Modelling Hydrogen Migration and Trapping – PHASE 1

Box-Size Numerical Modelling of Hydrogen Migration and Trapping: Testing the Geological Setting and Analogies with the Petroleum Systems

Integrated Geochemistry Interpretation (IGI Ltd)

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Hydrogen (H_2) and hydrogen-related fuels are regarded as one of the pillars of a decarbonized economy. In the Sustainable Development Scenario (net-zero emissions) forecast from the International Energy Agency (IEA), hydrogen usage should reach 13% of the global energy demand by 2070.

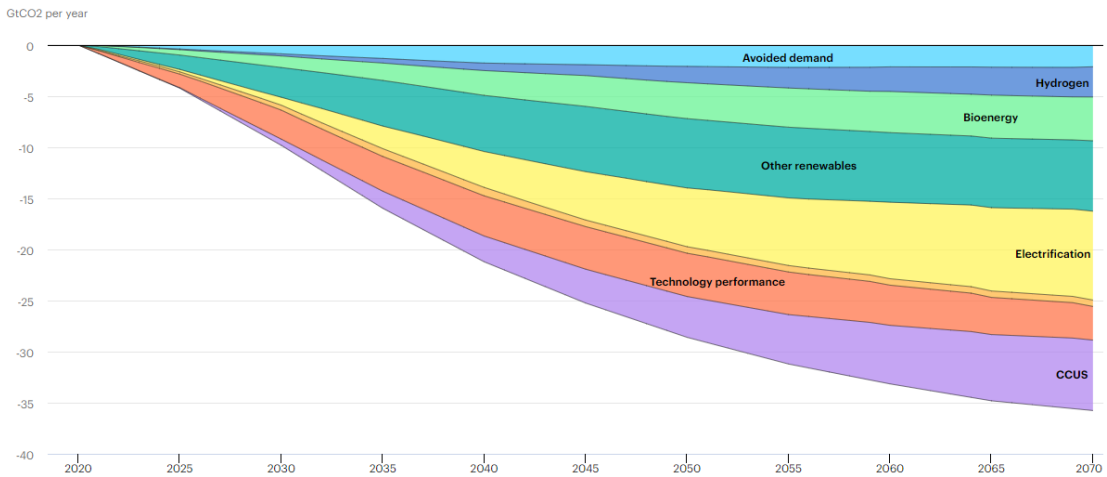

Figure 1. IEA, Global energy sector CO2 emissions reductions by measure in the Sustainable Development Scenario relative to the Stated Policies Scenario, IEA, Paris https://www.iea.org/data-and-statistics/charts/global-energy-sector-co2-emissions-reductions-by-measure-in-the-sustainable-development-scenario-relative-to-the-stated-policies-scenario, IEA. Licence: CC BY 4.0

At present, 95% of the hydrogen used in the industry originates from steam methane reforming (SMR), without the capture of the carbon monoxide produced in the process (Grey Hydrogen). Grey hydrogen is used mostly for ammonia production and refining. Planned technological developments to reduce the greenhouse gases associated with hydrogen production focus on carbon capture and storage (Blue Hydrogen), and the production from renewable energies powering water electrolysis (Green Hydrogen), which may also contribute to mitigate the renewables' energy curtailment.

In both cases, there are considerable costs involved in infrastructure for the injection and storage of gases (CO_2 or hydrogen), and in the case of green hydrogen, a large consumption of fresh water and energy in the hydrolysis process. The exploitation of natural hydrogen, if available at industrial-scale volumes, could therefore be a significant breakthrough for the energy transition efforts, and simultaneously contribute for the re-cycling of the knowledge and expertise available in oil & gas industry.

From 2022, IGI has been collaborating with the MARUM Center for Marine Environmental Sciences, of the University of Bremen (Germany), and the Natural Hydrogen Study Group (NHSG, UK), to address a number of outstanding problems related to the generation, migration and trapping of natural hydrogen, and thus contribute to the future exploration of this natural resource. Two communications have been recently presented by the consortium at a meeting in the Geological Society - Natural Hydrogen: A New Frontier for Energy and Science:

1. The Natural Hydrogen System: how success can be achieved through the system and play approach (*O. Jackson, S. Lawrence, A. Stocks, A. Barnicoat, I. Hutchinson)*

2. Box-Size Numerical Modelling of Hydrogen Migration and Trapping: Testing the Geological Setting and Analogies with the Petroleum Systems *(J. García-Pintado, M. Pérez-Gussinyé, T. Abreu Cunha, M. Nuzzo, S. Lawrence, O. Jackson, A. Stocks, A. Barnicoat, I. Hutchinson)*

In the first of these communications, the authors argue that the exploration of natural hydrogen can be guided by the play-concept, well developed in the oil & gas industry, and presented a number of study cases, representative of different tectonic settings. According to the authors, the most likely source of natural hydrogen in these settings is the serpentinization of mafic and ultra-mafic rocks, which then migrates through the sediments and/or along fracture systems through a mix of advection and diffusion processes, and eventually accumulates in traps, sealed by capillary contrasts.

