Modelling of hydrogen reactivity in underground aquifer storage

GENERAL CONTEXT

Storengy, an Engie Group company, is one of the world's leading underground gas storage operators. Hydrogen (H_2) has a promising potential to enable a sustainable energy transition and meet carbon neutrality targets. Storengy studies and develops solutions for the underground storage of hydrogen, in mixture or pure, in deep aquifers. On the one hand, the production of natural gas from new industrial-scale processes leads to changes in the composition of the stored gas, where H_2 can reach a few per cent. On the other hand, in the context of hydrogen sector development in Europe, the (pure) H_2 produced in a renewable way can not only participate in the decarbonation of electricity production and industrial processes, but also bring flexibility to the energy networks when it is stored. The underground storage of hydrogen should then be studied.

Centre for Geosciences, Mines Paris – PSL, has been developing the HYTEC reactive transport code that couples geochemical reactions to flow and advective/dispersive transport in porous media (van der Lee et al., 2003). HYTEC can also simulate the flow, diffusion, and reactivity of a gas mixture in a porous medium (Sin et al., 2017) over a wide range of pressures and temperatures (Sin et al., 2019 and 2023). The geochemical module of HYTEC allows for the full range of water-gas-rock interaction processes in the aquifer but also simulates bacterial growth and kinetics.

The aim of this post-doctoral project, resulting from a collaboration between Storengy and Mines Paris – PSL, is to model the behaviour of H_2 storage in porous media. One of the challenges is to take into account the bio-geochemical reactions that may develop in the porous medium during the on-site operations. These biotic reactions (methanogenesis, sulfate-reduction, etc.) can modify the composition of the stored gas (loss of H_2, risk of H_2S production), the water chemistry and the petrophysical properties of the porous medium. This is a rapidly developing area of research within the international reactive transport community.

OBJECTIVE AND REALIZATION OF RECHERCHE STUDY

The main objective of this study is: (i) to understand and model biogeochemical processes in underground aquifer storage following the injection of a natural gas containing a certain concentration of H_2; (ii) to quantify the impact of this injection on the water, the stored gas and the rock of the reservoir over time; (iii) to simplify the modelling of the storage on an industrial scale (injection and withdrawal cycles).

1. Different laboratory experiments, e.g. Haddad et al. (2022), allowing to identify and characterize biogeochemical processes following H_2 injection will be modelled. The kinetics of physico-chemical and microbiological reactions related to the interaction between the water-gas-rock phases will be constrained by the experiments. When the experimental results will be reproduced by HYTEC, sensitivity studies will be performed on different parameters such as the amount of reagents (carbonates, sulfates, etc.), the competition between in-situ bacterial populations (sulfate-reducing and methanogenic in particular), the temperature, the pressure, the buffering effect performed by some minerals, etc.
2. Modelling on the scale of underground storage will be studied based on mineralogical and petrophysical data from Storengy's storage sites. The operating conditions (injection and withdrawal rates at the wells, thermal effects, etc.) will be taken into account and simplified configurations will be analysed. The simulation results will be compared with in-situ measurements obtained on the storage sites.

The results will be published (at least one scientific publication) and presented at international conferences or workshops.

REFERENCES

Haddad, P., Ranchou-Peyruse, M., Guignard, M., Mura, J., Casteran, F., Ronjon- Magand, L., Senechal, P., Isaure, M.-P., Moonen, P., Hoareau, G., et al. (2022) Geological storage of hydrogen in deep aquifers–an experimental multidisciplinary study. Energy & Environmental Science 15, 8, 3400–3415.

Sin, I., Lagneau, V., Corvisier, J. (2017). Integrating a compressible multicomponent two-phase flow into an existing reactive transport simulator. Advances in Water Resources 100, 62-77.

Sin, I., and Corvisier, J. (2019). Multiphase multicomponent reactive transport and flow modeling. In Reactive Transport in Natural and Engineered Systems, J. Druhan and C. Tournassat, Eds., Mineralogical Society of America ed., vol. 85. Reviews in Mineralogy and Geochemistry, Ch. 6, pp. 143–195.

Sin, I., De Windt, L., Banc, C., Goblet, P., and Dequidt, D. (2023). Assessment of the oxygen reactivity in a gas storage facility by multiphase reactive transport modeling of field data for air injection into a sandstone reservoir in the Paris Basin, France. Science of The Total Environment 869, 161657.

van der Lee, J., De Windt, L., Lagneau, V., Goblet, P. (2003). Module-oriented modeling of reactive transport with HYTEC. Computers and Geosciences 29, 265-275.

SKILLS

- Doctorate (Ph.D) degree (or engineer with a first experience);
- Experience in geochemical, multiphase flow or reactive transport modelling;
- Strong motivation for team work with the industrial partners;
- High level in English, intermediate level in French is desirable.

WORKPLACE AND CONTRACT

This postdoctoral contract is the result of a collaboration between Storengy and Mines Paris - PSL.
Duration: 18-month fixed-term contract at Mines Paris – PSL.
Starting date: second semester 2023.
Location: Mines Paris - PSL, Centre for Geosciences, Fontainebleau (77); frequent exchanges with Storengy, Bois-Colombes (92).

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