

Peer-reviewed Conference Contribution

Diffusion of dissolved gases: from lab scale to in situ scale

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Over the last decade, SCK CEN obtained a large set of diffusion coefficients for different gases in different Members of the Boom Clay. These diffusion experiments were performed in the lab on Boom Clay samples with diameter 80 mm and length 30 mm [1, 2]. When performing safety calculations, diffusion of gas is assumed to take place within an approximate domain over 100's of meters. This led to the question: is the lab-scale diffusion coefficient also valid on a larger (meter) scale? In the past, a similar question was raised for more classical tracers such as HTO and iodide, and several *in situ* diffusion experiments lead to the confirmation of lab results. Hence, SCK CEN, ESV Euridice and ONDRAF/NIRAS will perform a new *in situ* diffusion experiment with dissolved neon in the HADES URL with main objective to confirm/improve the current knowledge on diffusion of dissolved gas at a large scale. To perform an experiment under the most relevant conditions for the Boom Clay, i.e. without being perturbed by the presence of an excavation-damaged zone, the MEGAS setup (drilled in 1992) is re-used. The MEGAS setup consists of four piezometers in a 3D configuration. The most suitable location to inject dissolved gas is filter 17. Monitoring will take place in filters 18, 9 and 22, which allows assessing the anisotropy of diffusion (Figure 1 left).

In a geological disposal facility, hydrogen is the main gas that will be produced. Performing experiments with hydrogen is complicated due to microbial conversion of hydrogen into methane. Therefore, this experiment will make use of neon, the best proxy for hydrogen. The principle of this *in situ* gas diffusion experiment is similar to the experiments in the lab: gas (neon) is dissolved in water, and the water with dissolved neon is circulated over a filter that is in contact with the clay. After some time, dissolved neon will be present in the water in the monitoring filters. By circulating this water with dissolved neon through a vessel with a non-interfering gas phase (e.g. helium), an equilibrium reaction will occur and neon will be present in the gas phase of the monitoring vessel. The monitoring vessels are connected to a gas analyser that performs on line analysis of the neon concentration. By measuring the concentration increase of neon over time in the monitoring vessels at the different filters, the diffusion parameters can be determined. Note that the initial pressure in each vessel will be equal to the *in situ* pore water pressure, to minimize disturbing the *in situ* hydraulic field. A summary of the experiment is available from [3].

Prior to the start of the diffusion experiment with neon, and in order to better understand the performance of the setup and the processes in the host formation during the experiment, a trial in-diffusion experiment with helium was performed in filters 8 and 21. Both filters will not be involved in the neon through-diffusion experiment, but the processes and conditions around these filters during in-diffusion tests are considered relevant for the through-diffusion experiment. Two circuits are filled with 50% synthetic pore water and 50% helium at an initial pressure equal to the *in situ* pore water pressure at respective filters. Due to in-diffusion of helium in the host rock, the pressure in the circuits decreases over time, which in turn induces water inflow to the circuits and a subsequent increase of circuit pressure. The gas and water phase balance in the circuit is therefore dynamically adjusted by the whole system, until a steady state is reached.

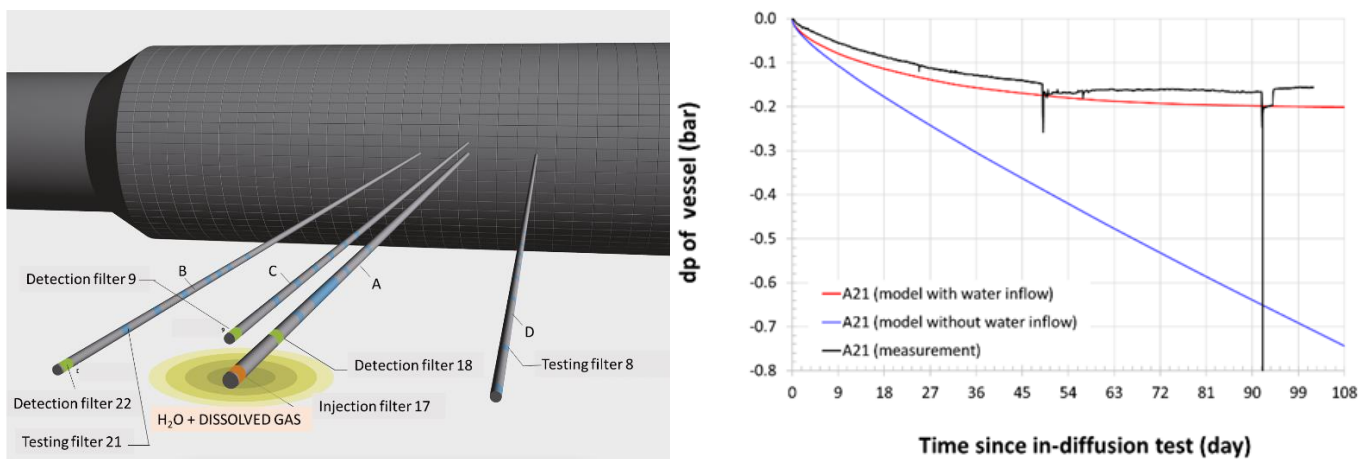


Figure 1: Schematic view of the location of the filters (left) and pressure evolution (measured vs. modelled) over time in the in-diffusion test in filter 21.

A numerical model was set up in COMSOL to predict pressure variations in both circuits. The diffusion coefficient of helium measured from the lab-scale diffusion test was used. The hydraulic conductivity of the clay comes from in situ permeability tests around these filters. If water flow is not considered in the model, the circuit pressure decrease of filter 21 follows the blue curve as shown in figure 1-right. The red curve gives the circuit pressure decrease considering diffusion of dissolved neon in clay as well as water flow under water pressure gradient. The three-month measurements follow well the red curve, which means that water inflow to the circuit plays a significant role in adjusting the circuit pressure. The good agreement between model results and field measurements confirms our lab scale test results. It also implies the good understanding of the in situ experimental system, which lays a good foundation for the long-term neon through-diffusion experiment afterwards.

Acknowledgement

EURAD programme has received funding from the European union's Horizon 2020 research and innovation programme under grant agreement n°847593. The work presented herein has been performed in the broader framework of a public-public cooperation between ONDRAF/NIRAS and SCK CEN.

Contributor statement

Conceptualisation and methodology: E. Jacops, G. Chen, L. Yu, A. Vanleeuw, J. Verstricht, D. Nackaerts; Writing and review: E. Jacops, G. Chen, L. Yu, S. Levasseur; Project administration: S. Levasseur, E. Jacops.

References

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