In the second communication, we presented the results from a box-size numerical model of miscible multiphase flow to improve our current understanding on the main factors controlling the migration and trapping of hydrogen in sedimentary basins. We discuss below the main findings from this work-in-progress model, illustrated with a figures and videos.

The box model is 25 m * 80 m, very high resolution (1 m high cells with laterally varying width), with near surface conditions P-T conditions (100 m depth at the top with 25°C), an injection zone of 24 m along the bottom half of the model and two levels of lower permeability (1mD Vs 1D – Figure 2). Other premises of the model are:

- Two-phase flow with pure water and hydrogen (or methane) components
- Equations of state for density, viscosity & specific enthalpy
- Migration by advection in gas & liquid phase plus diffusion in the liquid phase
- Henry coefficient (temperature-dependent) controlling the equilibrium between the gas and dissolved mass fractions
- Corey (1954) effective-saturation dependent relative permeability; residual saturations are 0.15 for liquid and 0.05 for gas
- Van Genuchten (1980) capillary pressure-saturation
- The models run for 10yr, after which they tend to reach dynamic equilibrium

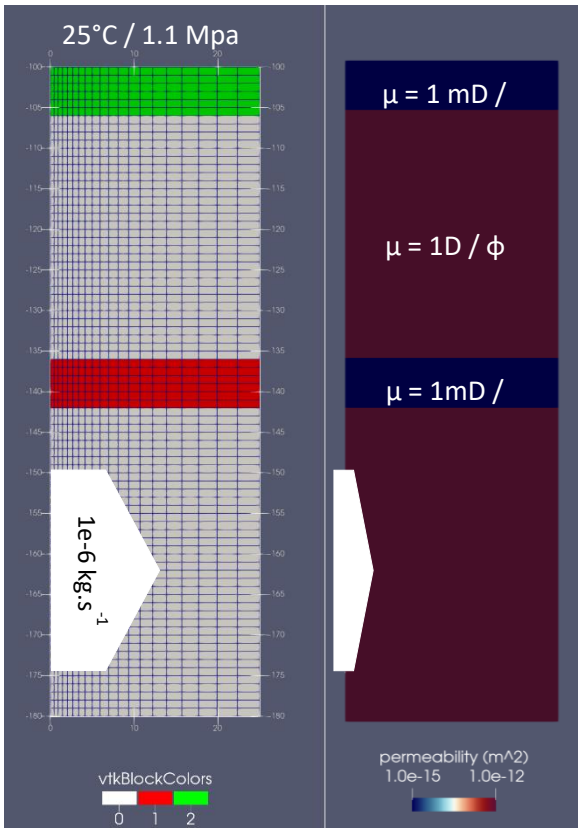

Figure 2. Model setup and parameterization

Initially, and at depth, the injected hydrogen is dissolved in the liquid phase (water) and migrates mainly as dissolved within the liquid phase. Further injection leads to free gas (increase in gas saturation), with a much faster upward migration controlled by the corresponding phase relative permeability. Towards the surface, decreasing pressures lead to further degassing, with a positive feedback on gas mobility. The relation between injection rates (hydrogen generation) and the development of a positive capillary pressure and dominance of the free trapped gas phase is controlled by the retarding capability of the lower permeability layers. These effects can be clearly observed in Video-1 [LINK], where we plot the most relevant parameters to follow the model predictions through time.

Video 1. Box model showing the migration and trapping of hydrogen (H_2) for the setup, boundary conditions and parameterization shown in Figure 2. The model runs over a 10 yr period, showing (from left to right): permeability (constant); total H_2 mass fraction (gas phase plus H_2 dissolved in the water); capillary pressure (pressure of the non-wetting phase minus the pressure of the wetting phase), with the velocities of the wetting phase; gas saturation (total gas ratio to porosity) with the velocities of the gas (arrow size reduced by a factor of 3 relative to the water velocities); liquid relative permeability; and gas relative permeability (ratio of effective permeability of a particular fluid at a particular saturation to absolute permeability of that fluid at total saturation).

