Hydrogen Intra-Diffusion Coefficients for Underground Storage




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Mixing between H_2 and the cushion gas (CH_4, N_2 or CO_2) during underground storage in porous media (UHSP) is characterised by two primary mechanisms: (1) Molecular diffusion and (2) mechanical dispersion. At low velocities (Péclet number < 0.1) mixing is dominated by diffusion. In this work, we measure the diffusion coefficient (*D*) of gaseous binary mixtures as a function of composition. This is performed using a custom-built Sapphire cell (**Figure 3**) which is integrated in a benchtop NMR spectrometer (**Figure 4**).

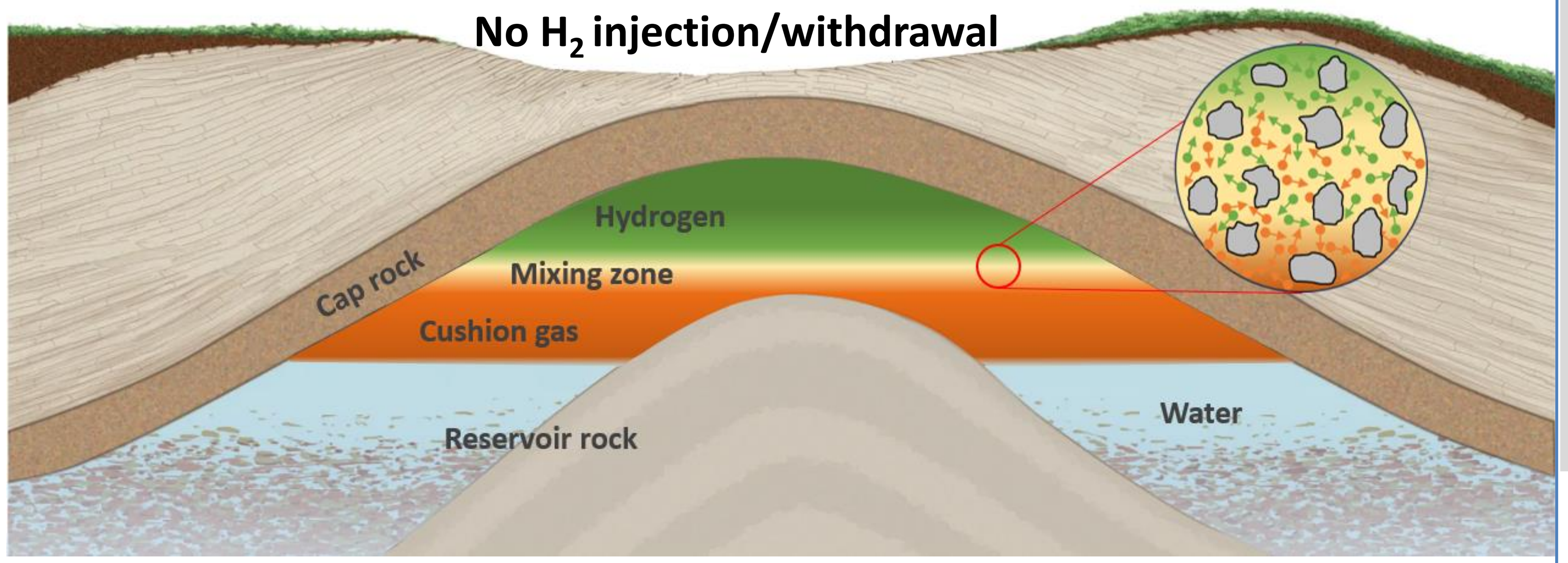

Figure 1. *Mixing between H_2 and cushion gas due to diffusion.*

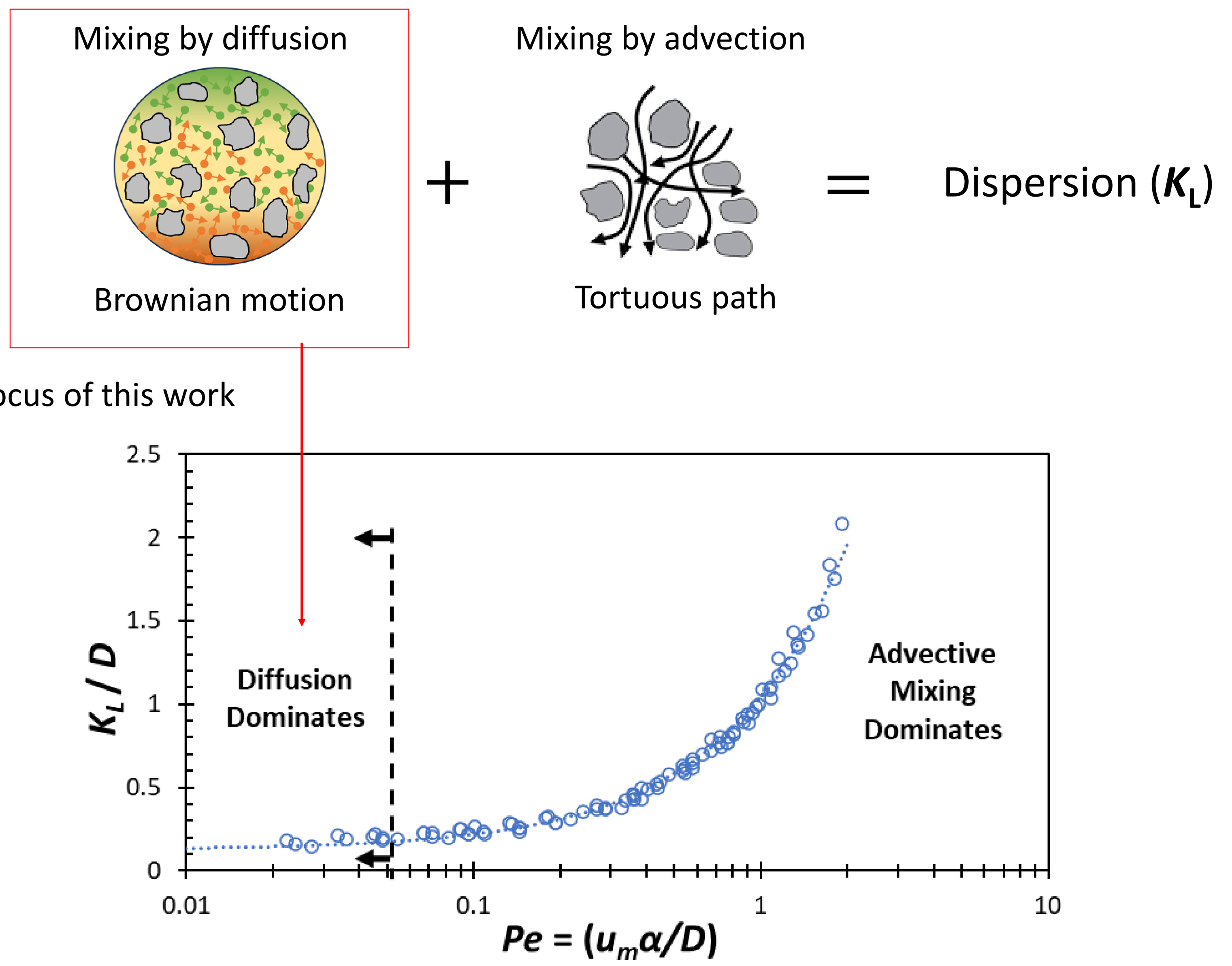

Figure 2. *K_L as a function of the Péclet number Pe_m (Kobeissi et al, 2024).*

Custom Designed Sapphire cell

The Sapphire cell (**Figure 3**) is designed to be integrated into the NMR spectrometer for diffusion measurements **(Figure 4).**

