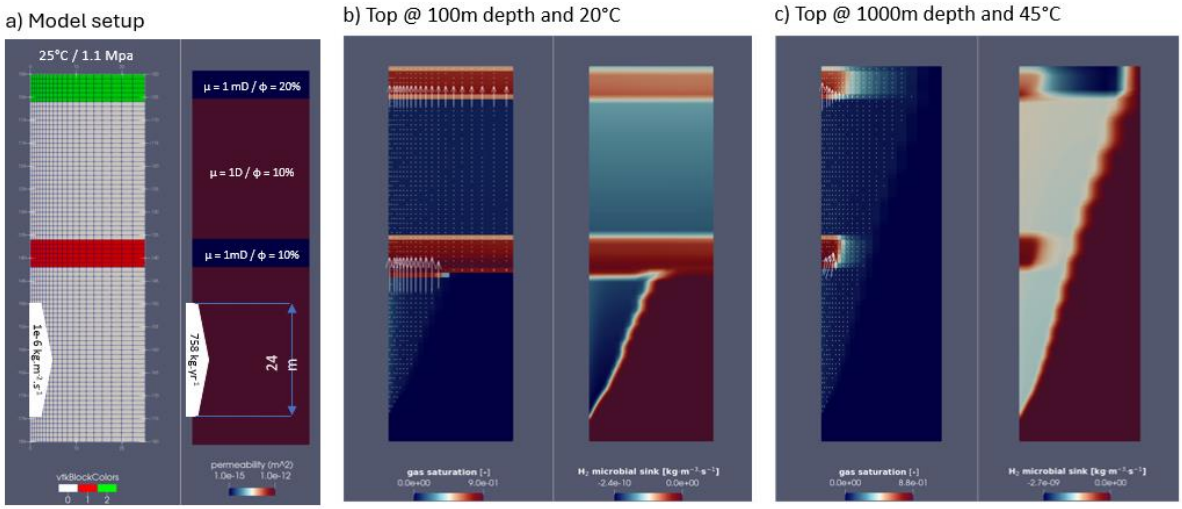

Fig. 2 – Box model predictions with varying P-T conditions for the development of microbial sinks. a) Setup of the high resolution box-model (see details in https://igiltd.com/news/modelling-hydrogen-migration-and-trapping-phase-1); b) Near surface conditions, with model top at 100 m (1.1MPa) depth and 20ºC. c) Top model at 1000m (10.1 MPa) depth and 45ºC.

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