The figure below corresponds to the near steady-state, or dynamic equilibrium reached after 10yr. Most of the gas is H_2, with minor H_2O (water vapour), while the mass fraction of H_2 in the liquid is very low (see numeric scale), due to its low solubility. The predicted storage for this particular model is of 40 kg of H_2 gas, at a mean density of ~1.8 kg.m^{-3} (~22 m^3 of gas), plus 2.7 kg of dissolved H_2. The low storage capacity in this model is partially controlled by the relatively high permeability of the seals (1 mD), but also by the low pressure, near surface conditions. In a similar experiment run for P-T conditions at 1 km depth the model predicts 115 kg of H_2 gas, at a mean density of ~6.85 kg.m^{-3} (~17 m^3 of gas), plus 20 kg of dissolved H_2.

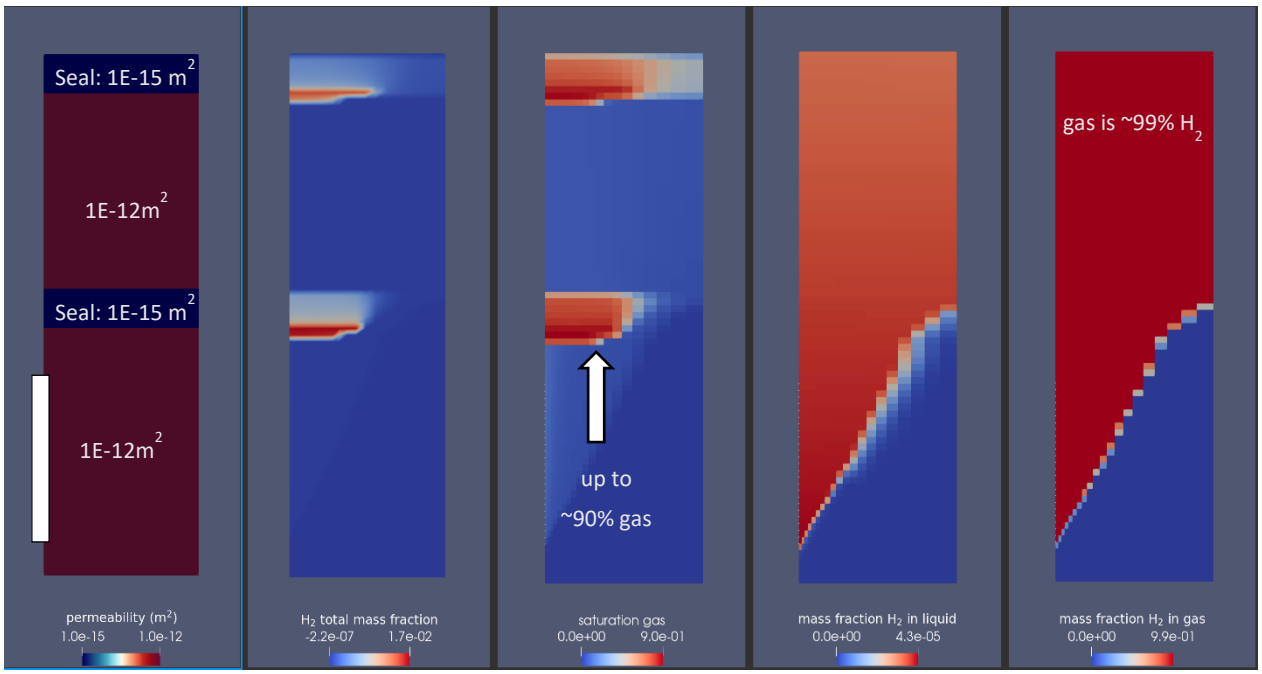

Figure 3. Box model predictions in near steady-state (after 10 yr.) assuming a constant H_2 injection of 1e^{-6} kg.s^{-1} (750 kg.yr^{-1}) – see [VIDEO-1] for dynamic model. Note the very low numbers in the mass fraction of H_2 in the liquid phase due to its low solubility. The gas saturation is the total gas ratio to porosity. Model setup and boundary conditions are shown in Figure 2.

A good parallelism can be established between the predictions from this simple box model and the observations at the Bourakebougou field, in the Taoudeni Basin (Mali), where several H_2 gas discoveries were made in carbonate reservoirs capped by dolerites intrusions. This field is described as a "*dynamic system, that is progressively recharged in H_2-rich gas at the production timescale*" (*in* Maiga et al., 2023a); the migration of gas bubbles through the water column in the carbonate fractures is clearly observed in the monitoring videos of the field (Maiga et al., 2023b). In the shallower, main carbonate reservoir of the Bourakebougou field, at 100 m depth, the gas composition is 98% H_2, with 1% nitrogen (N_2) and 1% methane (CH_4).

In another model experiment, we compare the model predictions for hydrogen and methane, a well-known gas from decades of oil and gas exploration ([VIDEO-2]).