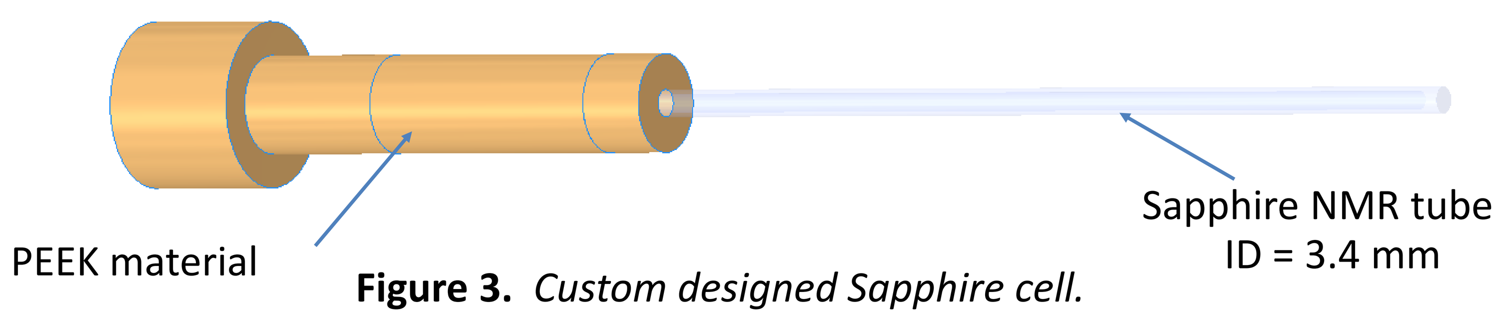

Figure 3. *Custom designed Sapphire cell.*

Apparatus

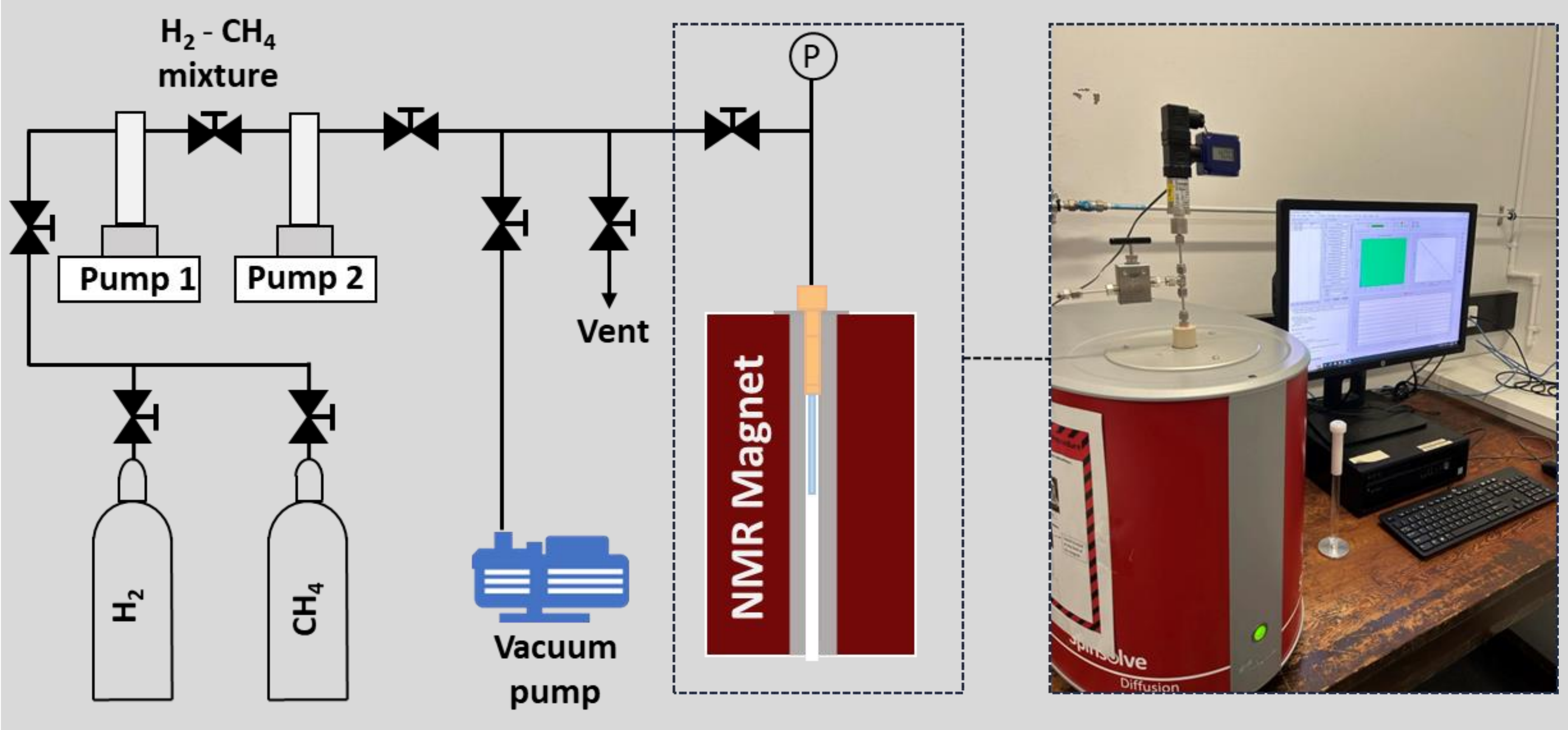

Figure 4. *Experimental setup for hydrogen diffusion measurements.*

Diffusion measurement technique

The diffusion coefficient (*D*) is measured using the NMR Pulsed field Gradient (PFG) technique (**Figure 5**).

