

Project number	6
Name/title of the PhD course	Geoscience & Engineering / Applied Mathematics
Name/Title of the PhD project	<i>Multiscale modelling and simulation of cyclic storage of H₂ in heterogeneous porous rocks</i>
Recruiting organisation and Department/Faculty of reference	TU Delft is the oldest, and with 25,000 students and 6000 employees, also the largest technical university of the Netherlands. The common mission of the 8 different faculties (offering 16 bachelor's and more than 30 master's programs) is: impact for a better society. TU Delft is home to one of the world's leading Geoscience and Engineering departments with subsurface storage as one of the key strategic multidisciplinary themes. The key scientific expertise includes characterization, modelling, simulation, monitoring, optimization and safety assessments of subsurface formations. Part of the training of the PhD students will be provided by the Delft Advanced Reservoir Simulation (DARSim) research group. DARSim is established in 2013 for development of advanced modelling and simulation methods for complex processes in the subsurface geological formations. In addition, the PhD student will have access to the state-of-the-art Laboratory of Geoscience & Engineering which is equipped with highly advanced instrumentations and set-ups to qualify and quantify chemical and physical processes in rocks and soils under deep and shallow in-situ conditions. Experimental equipment key to the proposed research project are the tri-axial stress/strain devices.
Scientific context and Objectives	Many of the existing performance analyses in the underground hydrogen storage community involve ad-hoc functions to describe the hydrogen through heterogeneous porous reservoirs. Beyond this, it is often assumed the reservoir is homogeneous. Very recently the first study which considered lab-based relative-permeability and capillary pressure functions were published by the TU Delft team in collaboration with the University of Queensland for an Australian Field. There we have found the great importance of the lab-based hysteretic data for hydrogen transport in porous media. In this SHINE project N.6, we aim to build on that and conduct systematic multiscale simulations to identify the trap efficiency, recoverability and sensitivity of the storage cycles to the heterogeneous and complex hysteretic functions. Very importantly we aim to carefully identify different element of the system including hydrogen, brine, cushion gas and the reservoir complex geology (i.e., heterogeneity and uncertainty).
Expected Results	Quantification of the reservoir performance and efficiency of cyclic H ₂ storage in heterogeneous porous reservoirs, and uncertainty assessments at reservoir scale.
Secondment opportunities	CSIC (V. Vilarrasa, 3 months, 12-15 month). ENI, 6 months, 24-30 month, perform multi-scale numerical simulation to test technical feasibility including purity assessments.
Brief CV of main Supervisor	Hadi Hajibeygi, associate Professor, leader of TU Delft Subsurface Storage Program, with long-term experience in supervising PhDs: 6 PhD Students graduated, currently advising 9 PhDs.
Publications	<ol style="list-style-type: none"> 1. M Naderloo, KR Kumar, E Hernandez, H Hajibeygi, A Barnhoorn, Experimental and numerical investigation of sandstone deformation under cycling loading relevant for underground energy storage, <i>Journal of Energy Storage</i> 64 (2023) 107198. https://doi.org/10.1016/j.est.2023.107198 2. S Krevor, H de Coninck, S Gasda, N Singh Ghaleigh, V de Gooyert, H Hajibeygi, R Juanes, J Neufeld, J Roberts & F Swennenhuis, Subsurface carbon dioxide and hydrogen storage for a sustainable energy future, <i>Nature Review Earth Environ</i> (2023). https://doi.org/10.1038/s43017-022-00376-8 3. WA van Rooijen, P Habibi, K Xu, P Dey, TJH Vlugt, H Hajibeygi, OA Moulto, Interfacial Tensions, Solubilities, and Transport Properties of the H₂/H₂O/NaCl System: A Molecular Simulation Study, <i>Journal of Chemical & Engineering Data</i> (2023) https://doi.org/10.1021/acs.jced.2c00707
Projects participation	<ol style="list-style-type: none"> 1. Project ADMIRE, funded by the Dutch National Science Foundation (€1m), 2019 – 2025. 2. Project SafeInCave, funded by Shell (€500k) 3. Project Science4Steer, funded by the Dutch National Science Foundation (€1.4m), 2019 – 2024. 4. Project EU ACT SHARP, €750k 5. Energi Simulation Chair, endowment €120k/year, since 2022—present.