Video 2. Box model predictions for hydrogen (H_2, left) and methane (CH_4, right), assuming the setup, boundary conditions and parameterization shown in Figure 2. The model runs over a 10 yr period, showing (from left to right): permeability (constant), with the velocities of the gas; total mass fraction (gas phase plus H_2 or CH_4 dissolved in the water); and gas saturation (total gas ratio to porosity).

The models show the mobility of H_2 to be about three times greater than that of CH_4, consistent with that predicted in other models (e.g. Lodhia and Clark, 2022; the velocity arrows in the video are proportional to the velocity). Similarly to the H_2 experiments, the CH_4 models reach dynamical equilibrium after less than 10 yr, but the differences in the mobility and solubility of the gases (CH_4 has much greater solubility) determine a much narrower distribution of CH_4 gas accumulation, as depicted in the figure below. The CH_4 model also predicts a greater mass of stored gas, of 124 kg for a mean density of 7.5 $kg.m^{-3}$, plus 33 kg of dissolved CH_4.

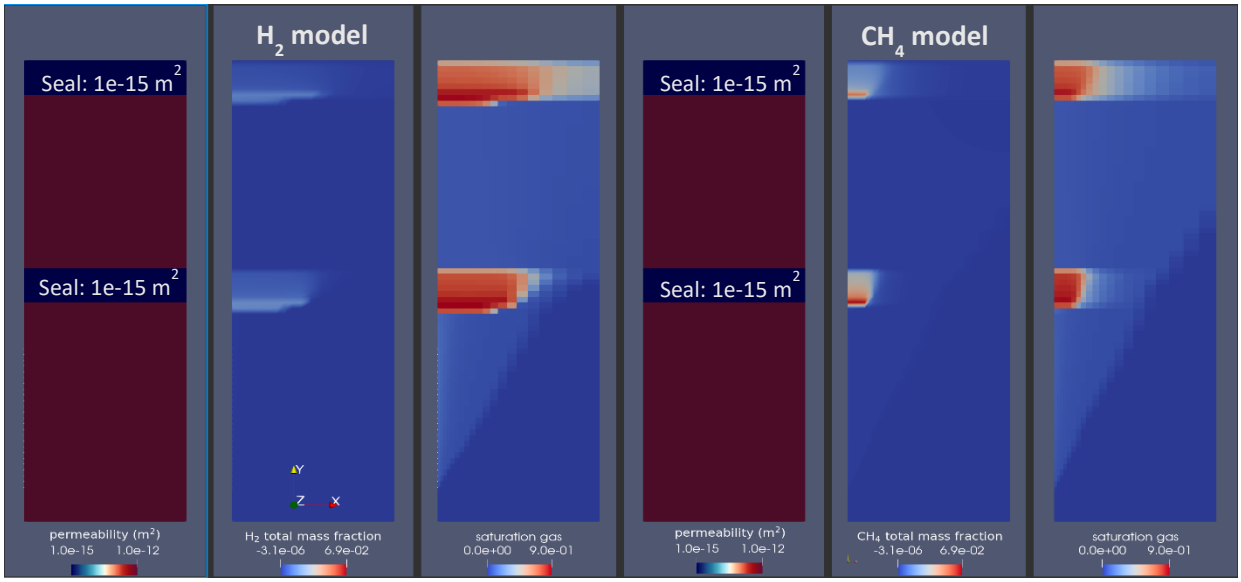

Figure 4. Comparison between H_2 (left) and CH_4 (right) model predictions after 10 yr, in steady-state - see [VIDEO-2] for dynamic models. Model setup and boundary conditions are shown in Figure 2. The differences in the movement and distribution of the gases are determined by the differences in the mobility and solubility of the gases.

The modelling results are particularly relevant since we only have sparse evidence of high hydrogen concentrations in sediments, and there is limited knowledge on the processes that control hydrogen migration and trapping in sedimentary basins. As future developments for the box-size models we aim to:

- Run the models over greater (eventually geological) timescales
- Parameterize other processes, such as adsorption, biological sinks and hydrodynamics
- Test multiple gases systems (ie. H_2O, H_2 and CH_4)
- Test sensitivities to a variety of realistic geological setting, such as lithologies, P-T conditions and H_2 generation rates

Following these initial tests, which are much more efficiently realized on box-size models, also to resolve potential issues of model stability, we plan to build basin-scale models, coupling sourcing, migration and trapping processes, and, where possible, calibrate the model to observations/data. We recognize the magnitude of the challenge in building natural-scale models, but are highly encouraged by the models developed by the Marum-Bremen team for evolution of passive margins and building of new oceans, which already incorporate crustal processes, including serpentinization, sedimentation, faulting and the circulation of fluids (García-Pintado et al., 2023; Pérez-Gussinyé et al., 2023).

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