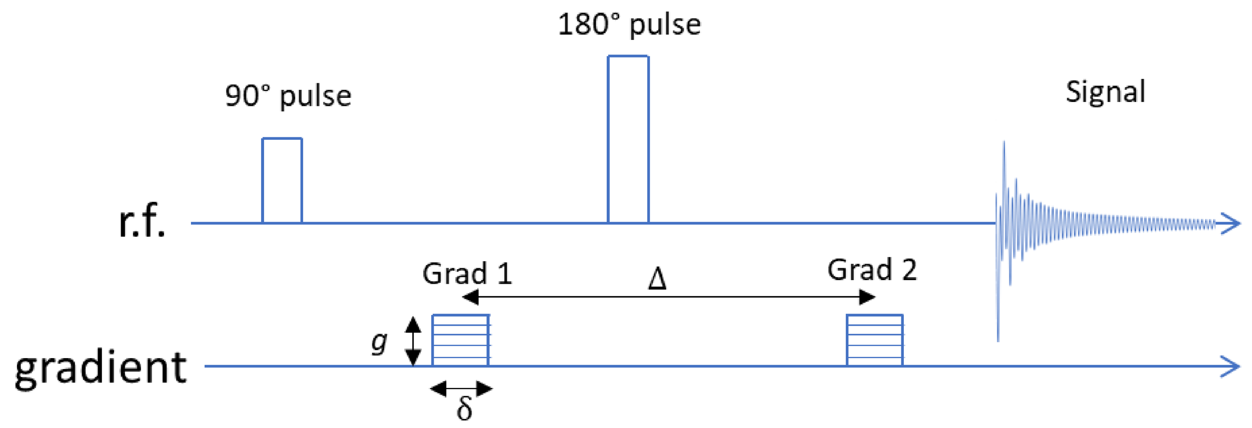

Figure 5. *Pulse sequence for diffusion measurements.*

The pulse sequence is performed for increasing magnetic field gradients (g). The NMR signal acquired for each gradient application is Fourier transformed to produce the NMR spectral peaks (**Figure 6**).

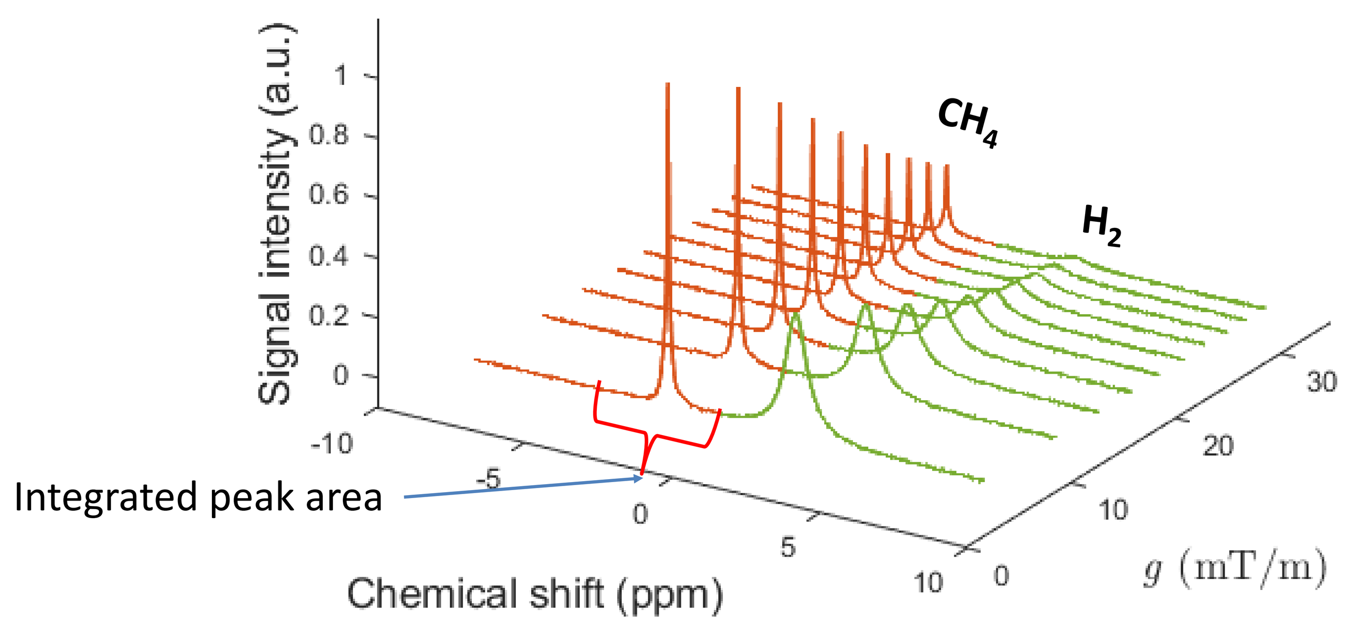

Figure 6. PFG measurement for a H_2-CH_4 mixture (x_{H2} = 0.9).

The two NMR peaks are integrated and plotted against the gradient (*g*) (**Figure 7**) to obtain their corresponding diffusion coefficients (D_{H2} and D_{CH4}).

$$\ln\left(\frac{S}{S_0}\right) = f(g, D), \qquad (1)$$

Gradient

Signal Loss

Diffusion coefficient

Results

Eq.(1) is regressed to the decay of the echo amplitude (S/S_0) (**Figure 7**) to obtain *D*.

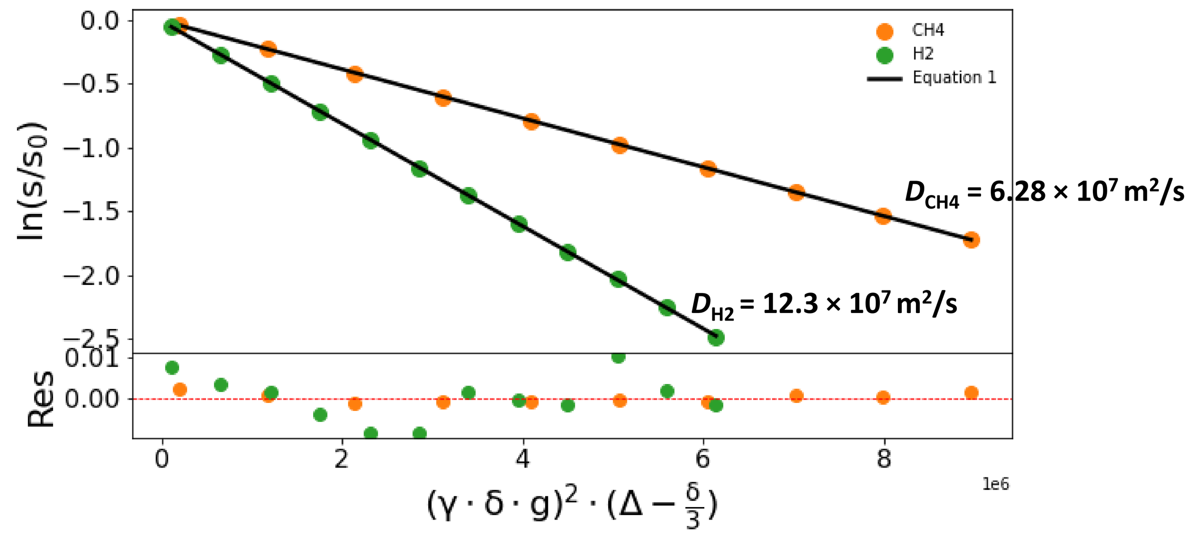

Figure 7. *PFG diffusion measurement of a H_2–CH_4 binary mixture (x_{H2} = 0.9). The integration of the NMR peaks (symbols) is regressed to Equation (1) (solid curve).*

- ❑ The diffusion coefficient is composition dependant (**Figure 8**).

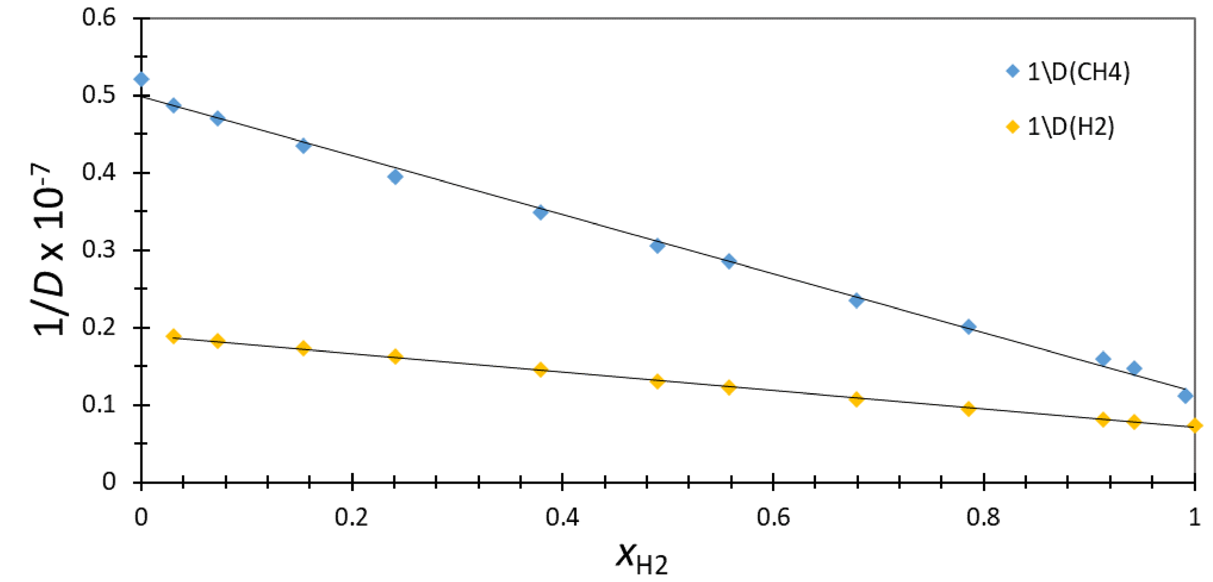

Figure 8. *Inverse of Diffusion coefficient of H_2 and CH_4 in a binary mixture as a function of composition.*

Mutual diffusion coefficients (D_{12}) of the binary mixture can be derived according to the Darken relation:

$$D_{12} = (x_{CH_4} D_{H_2} + x_{H_2} D_{CH_4}) B_2^x, \qquad (2)$$

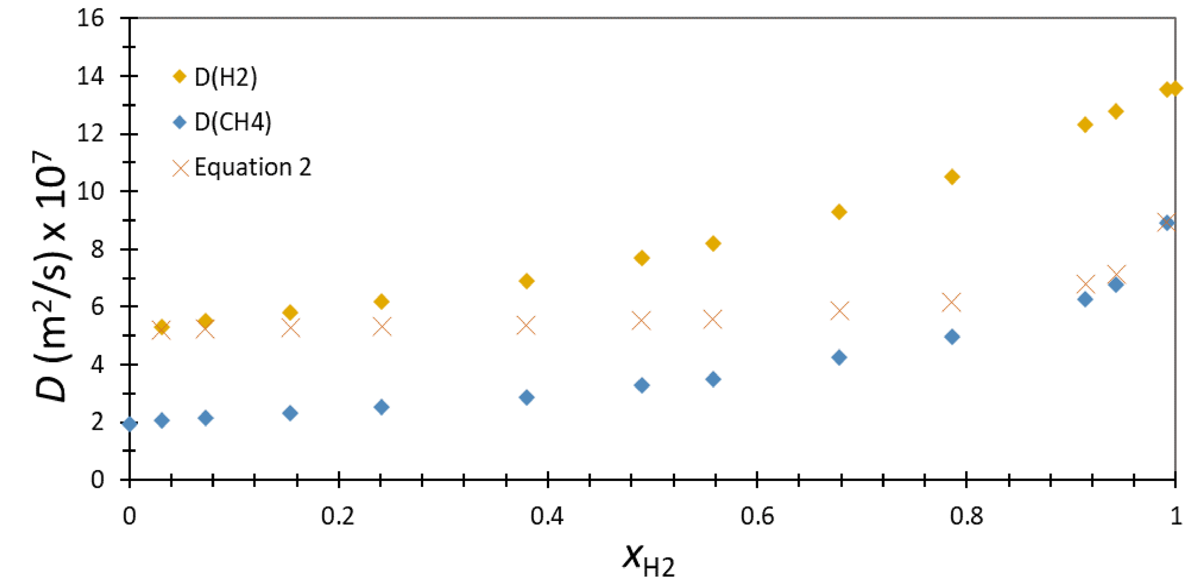

Figure 9. *Diffusion coefficient of H_2 and CH_4 in a binary mixture as a function of composition.*

Future work

- ❑ Validate the results from **Eq.(2)** via simulation.
- ❑ Expand measurements to UHS pressure conditions (50 - 250 bar).
- ❑ Expand measurements to UHS temperature conditions (20 - 60 °C).
- ❑ Perform H_2 diffusion measurements with N_2 and CO_2.